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Koopman Operator Theory and Dynamic Mode Decomposition in Data-Driven Science and Engineering: A Comprehensive Review

Ramen Ghosh ^{*} Marion McAfee [†]

Abstract

Poincaré’s geometric representation has long been fundamental in dynamical system analysis. However, its limitations in handling high-dimensional and uncertain systems have become increasingly apparent in modern engineering and data analysis. This article comprehensively reviews Koopman Operator Theory (KOT) and Dynamic Mode Decomposition (DMD) in the context of data-driven science and engineering. The survey introduces a conceptual shift towards the dynamics of observables, focusing on the Koopman operator’s ability to capture nonlinear dynamics in infinite-dimensional space. Examining spectral properties highlights the interconnectedness of various methodologies, aiming to enhance accessibility and applicability. The potential transition of KOT from theoretical to practical applications is underscored, emphasizing its efficacy in numerical analysis and industrial contexts. Drawing from the geometric framework established by Poincaré, the limitations of traditional approaches in handling high-dimensional and uncertain systems are discussed. Ergodic and operator theories offer elegant solutions to these challenges, enabling linear representations of nonlinear dynamics without sacrificing information. The practical considerations and computational challenges inherent in utilizing Koopman and Perron-Frobenius operators are explored, emphasizing the trade-offs between accuracy and computational efficiency. The article also addresses the rising importance of data-driven methodologies, particularly in the era of big data and machine learning. The Koopman operator theory is a promising approach for unsupervised learning in dynamically evolving systems, offering insights into system behaviour from limited data. This review provides a historical overview, theoretical foundation, and practical implications of Koopman operator theory and dynamic mode decomposition. It positions them as powerful tools for data-driven analysis and engineering design in complex dynamical systems.

1 Introduction and Motivation of Data-Driven Techniques

Poincaré’s geometric representation, which delves into the dynamics of states ([Poincaré, 2017](#)), underpins most of the methodologies employed in dynamical system analysis, particularly in applied contexts. Despite its century-long dominance in the field, this depiction has exposed limitations in handling high-dimensional, poorly described, and uncertain systems, which are increasingly prevalent in engineered system design and extensive data analysis.

This review article introduces a distinct conceptual framework for dynamical systems centred on the dynamics of observables. The primary focus is on the Koopman operator, a linear operator in infinite-dimensional space

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capable of accurately capturing nonlinear dynamics. The survey aims to demonstrate the interconnectedness of various approaches that have emerged across diverse publications and settings, all linked by the spectral properties of the Koopman operator. This examination of spectral properties serves two main objectives. Firstly, it will elucidate how these methodologies are interrelated. Secondly, it will present these methodologies concisely, facilitating accessibility for researchers seeking not only to implement them but also to extend and enhance them. The Koopman framework has proven successful in making the leap from academic theory to practical industry applications, demonstrating its versatility and effectiveness in real-world contexts. The study underscores its merits in both practical and numerical contexts while pinpointing areas requiring further investigation before the technique can serve as a readily applicable framework for analysis and design.

In his work on the three-body issue, Poincaré introduced a geometric framework that has become central to the analysis and design of dynamical systems today. This framework extensively utilizes concepts from differential geometry, trajectories, and invariant manifolds. Its effectiveness has been demonstrated across various contexts. There is little need to justify using geometric theory when addressing specific issues; it is widely accepted as a fundamental tool in dynamical systems analysis. However, it is essential to note that the geometric perspective is not universally applicable and may be suitable only for specific circumstances within natural systems. Real systems can exhibit complexities beyond the scope of geometric analysis. For example, unstable manifolds may lead to the emergence of locally exponentially divergent paths in systems characterized by hyperbolic regimes.

In the presence of noise or uncertainty within a system, multiple alternative trajectories may emerge from a given initial state, leading to an exponential increase in the breadth of trajectory collections. Addressing inquiries about the behaviour of specific trajectories under such conditions can pose significant challenges. Many geometric arguments, such as Bendixson's criterion ([Bendixson, 1901](#); [Andronov et al., 1974](#)) for demonstrating the absence of periodic orbits in the plane, are applicable only in low dimensions. Hence, systems with higher dimensions require reassessment. Even within these complex scenarios, practical implementations necessitate dimensional constraints. High-dimensional systems typically require unique symmetries or constraints to mitigate their dimensions. Furthermore, fundamental geometric analyses become complex in the absence of clear Ordinary Differential Equations (ODEs). Given the critical role of dynamical systems theory in addressing pressing issues such as big data, new methodologies must emerge to manage high-dimensional, ambiguous, and poorly characterized systems, especially when dealing with historical time-evolution data that requires precise mathematical interpretation.

Applying ergodic theory and operator theory to practical contexts presents an elegant solution to many of the challenges outlined above, facilitating the analysis and design of dynamical systems. When examining dynamical systems through certain linear operators, it becomes possible to represent nonlinear dynamics within a linear framework.

In contrast to other linearization methods, this linear approach enables spectral analysis to address nonlinear issues without sacrificing information. While traditional spectral techniques typically predict geometry locally in state space, the operator-theoretic method proves equally effective across low and high-dimensional state spaces. This framework is well-suited for investigating noisy systems by shifting the focus away from trajectories.

Moreover, data from simulations or experimental measurements can be used to construct, approximate, or examine the operators. This provides a flexible analysis method, particularly when the practitioner does not have a complete understanding of the system's internal mechanisms.

Like any approach, the benefits outlined earlier also come with inherent costs. Operator-theoretic frameworks, as discussed, tend to be more intricate to comprehend as they diverge from physical intuition. Instead of focusing on individual state space points, one must shift their perspective to functions, even in finite-dimensional state spaces where the technique remains infinite-dimensional. This trade-off allows linear systems to encapsulate nonlinear system information, albeit making the implementation of approximations

more nuanced. Furthermore, developing numerical methods remains a crucial area of focus, with direct computations—numerical proofs—predominantly employed in our methodologies.

Among the operators utilized for system analysis, Koopman and Perron-Frobenius (PF) operators stand out as the most commonly used. They are expected to function similarly when operating as duals in proper function spaces. However, practical considerations continually influence our approaches. Questions arise regarding the construction of the operator from issue descriptions and data. How well do finite approximations align with the ideal theoretical framework? Are numerical artefacts overshadowing genuine intuition? These are essential considerations underpinning these operators' practical application in system analysis.

The Perron-Frobenius operator portrays the dynamics of density through groups of trajectories. Extensive efforts have been dedicated to approximating the Perron-Frobenius operator with a Markov chain to compute invariant densities, representing objects over an infinite time horizon. However, the pursuit of accurate representations within specific areas of interest imposes limitations on the number of initial conditions that can be simulated. When simulating dynamics over short and long periods in large dimensions, the entire space often requires meshing, even for a low-dimensional attractor.

Constraining the mesh size becomes feasible when prior information about the low-dimensional subspace containing the attractor is available. However, for arbitrary systems, this information may not be readily accessible, necessitating the utilization of the entire mesh.

On the other hand, the Koopman operator encapsulates the evolution of observables. In fluid mechanics, the distinction between the Eulerian and Lagrangian perspectives finds a counterpart in the differentiation between the Koopman representation and the Eulerian view. The Koopman representation aligns with the Lagrangian viewpoint, where measurements are conducted along trajectories or paths.

The numerical construction of the Koopman operator offers the advantage of requiring fewer initial conditions, albeit at the expense of extended computational runtimes. This characteristic makes it well-suited for applications in physical investigations. For instance, in testing a jet engine, initiating the engine from a relatively limited set of initial conditions and allowing it to operate for an extended duration proves more practical than preparing numerous initial conditions and running the engine for only a few seconds under each condition.

Extensive research has concentrated on understanding system behaviour due to the necessity of prolonged run durations. Nonetheless, a deeper exploration is warranted to grasp these scenarios' transient dynamics comprehensively.

When visualizing high-dimensional dynamical systems, focusing on a few two-dimensional cross-sections in the state space allows examination of overlapping invariant structures; however, using the Perron-Frobenius operator complicates this approach, as it requires computing the invariant density for the entire state space before deriving the densities on the specific slices of interest.

The closing years of the 20th century and the dawn of the 21st century witnessed a revolutionary surge in data availability, marking what can be termed a sensing revolution. This revolution spans a broad spectrum of data acquisition methods. Unfortunately, a significant portion of this data remains unprocessed and untapped in its potential, leading to missed opportunities across various domains like health, commerce, technology, and network security.

Various mathematical methodologies have emerged in response to this need, with Deep Neural Networks gaining particular prominence. These networks feature neuron functions inspired by biological neurons and have achieved remarkable success in realms such as image recognition, speech recognition, and natural language processing, rooted in the philosophy of supervised machine learning.

The introduction of convolutional neural networks, mirroring the hierarchical architecture of the animal visual cortex, has led to significant advances in image recognition and the generation of realistic images through

Generative Adversarial Networks (GANs). While these accomplishments are remarkable, they primarily pertain to static pattern recognition or generation tasks. Deep learning methodologies encounter more significant challenges in dynamically evolving contexts, such as autonomous driving, where accommodating the intrinsic characteristics of the temporal variable poses substantial obstacles.

In contrast, the Koopman operator framework naturally encapsulates the symmetry associated with temporal translation, endowing it with a fundamental group structure that aligns with dynamic processes where time plays a pivotal role. This framework has emerged as a formidable contender for machine learning of dynamic processes, offering a potent framework for unsupervised learning capable of extracting insights from limited data. This paper provides a concise historical overview, tracing its lineage from its roots in quantum mechanics and elucidating its contemporary focus within the innovative concept of dynamic process representation. Along this journey, connections to geometric dynamical systems theory methods are drawn, facilitating the data-driven discovery of essential components of the theory, including stable and unstable manifolds. This intricate interplay offers a robust framework for unsupervised learning, enabling self-supervised learning aligned more closely with human cognition principles than past machine learning paradigms.

As emphasized at the outset of this article, linear systems offer a more tractable path to solutions, as they can be decomposed into manageable components through techniques like Fourier analysis and Laplace transforms. However, conventional methods falter when confronted with nonlinear systems due to the intricate nonlinear interactions at play. Introducing external forces is particularly challenging, which further complicates the solution process.

In traditional practice, nonlinear systems are often linearized around equilibrium points to facilitate analysis. However, what if the system exhibits a high dimensionality, rendering numerical solutions impractical? Take, for instance, turbulent systems or power networks, both characterized by extreme nonlinear dynamics and vast dimensions. In the case of power systems, the uncertainties stemming from renewable energy sources (RESs) add layers of complexity, introducing countless degrees of freedom as these sources fluctuate with changing weather patterns and temperatures (Wang et al., 2016; Netto, 2019). Moreover, human intervention often amplifies model complexity (Wang, 2014). Consider the human brain, whose internal neural networks defy simple differential or difference equations, rendering the basic geometric properties and system characteristics exceedingly elusive. Furthermore, how do we address systems perturbed by significant disturbances far from equilibrium? Is there a robust model capable of handling such disruptions?

These challenges prompt the exploration of alternative methodologies. The proliferation of computational power has propelled data-driven approaches into the spotlight, particularly in system identification and control, where big data and machine learning have sparked a paradigm shift (Yang et al., 2017; Wang et al., 2019; Yang, 2017b,a). By their very nature, data-driven methodologies scrutinize systems through the lens of data, making them especially well-suited for systems characterized by solid nonlinearities and high dimensionality.

One such data-driven methodology garnering substantial research attention is the Koopman operator theory. This systematic framework offers a means to obtain linear representations of nonlinear systems, a topic we delve into in the following sections.

2 Koopman Operator and Dynamic Mode Decomposition: Basic Results

The genesis of the Koopman operator traces back to the seminal contributions of B. Koopman (Koopman, 1931), who introduced an operator facilitating unitary transformations within Hamiltonian dynamical systems. This foundational endeavour was further illuminated through collaborative efforts with John von Neumann in

1932 (Koopman and v. Neumann, 1932), wherein the spectral theory delineated a spectrum intrinsic to the Koopman operator unveiled the preceding year (Koopman, 1931). Despite its conceptual significance, this line of inquiry lay dormant for seven decades, owing to the formidable computational challenges inherent in its application without external support.

The early 2000s marked a resurgence of interest in the Koopman operator, catalyzed by the pioneering investigations of (Mezić and Banaszuk, 2000, 2004). Mezić demonstrated the reduction and reconstruction of high-dimensional state spaces from empirical data, leveraging salient eigenvalues of the Koopman operator to discern and characterize trends in ostensibly chaotic dynamics, colloquially referred to as Koopman modes.

Subsequently, (Rowley et al., 2009) harnessed the Koopman operator to analyze complex fluid dynamics, showcasing the efficacy of capturing pertinent structures through Koopman mode decomposition (KMD). This data-driven approach established a direct link between system measurements and the underlying dynamics in the state space, facilitated by dimensional reduction algorithms advanced by (Schmid, 2010). Schmid et al.'s methodological breakthroughs, particularly in dynamic mode decomposition (DMD), elucidated the dynamic information extraction from flow fields, exemplified by studies on cylinder wake dynamics (Schmid, 2010).

The symbiotic relationship between KMD and DMD, elucidated by (Schmid, 2010) and (Rowley et al., 2009), has emerged as a cornerstone in investigating nonlinear flows (Sayadi et al., 2014; Tu, 2013; Kutz et al., 2016; Kaiser et al., 2021) and other interdisciplinary domains, as elaborated further Sections.

2.1 Koopman Operator of Autonomous Nonlinear System

In seminal work, B. O. Koopman established that a linear operator may elegantly represent a nonlinear dynamical system within the infinite expanse of Hilbert space, a notion detailed in (Koopman, 1931). This operator, known as the Koopman operator, embodies unitary properties, signifying a bijection of points in Hilbert space while preserving the inner product of any two observables (Koopman, 1931). Numerous investigations have unveiled that classical attributes of dynamical systems seamlessly translate into the Koopman formalism. Notably, it has been demonstrated that the level sets of Koopman eigenfunctions can serve as invariant partitions within the dynamical system's state space (Budišić and Mezić, 2012). Moreover, an expansion of the local linearization, rooted in the Hartman–Grobman theorem, to encompass the entire basin of attraction of a stable equilibrium or limit cycle has been achieved through the adept utilization of the Koopman operator. Remarkably, this linearization extends to both flows and maps (Lan and Mezić, 2013).

Employing the Koopman operator transforms the nonlinear system into a linear, high-dimensional construct, introducing novel challenges. Researchers are actively pursuing methodologies to derive a finite approximation of the Koopman operator while retaining the dynamical essence of the original system (Brunton et al., 2016b). This approximation holds promise for both controlling and predicting nonlinear systems.

Obtaining the Koopman operator requires initial measurements of observables. The Koopman operator's appeal in big data lies in its reliance on measurement data and ability to linearly approximate nonlinear systems without traditional linearization around specific fixed points. This approximation often expands the stability region around the equilibrium, as discussed in the case study by (Li, 2019, Chapter 7). However, a crucial question arises: Which data should be used? The variables vital for constructing the Koopman operator, termed observables, deserve careful consideration. Typically, observables consist of functions of system states that encapsulate the dynamics of interest. For example, rotor speeds and angles are pivotal in dictating system dynamics in a power system governed by the swing equation. Thus, terminal bus voltages, generator electrical power, and system frequency emerge as primary candidates for observables due to their correlation with system states. Conversely, the reactive power of the generator is deemed suboptimal as an observable due to its minimal dependence on rotor angle and speed.

Nevertheless, the complexity of controlling the system depicted in (Li, 2019, Chapter 1, Figure 4.1) precludes

unfettered access to all system states or the straightforward determination of observables using conventional power system knowledge (Gupta et al., 2019). Consequently, a methodology for discerning observables capable of accommodating partial states or even devoid of state information is imperative. To this end, the forthcoming sections will elucidate a method of constructing the Koopman operator tailored to such systems, particularly those characterized by input-output dynamics. Let us embark on a journey delving into the foundational theory underpinning the Koopman operator.

2.2 Koopman Operator for Discrete-Time System

In the context of nonlinear dynamical systems, a conventional depiction entails a collection of states governed by a functional relationship dictating their temporal evolution or interrelation (Kutz et al., 2016; Brunton and Kutz, 2022). Such systems are typically elucidated through continuous and discrete methodologies. For a generalized continuous system represented by:

$$\frac{d}{dt}x(t) = F(x(t), t; \mu), \quad (1)$$

where $x(t) \in \mathbb{R}^n$ denotes the state of the dynamical system at time t , n signifies the number of state components, μ encapsulates parameters dictating system dynamics, and $F(\cdot)$ delineates the continuous-time state evolution. Concurrently, these continuous dynamics can be discretely modelled and evaluated at finite intervals Δt , expressed as $x_k = x(k\Delta t)$, with subscript k . The discrete-time system evolution can be formally articulated as follows:

$$x_{k+1} = F(x_k), \quad (2)$$

where x_k represents an n -dimensional column vector of system states at time t_k , $k = 1, 2, 3, \dots, m$, for m time steps, and x_{k+1} signifies the subsequent states following x_k (Proctor et al., 2016, 2018; Franklin et al., 2002). The rules dictating system state advancements typically manifest as nonlinear equations, thereby capturing the complexities of practical systems. However, the analytical resolution of nonlinear system dynamics presents a formidable challenge. Consequently, contemporary control methodologies often resort to approximations when designing high-fidelity controllers. Nevertheless, linear representations offer a notable advantage in predicting system advancements accurately. We aim to demonstrate this phenomenon through the lens of Koopman operator theory.

In the context of employing Koopman operator theory, we introduce a novel function $g : \mathbb{R}^n \rightarrow \mathbb{M}^p$, where p denotes the dimensionality of an almost infinite column vector representing the observables of x at a specific time step. Consequently, the Koopman operator extends across all observables, resulting in an infinite-dimensional operator \mathcal{K} . Strategies for addressing this infinite dimensionality will be subsequently explored. Here, g denotes a real-valued, scalar measurement function belonging to an infinite-dimensional Hilbert space referred to as an observable. The action of the Koopman operator on this observable is defined as:

$$\mathcal{K}_t g = (g \circ F)(x(t)) \quad (3a)$$

$$\mathcal{K}_{\Delta t} g(x_k) = (g \circ f)(x_k) \quad (3b)$$

In continuous and discrete representations, respectively. Equation (3a) illustrates the constant evolution of the observable under the Koopman operator over time, while in (3b), it governs the discrete-time dynamics with

Δt representing the interval between k and $k + 1$ in the time series m . Further elucidation of the interrelations between these representations is provided in (Proctor et al., 2016; Korda and Mezić, 2018b; Mauroy et al., 2020; Kaiser et al., 2021; Brunton and Kutz, 2022). Equations (3a) and (3b) enable the formulation of analogues for continuous and discrete-time dynamical systems, respectively, as depicted below:

$$\frac{d}{dt}g = \mathcal{K}g \quad (4a)$$

$$g(x_{k+1}) = \mathcal{K}_{\Delta t}g(x_k) \quad (4b)$$

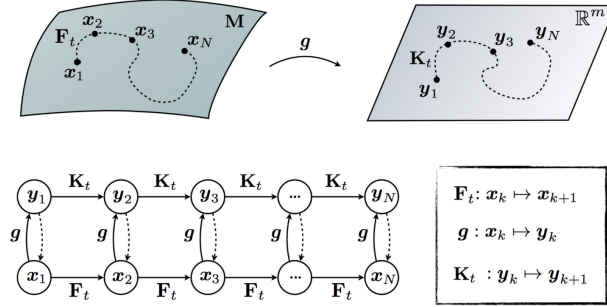


Figure 1: Schematic for illustrating the advancement of a dynamical system as defined by the Koopman operator on nonlinear dynamical systems (Brunton et al., 2016b)

However, as depicted in Figure 1, this operator facilitates the measurement of dynamic evolution over time (Brunton and Kutz, 2022; Proctor et al., 2016; Korda and Mezić, 2018b). Revisiting (2) where the rule F maps x_k from $F: \mathbb{R}^n \rightarrow \mathbb{R}^n$, introducing Koopman operator theory presents an alternative rule, g , where g maps x_k from \mathbb{R}^n to \mathbb{M}^p , with p denoting the dimensionality of the nearly infinite column vector characterizing the observable at that time step of x_k . Consequently, the Koopman operator is defined across all observables, implying that the Koopman Operator \mathcal{K} is also infinite-dimensional. Here, g represents a real-valued, scalar measurement function within an infinite-dimensional Hilbert space \mathcal{H} , denoted as an observable. The Koopman operator operates on g as follows:

$$\mathcal{K}g(x) = (g \circ F)(x) \quad (5)$$

The Koopman operator \mathcal{K} provides a linear representation of the nonlinear dynamical system in the space \mathcal{H} , signifying that it advances the observables linearly:

$$g(x_{k+1}) = \mathcal{K}g(x_k) \quad (6)$$

This operator effectively captures the dynamics of the underlying system within the space of observables \mathcal{H} , encompassing the components of x , including x itself. The fundamental property of the Koopman operator is its linearity, expressed as:

$$\mathcal{K}(\alpha g_1 + \beta g_2) = \alpha \mathcal{K}g_1 + \beta \mathcal{K}g_2, \quad (7)$$

where α and β are constants, and $g_1, g_2 \in \mathcal{H}$.

We define a pair (ϕ_i, λ_i) as an eigenfunction-eigenvalue pair of the Koopman operator if they satisfy (Brunton et al., 2016b)

$$\mathcal{K} \phi_i = e^{\lambda_i t} \phi_i \text{ where } \lambda_i \in \mathbb{C}. \quad (8)$$

Koopman eigenfunctions have the property that if (ϕ_i, λ_i) and (ϕ_j, λ_j) are two distinct eigenfunction-eigenvalue pairs, then $(\phi_i \phi_j, \lambda_i + \lambda_j)$ is also an eigenfunction-eigenvalue pair. The spectral properties of the Koopman operator can characterize the state space dynamics. For instance, since the Koopman eigenvalues are the point spectra of the Koopman operator, we can use Koopman eigenvalues to evaluate the system's stability. More properties can be found in (Mauroy and Mezić, 2016; Mauroy et al., 2013; Mezić, 2015).

With the assumption that all the observables of the system lie in the linear span, i.e.,

$$g(x) = \sum_{i=0}^{\infty} \nu_i \phi_i(x), \quad (9)$$

where ν_i 's are the coefficients of the Koopman expansion, namely ν_i 's are Koopman modes associated with the Koopman eigenfunction-eigenvalue couple (ϕ_i, λ_i) . According to (9), Koopman modes can be obtained by the projection of the corresponding observable and the eigenfunction. Then, we can describe the evolution of the observables as

$$\mathcal{K} g(x) = \sum_{i=0}^{\infty} \nu_i \phi_i(x) e^{\lambda_i t}. \quad (10)$$

It has been proved that Koopman linear expansion in (10) applies to a large class of nonlinear dynamical systems such as those with limit cycles and hyperbolic fixed points. See (Mezić, 2017) for detailed examples.

2.3 Koopman Operator for Continuous-Time System

We have directed our attention to the Koopman operator formalism for discrete-time systems to maintain consistency with the measurement data obtained from real-life experiments or simulations. However, for the sake of completeness in our discourse, the analysis extends to continuous-time systems. Consider the continuous-time system described by

$$\dot{x} = f(x). \quad (11)$$

Given that it is a continuous-time system, we can define a one-parameter semi-group of Koopman operators $\{\mathcal{K}^t\}_{t \geq 0}$ such that each component of this group is given by

$$\mathcal{K}^t g(x) = g(x) \circ F^t(x), \quad (12)$$

Where g represents the observable of the system. Equation (12) can be equivalently expressed as

$$\mathcal{H}^t g(x) = g(F^t(x)), \quad (13)$$

This system also adheres to the linearity of the composition operation, thereby possessing the same properties as the Koopman operator for discrete systems. The evolution of observables is thus represented as

$$\mathcal{H}^t g(x) = \sum_{i=0}^{\infty} v_i \phi_i(x) e^{\lambda_i t}. \quad (14)$$

2.4 Dynamic Mode Decomposition

The original Dynamic Mode Decomposition (DMD) algorithm, as introduced by Schmid and Sesterhenn (Schmid, 2010), was initially conceptualized as a Companion matrix. Subsequently, Rowley et al. (Rowley et al., 2009) established a connection between the DMD algorithm and the modified Arnoldi algorithm, along with Koopman operator theory. However, Tu et al. (Tu, 2013) argue that an algorithm founded on the Singular Value Decomposition (SVD) offers superior numerical stability. We shall elucidate this algorithm presently.

Consider a scenario where sequential data stems from linear dynamics, as described by:

$$x_{k+1} = Kx_k, \quad k = 0, 1, 2, \dots, \quad (15)$$

with the matrix K remaining unknown. Despite the potential nonlinear origins of the data, it is presumed that an operator K can approximate the underlying dynamics. Sequential data from the linear dynamics (15) is represented as:

$$X_1 = [x_0 \quad x_1 \quad x_2 \quad \dots \quad x_{N-1}], \quad (16)$$

$$X_2 = [x_1 \quad x_2 \quad x_3 \quad \dots \quad x_N]. \quad (17)$$

We proceed by computing the Singular Value Decomposition (SVD) of X_1 :

$$X_1 = U\Sigma V^*, \quad (18)$$

where U is an $n \times r$ real or complex matrix, Σ is an $r \times r$ diagonal matrix with non-negative real numbers on the diagonal, V is an $m \times r$ real or complex matrix, and r denotes the rank of X_1 . Subsequently, we define the matrix \tilde{K} as follows:

$$\tilde{K} = UX_2V\Sigma^{-1}. \quad (19)$$

We then compute the eigenvalues and eigenvectors of \tilde{K} , denoted by:

$$\tilde{K}w = \lambda w. \quad (20)$$

The DMD mode associated with the DMD eigenvalue λ is expressed as:

$$\tilde{v} = Uw. \quad (21)$$

Following the insights of Tu et al. (Tu, 2013), \tilde{v} represents the projected DMD modes.

2.5 Exact Dynamic Mode Decomposition

The Dynamic Mode Decomposition (DMD) algorithm, formulated initially under the assumption of sequential and ordered data vectors $\{x_0, x_1, x_2, \dots, x_n\}$ satisfying the dynamics (15), has been extended by Tu et al. (Tu, 2013). This extension relaxes the constraints on the data by considering pairs $\{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$, leading to the definition of data matrices as follows:

$$X_1 = [x_1 \quad x_2 \quad \dots \quad x_N]; \quad X_2 = [y_1 \quad y_2 \quad \dots \quad y_N]. \quad (22)$$

The Comparison between data matrices for the standard DMD and the extended DMD is illustrated in Table 1, highlighting that the data matrices for the DMD algorithm are a particular case of those for the exact DMD, with $y_k = x_{k+1}$.

Data Matrix	DMD	Exact DMD
X_1	$[x_0 \quad x_1 \quad \dots \quad x_{n-1}]$	$[x_1 \quad x_2 \quad \dots \quad x_n]$
X_2	$[x_1 \quad x_2 \quad \dots \quad x_n]$	$[y_1 \quad y_2 \quad \dots \quad y_n]$

Table 1: Comparison between data matrices

For a dataset given by (22), the operator K is defined as:

$$K = X_2 X_1^\dagger. \quad (23)$$

The dynamic mode decomposition of the pair (X_1, X_2) involves the eigendecomposition of K , where the DMD modes and eigenvalues correspond to the eigenvectors and eigenvalues of K .

The exact DMD algorithm proceeds as follows: arrange the data pairs $\{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$ into matrices X_1 and X_2 as defined in (22). Compute the reduced Singular Value Decomposition (SVD) of X_1 :

$$X_1 = U \Sigma V^*. \quad (24)$$

Next, define the matrix \tilde{K} as:

$$\tilde{K} = U X_2 V \Sigma^{-1}. \quad (25)$$

Compute the eigenvalues and eigenvectors of \tilde{K} , denoted by:

$$\tilde{K} w = \lambda w. \quad (26)$$

Finally, the DMD mode corresponding to the DMD eigenvalue λ is expressed as:

$$v = \frac{1}{\lambda} X_2 V \Sigma^{-1} w. \quad (27)$$

Interested readers are directed to (Tu, 2013) for a more in-depth exploration of the exact DMD.

2.6 Extended Dynamic Mode Decomposition

The extended Dynamic Mode Decomposition (EDMD), initially proposed by (Williams et al., 2015a), underwent a modification presented by (Klus et al., 2016). Unlike the original formulation, (Klus et al., 2016) employed left eigenvectors of the finite-dimensional approximation of the Koopman operator for a similarity transformation, while (Williams et al., 2015a) utilized right eigenvectors. This nuanced difference proves

pivotal for the participation factors developed in (Li, 2019, Chapter 7). Following the methodology of (Klus et al., 2016), consider a series of snapshots of system states denoted by x_k . Define the matrices as follows:

$$X_1 = [x_1 \ x_2 \ \dots \ x_N]; \quad X_2 = [y_1 \ y_2 \ \dots \ y_N], \quad (28)$$

where $X_1, X_2 \in \mathbb{R}^{n \times N}$. Additionally, define a vector of observable functions:

$$g(x_k) = [g_1(x_k); \ g_2(x_k); \ \dots; \ g_q(x_k)]^\top, \quad (29)$$

where $g : \mathbb{R}^n \rightarrow \mathbb{R}^q$, and the matrices of observables:

$$O_{X_1} = [g(x_1) \ g(x_2) \ \dots \ g(x_N)], \quad (30)$$

$$O_{X_2} = [g(y_1) \ g(y_2) \ \dots \ g(y_N)], \quad (31)$$

where $O_{X_1}, O_{X_2} \in \mathbb{R}^{q \times N}$. A finite-dimensional approximation to the Koopman operator is formed as:

$$K = O_{X_2} O_{X_1}^\dagger, \quad (32)$$

where $K \in \mathbb{R}^{q \times q}$. The eigenvalues of K provide a finite-dimensional approximation to the Koopman eigenvalues, while the Koopman eigenfunctions, ϕ_i , are expressed as:

$$\phi(x_k) = \Psi g(x_k), \quad (33)$$

where $\Psi = [\psi_1^\top; \psi_2^\top; \dots; \psi_q^\top]$ contains the left eigenvectors of K , and $\phi(x_k) = [\phi_1(x_k); \phi_2(x_k); \dots; \phi_q(x_k)]^\top$.

To derive the Koopman modes for the full-state observable, $g(x_k) = x_k$, let $B \in \mathbb{R}^{n \times q}$ be a matrix defined such that:

$$x_k = Bg(x_k). \quad (34)$$

From (33), we have $g(x_k) = \Psi^{-1}\phi(x_k)$, and:

$$x_k = Bg(x_k) = B\Psi^{-1}\phi(x_k), \quad (35)$$

where Ψ^{-1} contains right eigenvectors. Therefore, the Koopman modes are the column vectors, v_i , $i = 1, 2, \dots, q$, of $\Upsilon = B\Psi^{-1} \in \mathbb{C}^{n \times q}$, and:

$$x_k = \sum_{i=1}^q \phi_i(x_k) v_i = \sum_{i=1}^q \phi_i(x_0) v_i \lambda_i^k. \quad (36)$$

The convergence of the EDMD to the Koopman operator was demonstrated in (Korda and Mezić, 2018c; Arbabi and Mezić, 2017a).

3 Resurrection of Koopman Operator Theory: Spectral Theory of Dynamical Systems

(Mezić and Banaszuk, 2000, 2004) presents a formalism that utilises the spectral properties of the Koopman operator to compare the asymptotic dynamics of dynamical systems with the physical systems they model. The formalism includes a *statistical Takens theorem* (Takens, 2006) and an *ergodic-theoretic* treatment of spectral functionals, enabling parameter identification and model validation of nonlinear models with complex behaviour, as demonstrated through a comparison between the asymptotic behaviour of an experimentally measured combustion system and a class of random dynamical system models.

(Mezić, 2005) addresses two critical aspects of model reduction and validation for complex dynamical systems. Firstly, it explores the relationship between the spectral properties of the original high-dimensional system and the possibilities for model reduction. They propose a decomposition method to extract the system's dynamics' periodic and continuous spectrum components by leveraging the *spectral theory of dynamical systems and the linear Koopman operator*. Secondly, the paper discusses model validation, where the original dynamics are compared with those of a reduced model in terms of a statistical measure derived from the *statistical Takens theorem* (Takens, 2006). This measure helps assess the accuracy of the reduced model by evaluating the energy contained in the finite-dimensional projection. Overall, the paper provides insights into the spectral analysis of dynamical systems, model reduction techniques, and the validation of reduced models.

Hartman–Grobman Theorem establishes the linearization of nonlinear systems near hyperbolic stationary points. (Lan and Mezić, 2013) applied this linearization concept to stable or unstable equilibria and periodic orbits and extended it to encompass the entire basin of attraction. This extension is pertinent for both discrete diffeomorphisms and continuous flows. In this endeavour, they delve into the correlation between the linearizing transformation and the spectrum of the Koopman operator. This operator, a central construct in our study, plays a pivotal role in capturing the dynamic behaviour and changes within the system. By examining the interplay between the linearization process and the Koopman operator's spectrum, they gained more profound insights into the intricate dynamics of the nonlinear system across its entire basin of attraction. This connection bridges the theoretical underpinnings of linearization with the practical implications of the Koopman operator, enriching our understanding of the system's behaviour in diverse contexts.

(Mauroy et al., 2013) showcases several noteworthy contributions: First, it explores the intrinsic connection between Lyapunov functions and densities, revealing their interrelation through the duality established between the *Koopman and Perron-Frobenius operators*. Secondly, the paper introduces an innovative stability theory founded on spectral operator-theoretic methodologies. Thirdly, it investigates the intricate interplay between global stability and the existence of specific eigenfunctions. Additionally, the paper puts forth a numerical technique designed for the computation of smooth eigenfunctions while offering practical instances that demonstrate the application of these methodologies. In particular, the paper's critical focal points involve leveraging eigenfunctions in the comprehensive analysis of global stability within a system. It formulates a proposition that asserts the global asymptotic stability of a specified set predicated upon certain eigenvalues and substantiates these propositions through rigorous proofs. The intricate relationship connecting eigenfunctions with Lyapunov functions is also delineated. Moreover, the paper establishes an inequality that governs trajectory convergence using Koopman eigenfunctions and presents a numerical algorithm tailored to calculate smooth Koopman eigenfunctions. The method's versatility extends to diverse types of attractors and systems, underlining its wide-ranging applicability.

(Mauroy and Mezić, 2013) discuss asymptotically periodic systems, a highly effective approach to simplifying the dynamics involves determining what are known as *isochrons*. These isochrons correspond to sets of points that ultimately converge towards the same trajectory on a limit cycle. The study of excitable systems has inspired the concept. A similar reduction technique has been explored for systems that are not strictly periodic but possess a stable fixed point. In this scenario, isochrons can still be defined, but they do not

accurately capture the long-term behaviour of trajectories. Instead, the concept of *isostables* comes into play. Isostables are points identified in the literature that exhibit convergence towards the same trajectory on a stable slow manifold associated with the fixed point. However, it is essential to note that this notion of isostables applies only to systems with a mix of slow and fast dynamics. Furthermore, practical methods for calculating these isostables have yet to be developed. (Mauroy and Mezić, 2013) introduces a comprehensive framework for defining and computing the isostables linked to stable fixed points. This framework is grounded in the spectral properties of the Koopman operator, a mathematical construct. More specifically, isostables are defined as the Koopman operator’s level sets of a specific eigenfunction. This approach establishes isostables as well-defined and unique entities directly linked to the system’s asymptotic properties. Additionally, this framework unveils the distinct yet complementary nature of isostables and isochrons, which collectively establish a set of coordinates termed *action-angle coordinates* for characterising the system’s dynamics. The paper also outlines an efficient algorithm for computing isostables. This algorithm relies on calculating Laplace averages along trajectories. To exemplify the method’s effectiveness, the research employs the *FitzHugh–Nagumo model* (Sherwood, 2013), which represents excitable behaviour, and the Lorenz model. Finally, the paper delves into how these techniques rooted in the Koopman operator framework correlate with broader mathematical concepts. This includes their connection to the system’s global linearisation and relevance in deriving specialised Lyapunov functions.

The innovative operator-theoretic framework introduced by (Mauroy and Mezić, 2016) explores global stability in nonlinear systems. Leveraging the spectral characteristics of the Koopman operator, this approach seamlessly extends the traditional realm of linear stability analysis to nonlinear systems. The principal outcomes of the study establish a conclusive correlation (both necessary and sufficient) between the presence of specific eigenfunctions associated with the Koopman operator and the global stability attribute observed in hyperbolic fixed points and limit cycles. To enhance these findings, computational techniques are incorporated to approximate the attraction region of fixed points. Moreover, a systematic methodology is presented to substantiate the global stability of attractors within designated areas of the state space.

Employing an operator-theoretic framework, (Govindarajan et al., 2016) delve into a category of non-smooth dynamical systems characterized by event-triggered state resets. The focal point of their investigation centres on the archetype of a pendulum subject to downward impulses at specific fixed angles. This pendulum is mathematically formalized as a hybrid automaton, inviting scrutiny from both a geometric vantage point and through the lens of Koopman operator theory. They connect these dual perspectives of dynamical systems, establishing a profound correlation between the Koopman operator’s spectral attributes and the state space’s geometric characteristics.

(Mohr and Mezić, 2016) delves into a nonlinear dynamical framework within a complex, finite-dimensional Banach space, boasting an asymptotically stable and hyperbolic fixed point. Their exploration revolves around elucidating the intricate interplay between the principle eigenfunctions of the Koopman operator and the emergence of a topological conjugacy bridging the nonlinear dynamics with its linearization within the fixed point’s vicinity. Of particular significance, the principle eigenfunctions serve as architects of an algebra of observables, aptly named the *principle algebra*, within the linear dynamics. This algebra then propels the formulation of a series of approximative conjugacy mappings, mirroring the techniques harnessed in the realm of *standard form theory*. Each constituent of the principle algebra unfolds into a spectrum of Koopman operator eigenfunctions. Fusing these eigenfunctions with the approximate topological conjugacies yields approximative eigenfunctions associated with the nonlinear dynamical construct. In instances where the limit of these approximative conjugacy materializes and focus narrows to natural Banach spaces, an elegant application of the *Stone-Weierstrass* theorem unveils the uniform density of both the principle algebra and the pull-back algebra. This latter algebra, defined by merging the principle algebra with the topological conjugacy, permeates the continuous function space or the maximal ideal of constant functions vanishing at the fixed point. The crux of these findings resides in providing a solution to the problem of selecting an appropriate space of observables for dissipative nonlinear dynamical systems, whose components are characterized by

spectral expansions into eigenfunctions. The conclusions elegantly affirm that any continuous observable can be approximated to arbitrary proximity by one harbouring such an expansion.

(Mezić and Surana, 2016) presents a novel extension of the Koopman operator framework tailored for *non-autonomous systems* exhibiting periodic and quasi-periodic temporal variations. By utilizing a family of Koopman operators parameterized by time, alongside time-varying eigenvalues eigenfunctions, and incorporating principles from *Floquet theory*, that advance the concept of Koopman mode decomposition to encompass these broader classes of systems.

(Mohr and Mezić, 2017) delve into the evolution of Koopman principal eigenfunctions within cascaded dynamical systems. When each component subsystem demonstrates asymptotic stability, strict and successive growth characterizes the matrix norms of the linear components inherent to these subsystems, and disjoint spectra are observed among these subsystems. Under these conditions, perturbation functions for the initial conditions associated with each component subsystem can be established. These perturbation functions generate a remarkable outcome: both the orbits of the cascaded system and the isolated component subsystems exhibit zero asymptotic relative error. This pivotal finding implies an intrinsic equivalence in their asymptotic behaviours, consequently establishing the stability of cascaded compositions derived from stable systems. Notably, these conclusions remain applicable to both cascaded systems featuring linear component subsystem dynamics and linear coupling terms and nonlinear cascades that are topologically congruent to the linear case. Furthermore, the study showcases the mutual correspondence between the Koopman principal eigenvalues of each component subsystem and the Koopman eigenvalues of the overall cascaded system. Extending the domain of definition for the principal eigenfunctions of the component systems and subsequently intertwining them with the perturbation function can systematically formulate the corresponding Koopman eigenfunctions for the cascaded system.

The study in (Mezić, 2017) focuses on scrutinizing spectral operator-theoretic attributes inherent in linear and nonlinear dynamical systems, encompassing a spectrum spanning equilibrium and quasi-periodic attractors. Leveraging these intrinsic properties, the article characterizes a specific class of datasets, introducing the novel concept of the principal dimension of the data. The exploration begins by harnessing the *Kato Decomposition* (Kato, 1958) to forge a spectral expansion tailored to general linear autonomous dynamical systems featuring analytic observables. This intricate development lays the groundwork for defining generalized eigenfunctions of the associated Koopman operator. A compelling revelation emerges as the article decodes the significance of stable, unstable, and centre subspaces, revealing their essence as zero-level sets of generalized eigenfunctions. This discernment extends to nonlinear dynamical systems featuring an equilibrium, thanks to the profound impact of Koopman eigenfunctions and the innovative concept of open eigenfunctions—entities defined on subsets of state space. Expanding upon these foundations, the study delves into the dynamic interplay of nonlinear systems, highlighting their intricate properties. The characterization of (global) centre, centre-stable, and centre-unstable manifolds is unravelled by scrutinizing the zero-level sets of Koopman operator eigenfunctions associated with the nonlinear system. This narrative unfolds as the study engages with dynamical systems boasting globally stable limit cycles and limit tori. In these scenarios, spectral expansions seamlessly integrate square-integrable observables in on-attractor variables and analytic observables in off-attractor variables, redefining stable, unstable, and global centre manifolds intertwined with the zero-level sets of Koopman operator eigenfunctions. The discourse extends its reach to embrace a broader class of nonlinear systems, introducing the notion of isostables. Concurrent with this rich tapestry, the study provides a compelling example: a measure-preserving system that, despite evading chaos, harbours a continuous spectrum. Experimental spectrum observations within such systems are also explored, enriching the discourse. Concluding the journey, the study encapsulates the implications of these theoretical strides by defining data characteristics and elucidating the principal dimension across a distinct class of datasets. This principal dimension is grounded in the lattice-like principal spectrum of the associated Koopman operator, drawing the expedition into the depths of spectral operator-theoretic exploration.

In (Mezić and Arbabi, 2017), the Koopman operator framework assumes a central role as an essential

mathematical tool in nonlinear control. Within this framework, operators manipulate observables to capture the intricate evolution of dynamical systems. Dynamic Mode Decomposition (DMD), a prominent technique, emerges as a robust method for computing Koopman modes. A compelling connection emerges, linking DMD with the Koopman Mode Decomposition (KMD), enriching the understanding of their interplay. Expanding the exploration, the study delves into the computation of isostables and isochrons, navigating this realm through the lens of DMD. This journey uncovers the intricate threads binding these concepts to the overarching Koopman operator. This comprehensive analysis unveils the intricate synergy among the Koopman operator framework, DMD, and the characterization of isostables and isochrons.

In (Kurdila and Bobade, 2018), Koopman theory investigates dynamical systems by examining the operator-theoretic properties of the Perron-Frobenius and Koopman operators denoted as \mathcal{P} and \mathcal{U} , respectively. This paper is dedicated to deriving convergence rates for estimates of these operators, applicable to a wide range of generally nonlinear dynamical systems across various scenarios. Additionally, the article establishes convergence rates for specific probability measures associated with these operators and for specific data-driven algorithms constructed based on them. A central element of this paper introduces a suitably general class of priors, describing the information available for creating these approximations. These priors are designed to facilitate the development of error estimates in numerous applications of interest. The definition of these priors is framed in terms of the action of \mathcal{P} or \mathcal{U} within specific linear approximation spaces. In cases where obtaining eigenfunctions of either the Perron-Frobenius or Koopman operator is feasible, priors are defined with respect to the “spectral approximation space” denoted as $A_\lambda^{r,2}(H)$, where $r > 0$ represents the approximation rate, T is a given self-adjoint and compact operator on H , $\lambda := \lambda(T)$ represents the eigenvalues of T , and H constitutes a Hilbert space of functions defined over the domain $\Omega \subseteq \mathbb{R}^d$. In a more general context, the article employs priors expressed to *Banach spaces of linear approximation* denoted as $A^{r,q}(X)$, with X representing a Banach space of functions defined on the domain Ω , $r > 0$ indicating the approximation rate (or smoothness), $\{A_j\}_{j \in \mathbb{N}_0}$ comprising a sequence of approximant spaces, and $1 \leq q \leq \infty$. Most frequently, this paper focuses on scenarios where the Hilbert space H is either $U := L_\mu^2(\Omega)$ with μ representing a measure or $V \subset U$ denoting a reproducing kernel Hilbert space (RKHS). The paper proceeds to characterize the convergence rates for \mathcal{P} approximations or \mathcal{U} generated through finite-dimensional bases like wavelets, multiwavelets, and eigenfunctions. Furthermore, it delves into approaches incorporating samples of the system’s input and output in conjunction with these bases. Given that the wavelets and multiwavelets are specifically selected to reproduce piecewise polynomials of a particular order, the results derived here shed light on the achievable approximation rates for joint spline or finite element approximations, particularly in *Petrov-Galerkin* approximations of the *Frobenius-Perron* or Koopman operators. In cases where the operator estimates are sample-based, the paper demonstrates that the error in the approximation of the Perron-Frobenius or Koopman operators can be decomposed into two components: the approximation error and the sampling error. This finding underscores the well-known trade-off between bias and variance contributing to the error. This balance also plays a prominent role in nonlinear regression and statistical learning theory.

In (Maćešić et al., 2018), for any nonautonomous dynamical system, the family of Koopman operators and associated Koopman eigenvalues and eigenfunctions is parameterized by a time pair. Consequently, a logical approach within data-driven algorithms for nonautonomous Koopman Mode Decomposition involves implementing a dynamic mode decomposition (DMD) technique on moving stencils of snapshots to capture the time-dependent nature of the system. This paper thoroughly examines the challenges that arise when pursuing such an approach. These challenges do not surface when employing the moving stencil approach as the model fitting method. Instead, they become apparent in substantial errors in the computed eigenvalues of the nonautonomous Koopman operator. The first challenge manifests in hybrid dynamical systems when the moving stencil traverses a nonautonomous switching point. The article demonstrates that such stencils can be identified by evaluating the Krylov subspace projection error and introducing an algorithm that computes accurate eigenvalues by circumventing these problematic stencils. The second challenge emerges in the context

of continuous-in-time nonautonomous systems. Even if one applies techniques to identify suitable observables capable of addressing all issues in autonomous scenarios, the computation of nonautonomous Koopman eigenvalues still incurs significant errors. The article’s theorems elucidate this error’s nature and propose a secondary algorithm grounded in stencil size reduction. Applying these two novel data-driven algorithms to various nonautonomous systems demonstrates their efficacy in rectifying the errors that typically arise in the computation of nonautonomous Koopman operator eigenvalues.

In (Mezić, 2022), the focus is on the study of numerical approaches for computing the spectral properties of composition operators. The characterization of Koopman Modes in Banach spaces is achieved by applying *generalized Laplace analysis*. The context of the finite section theory of infinite-dimensional operators is utilized to frame dynamic mode decomposition-type methods, along with the presentation of an illustrative example involving a mixing map where the finite section method encounters challenges. Subject to assumptions concerning the underlying dynamics, the initial result is presented regarding the convergence rate as the sample size increases in the finite-section approximation. Furthermore, investigating the error within the Krylov subspace version of the finite section method leads to establishing convergence in a pseudospectral sense for operators characterized by a pure point spectrum. This outcome is particularly noteworthy as *Krylov sequence*-based approximations possess the potential to mitigate the curse of dimensionality, indicating that they may maintain low spectral error without necessitating an exponential increase in the number of required functions.

4 Data Driven Techniques in Nonlinear Dynamics

(Williams et al., 2015a) introduces a data-driven technique for approximating the principal eigenvalues, eigenfunctions, and modes associated with the Koopman operator. This method relies on a dataset containing pairs of snapshots and a predefined collection of scalar observables without requiring explicit governing equations or interaction with a *black box integrator*. The article will demonstrate that this approach can be viewed as an extension of dynamic mode decomposition (DMD), a technique utilized for approximating Koopman eigenvalues and modes. Additionally, if the dataset originates from a Markov process rather than a deterministic dynamical system, the algorithm provides approximations of the eigenfunctions of the *Kolmogorov backward equation*. This extension could be regarded as the representation of the *stochastic Koopman operator*. To provide clarity, the article presented four illustrative examples. Two of these examples showcase the method’s quantitative performance when presented with either deterministic or stochastic data, while the other two highlight potential applications of the Koopman eigenfunctions. For further results in this direction, see (Klus et al., 2016; Korda and Mezić, 2018c)

(Williams et al., 2015b) introduces a novel technique for integrating measurements acquired from disparate sensors within nonlinear systems. This method capitalizes on the Koopman operator and its associated eigenfunctions, treated as inherent coordinates, which are approximated through an extended version of dynamic mode decomposition. The algorithm mandates time series data from each sensor and a modest quantity of shared measurements. Its applicability extends to systems featuring two distinct measurement sets, provided invertible mappings, and constant sampling intervals exist. The procedure entails the approximation of eigenfunctions through data-driven means and establishing mappings between observations via parameter values and principal-component analysis. By combining static and dynamic state estimation methodologies through interpolation, the method facilitates the creation of approximations for Koopman eigenfunctions and eigenvalues. These approximations are the foundation for parameterizing the data and characterizing the slow manifold. Moreover, the algorithm computes principal-component coefficients for new data points, effectively identifying minor numerical discrepancies in the reconstruction process. Notably, this approach empowers the generation of independent mappings connecting diverse measurement sets as long as each set possesses a mapping to the system state. The method aligns well with contemporary data-driven techniques

like Extended DMD, enhancing its practical feasibility.

(Raak et al., 2016) delve into applying Koopman Mode Decomposition (KMD) to dynamic datasets characterized by low spatial dimensions compared with the well-established Dynamic Mode Decomposition (DMD). Their investigation thoroughly examined diverse algorithms tailored for KMD and an intricate analysis of the system’s dynamical attributes as delineated by these modes. A pivotal focus of the discourse is the strategic mitigation of rank deficiencies in power system test data, skillfully achieved through incorporating the Prony method. To substantiate the methodologies, the article subjects the algorithms—namely DMD, Arnoldi KMD, and Prony to empirical testing using data emanating from a power system harbouring seven buses and three synchronous generators. This complex system is characterized by a constant impedance load and is perturbed by various disturbances. In this empirical crucible, DMD exhibits a conspicuous performance shortfall compared to its algorithmic counterparts, particularly as the dataset’s size augments. Contrarily, the Prony algorithm showcases commendable performance in low frequencies, exhibiting a distinct peak at a specific value. Both the Arnoldi and Prony algorithms display robustness in frequency identification even when confronted with voluminous datasets. Furthermore, employing a timeshifted time-series approach vividly portrays a linear attenuation of oscillations—notably, the algorithms under scrutiny yield congruent outcomes when the function subspace undergoes expansion. In a comparative vein, DMD and Arnoldi yield similar results when juxtaposing the algorithms in scenarios featuring distinct measurement locales. Intriguingly, DMD’s efficacy evinces signs of diminishment as the parametric values ascend beyond a certain threshold. In sum, this erudite exposition navigates the intricate landscape of KMD’s application to dynamic data with parsimonious spatial dimensions, drawing meaningful comparisons against the backdrop of DMD. The algorithms’ performances are meticulously scrutinized within the context of power system dynamics, elucidating their merits and limitations under varying conditions.

(Mezić, 2016) studied comparing dynamical systems or aligning them with empirical data—a challenge of paramount significance within the domains of dynamical systems and control theory. This endeavour assumes heightened complexity when addressing systems and data characterized by nonlinear behaviours and non-Gaussian noise profiles. It presents a novel theoretical framework that capitalizes upon the spectral theory of linear operators, precisely composition or Koopman operators. Initially devised for systems endowed with measure-preserving attributes, this theoretical construct is judiciously extended to encompass the intricate realms of dissipative and finite-time dynamics. Central to their methodological approach is the synergistic amalgamation of an advanced iteration of ergodic partition theory with the sophisticated underpinnings of Hardy space theory. Remarkably, this fusion is instantiated within the ambit of the observable space, thereby deviating from the conventional temporal framework. It is envisaged that this contribution significantly enriches the discourse surrounding comparing dynamical systems and their correspondence with empirical data in nonlinear and noise-affected scenarios. As such, this work bears implications for fundamental research and practical applications within the purview of various scientific and engineering disciplines.

In (Brunton et al., 2017), the focal theme revolves around data-driven approaches for analyzing chaotic systems, emphasizing the pivotal role of big data and machine learning. Integral to this discussion is exploring the Takens embedding theorem, which interfaces with utilizing Koopman operator theory to facilitate linear representations of inherently nonlinear dynamics. The exposition delves into the HAVOK model, which is distinguished for its ability to predict lobe-switching events with precision. Moreover, the article engages in a comprehensive dialogue concerning estimating nearly invariant sets through the lens of the Perron-Frobenius operator. The HAVOK method, a centrepiece of the discourse, demonstrates its prowess in effectively modelling and predicting various systems. It adeptly captures the nuanced interplay of attractor dynamics, significant transients, and intermittent phenomena. A word of caution surfaces regarding applying time-delay coordinates in real-time scenarios, underscoring the importance of prudent implementation. The imperatives of model order and sparse regression are highlighted as critical considerations to counteract overfitting and instability. In a harmonious convergence of methodologies, the HAVOK analysis seamlessly integrates machine learning regression, *Takens’ embedding theorem*, and Koopman’s theory. This fusion collectively culminates

in identifying a linear system representation underlying chaotic dynamics. Embedded within this analytical framework lies the strategic determination of timestep and truncation rank, thereby refining the robustness and precision of the analysis.

(Takeishi et al., 2017a) introduces a data-driven methodology for modal decomposition utilizing the Koopman operator. The approach involves estimating parametric functions through linear regression and integrating them into *neural networks*. This integration serves to convert the original data into a linear regression format. Furthermore, the method encompasses reconstructing original states from observed data via delay-coordinate embedding. This reconstruction is complemented by training a linear embedder, a critical step in selecting optimal embedding parameters. The underpinning of this decomposition is the LKIS framework, which incorporates a tailored loss function designed to encompass the reconstruction of the original measurements. In modelling functions, *neural networks*, specifically multi-layer perceptrons, come into play. The optimization procedure hinges on gradient descent facilitated by batch normalization techniques. The genesis of this proposed framework emanates from an operator-theoretic perspective on nonlinear dynamical systems. LKIS-DMD, the specific algorithm in this framework, can discern eigenvalues and accurately withstand observation noise. Its utility extends to predictive analysis and the identification of unstable phenomena. Moreover, the framework can be adeptly adapted to assimilate data uncertainties.

(Arbabi and Mezić, 2017b) explores the Koopman Mode Decomposition (KMD), a data-analysis technique renowned for extracting intricate spatiotemporal patterns from complex flows. The focus of the article centres on employing KMD to investigate the dynamics of a lid-driven flow within a two-dimensional square cavity. Drawing upon theorems rooted in the spectral theory of the Koopman operator, the article delves into the intricate interplay of dynamics. The article harnesses two established algorithms derived from classical Fourier and power spectral analysis methodologies. These algorithms are adeptly adapted to compute both the discrete and continuous spectra of the Koopman operator as applied to post-transient flows. The spectral properties of the Koopman operator become instrumental in unravelling the sequence of distinct flow regimes observed within the Re range of 10000 to 30000. This transitional spectrum reflects the evolution of flow nature, transitioning from a steady state to an aperiodic regime. The construction of Koopman eigenfunctions for diverse flow regimes, encompassing those with mixed spectra, hinges on the assumption of ergodicity within the state space. Intriguingly, the associated Koopman modes exhibit remarkable robustness even amidst substantial shifts in the temporal character of the flow. Our investigation reveals that KMD performs better than proper orthogonal decomposition when reconstructing flows characterized by quasi-periodic solid components. This finding underscores the efficacy and potential of KMD in capturing the intricate features of dynamic systems.

(Arbabi and Mezić, 2017a) focus on establishing the convergence of a specific class of numerical algorithms known as dynamic mode decomposition (DMD). These algorithms serve as valuable tools for computing the eigenvalues and eigenfunctions of the infinite-dimensional Koopman operator. The foundation of these algorithms lies in their manipulation of data derived from observables within a state space, organized into matrices reminiscent of Hankel matrices. The theoretical investigations draw strength from the assumption of ergodicity inherent to the underlying dynamical system. This assumption encompasses classical measure-preserving systems characterized by attractors supporting physical measures. Central to their approach is the observation that the vector projections within DMD can effectively approximate function projections, leveraging Birkhoff’s ergodic theorem. Leveraging this insight, the article demonstrates that the application of DMD to Hankel data matrices, as the observation time tends to be infinite, culminates in precisely determining Koopman eigenfunctions and eigenvalues. Additionally, they elucidate that the singular value decomposition—a cornerstone of most DMD algorithms—converges to the proper orthogonal decomposition of observables. This pivotal result enhances the theoretical understanding and enables a novel representation of the dynamics of systems characterized by continuous spectra. This representation is rooted in the elevation of coordinates to the realm of observables. The article turns to numerical applications to showcase the practical utility of these methods. The article illustrates these newly developed techniques’ tangible benefits

and insights by delving into well-known dynamical systems and drawing examples from computational fluid dynamics.

In (Fonoberova et al., 2018), the research pivots around using agent-based modelling to comprehensively investigate the dynamics of social processes, particularly those underlying urban insurgency. Koopman Mode Analysis (KMA) is a pivotal tool employed to dissect the models, unravelling the multifaceted impacts various factors exert on simulation outcomes. The financial support for this study through an AFOSR grant and the consequent availability of data in a Zenodo public repository are worth noting. The agent-based model’s behaviour within the simulation realm finds expression through a tensor and an array of random vectors. Notably, the interplay of diverse factors—lattice size and the count of gathering sites—exerts a palpable influence on the number of active citizens and the emergence of large-scale outbursts. While an initial increase in the number of outbursts is observed upon augmenting gathering sites, a threshold subsequently leads to a decrease. Moreover, the zenith of active citizens during an outburst dwindles in tandem with growing gathering sites and lattice size. The dynamics of insurgency exhibit a nuanced relationship with variables such as waiting time between outbursts and the count of active and intimidated citizens. A peak in the number of revolutions per 1,000 days is discerned for lattices of average dimensions. Notably, the spatial distribution of active citizens and law enforcement officers undergoes meticulous analysis via Koopman Mode Decomposition. A strategic insight emerges, highlighting the necessity for law enforcement officers to cover the zones connecting gathering sites, thus thwarting large-scale outbursts. Introducing preferential gathering sites introduces captivating non-monotonic behaviour in large-scale insurgency outbursts. Remarkably, including numerous gathering sites fosters spatial dispersion among citizens, alleviating local concentrations. By leveraging Koopman Mode Analysis, meaningful spatial patterns are adeptly extracted from the dynamic data, fostering deeper insights into the studied phenomena. Further unravelling this investigation, the discourse traverses the realm of agent-based modelling concerning urban insurgency. The spotlight rests on the impact of organized gathering sites, offering a novel vantage point. This exploration unearths intriguing dynamics wherein a limited number of gathering sites wield a more significant insurgency impact than their more distributed counterparts. Law enforcement officers’ spatial distribution starkly contrasts with that of active and intimidated citizens, a noteworthy observation. It is imperative to clarify that the study refrains from advocating policy recommendations, instead focusing on introducing the concept of environmental morphology within insurgency organizations.

In (Drmač et al., 2019), this paper presents a two-fold objective. Firstly, it introduces a novel computational tool for data-driven Koopman spectral analysis, addressing the formidable challenge of devising a numerically robust algorithm. This is achieved by adopting a natural formulation involving the Krylov decomposition with the Frobenius companion matrix and the explicit utilization of its eigenvectors, which are, by definition, the inverses of the notoriously ill-conditioned Vandermonde matrix. Crucially, ill-conditioning mitigation hinges on the discrete Fourier transform of the snapshots. In this new framework, the Vandermonde matrix transforms a generalized Cauchy matrix, facilitating precise computations through specialized algorithms in numerical linear algebra. Secondly, the paper aims to illuminate the relationship between formulas for optimal reconstruction weights in reconstructing snapshots using subsets of the computed Koopman modes. It demonstrates how adopting a specific variant of generalized inverses yields explicit reconstruction formulas that align with the abstract findings of Koopman spectral theory, particularly those about the Generalized Laplace Analysis.

In (Li et al., 2019), a novel methodology is introduced, combining compositional Koopman operators and graph networks to enable efficient and adaptable dynamics modelling of intricate systems. This innovative approach effectively circumvents the limitations associated with neural networks by employing a linear approximation strategy. The primary hurdle faced in this endeavour is scalability, a challenge mitigated through leveraging the inherent structure of the system. At the heart of this model lies the utilization of graph networks to represent the compositional nature of fluid control systems. This framework exhibits remarkable versatility, capable of generalizing across diverse environments and shapes while adeptly handling

uncertainty and enhancing the efficiency of solving control problems. The Koopman operator, serving as a linear transformation mapping the state space of a dynamical system into an embedding space, plays a pivotal role in this context. The paper delves into the intricacies of modelling and controlling multi-object systems, introducing compositional Koopman operators to accommodate compositionality. It achieves this by employing object-centric sub-embeddings and structuring the Koopman matrix block-wise. The method further leverages a graph neural network to generate object-centric Koopman embeddings. The key to its effectiveness is a least squares problem-solving approach employed to identify the Koopman and control matrices, effectively reducing the number of parameters involved in the process. This optimization strategy hinges on minimizing a training loss and a total cost function facilitated by quadratic programming techniques. The practical application of this model extends to simulations and control of diverse systems, including ropes and soft robots. Remarkably, the model surpasses other baseline models in tasks related to ropes, soft materials, and swimming, rendering it particularly advantageous in real-world scenarios where physical parameters remain unknown. Furthermore, introducing metric loss within the methodology significantly enhances prediction accuracy, acting as an effective regularization tool. While preserving distances and mitigating simulation errors, this regularisation remarkably enhances distance preservation without compromising the accuracy of dynamics modelling and control. It is precious in novel, uncharted environments where physical parameters remain elusive. Consequently, the model trained with metric loss excels in distance preservation and control performance compared to alternative models.

In (Mezić, 2020), the examination of spectral operator-theoretic properties within linear and nonlinear dynamical systems, marked by globally stable attractors, is undertaken. Using the Kato decomposition, a spectral expansion is formulated for general linear autonomous dynamical systems boasting analytic observables. In tandem, the notion of generalized eigenfunctions linked to the Koopman operator is introduced. Stable, unstable, and centre subspaces are elucidated by expressing them in the zero-level sets of these generalized eigenfunctions. Subsequently, the extension of these findings to nonlinear dynamical systems with an equilibrium point is facilitated by leveraging the conjugacy properties of Koopman eigenfunctions and introducing the innovative concept of open eigenfunctions defined within the state space’s subsets. A comprehensive characterization of (global) centre manifolds, centre-stable, and centre-unstable manifolds associated with the nonlinear system is provided. These characterizations are rooted in the joint zero-level sets of families of Koopman operator eigenfunctions. Furthermore, a novel class of Hilbert spaces is introduced, designed to encapsulate dissipative dynamics’ on- and off-attractor properties. The concept of modulated Fock spaces is also presented, enabling the development of spectral expansions for a specific class of dynamical systems characterized by globally stable limit cycles and limit tori. These expansions apply to square-integrable observables in on-attractor variables and analytic in off-attractor variables. Moreover, discussions revolve around the definitions of stable, unstable, and global centre manifolds in nonlinear systems featuring (quasi)-periodic attractors, expounded in terms of zero-level sets of Koopman operator eigenfunctions. The article introduces the notion of isostables for a broad category of nonlinear systems, distinguishing them from systems with discrete Koopman operator spectra. A notable departure arises as a straightforward example of a measure-preserving system devoid of chaos yet featuring a continuous spectrum. Furthermore, it discusses experimental observations of the spectrum within such systems. In addition, it briefly outlines the data types corresponding to the acquired theoretical results. It defines the coherent principal dimension for a specific class of datasets grounded in the lattice-type principal spectrum associated with the Koopman operator.

In (Korda et al., 2020), a method emerges for computing the fine structure of the Koopman operator’s spectrum, accompanied by rigorous convergence guarantees formulated from measured data. This method is predicated on the observation that, within the measure-preserving ergodic context, the computability of the moments of the spectral measure linked to a particular observable arises from a solitary trajectory of that observable. Employing a finite array of moments, the classical *Christoffel–Darboux* kernel is utilized to partition the spectrum into atomic and continuous components. Importantly, this partitioning enjoys convergence guarantees as the number of moments approaches infinity—Furthermore, a novel technique surfaces for identifying the singular continuous portion of the spectrum. Additionally, two distinct approaches

are presented for approximating the spectral measure, each boasting guaranteed convergence in the weak topology. This holds irrespective of the presence or absence of the singular continuous component. The implementation of this method is characterized by its simplicity and adaptability to large-scale systems. This convenience stems from the computational complexity, primarily determined by the inversion of an $N \times N$ Hermitian positive-definite Toeplitz matrix. Fortunately, specialized and numerically stable algorithms tailored for this task are readily available. Notably, the approach’s complexity remains unaffected by the dimensionality of the underlying state space. Furthermore, computing the spectral projection onto a specified segment of the unit circle based on measured data is thoroughly elucidated. This process enables the derivation of a finite approximation of the operator, explicitly encompassing both the point and continuous facets of the spectrum. Finally, a connection is drawn between the proposed method and the Hankel Dynamic Mode Decomposition (DMD), offering novel insights into the behaviour of the eigenvalues associated with the Hankel DMD operator. A series of numerical examples illustrate the approach’s efficacy, including a comprehensive spectrum examination within the lid-driven two-dimensional cavity flow.

In (Nakao and Mezić, 2020), an overview is provided of Koopman-operator analysis as applied to a class of partial differential equations that describe the relaxation of the field variable towards a stable stationary state. The presentation commences by introducing Koopman eigenfunctions for this system and utilizes the concept of conjugacy to construct a spectral expansion for the Koopman operator. Within linear systems, such as the diffusion equation, Koopman eigenfunctions manifest as linear functionals of the field variable. A pivotal insight is revealed as the notion of inertial manifolds aligns with the joint zero-level sets of these Koopman eigenfunctions. Furthermore, isostables are the level sets associated with the slowest decaying Koopman eigenfunctions. Specific examples are analyzed to concretize these theoretical ideas, including the linear diffusion equation, the nonlinear Burgers equation, and the nonlinear phase-diffusion equation.

In (Rabben et al., 2020), the challenge of ascertaining the occurrence rate of infrequent events within dynamical systems is widely recognized, yet it remains a formidable task. Recent endeavours to surmount this challenge capitalize on the premise that linear operators can effectively encapsulate dynamic systems, exemplified by the Koopman operator. From a mathematical standpoint, the crux of the rare event problem lies in the intricate quest for invariant subspaces embedded within these Koopman operators. An approach is expounded upon in the following exposition, outlining the process of acquiring foundational functions for these invariant subspaces through an artificial neural network.

In (Susuki et al., 2021), the research motivation lies in establishing a Laplace-domain theory, offering principles and methodology for analyzing and synthesizing systems with nonlinear dynamics. At the core of this study resides a semigroup of composition operators tailored for nonlinear autonomous dynamical systems—the Koopman semigroup and its corresponding Koopman generator. The Koopman generator’s resolvent, referred to as the Koopman resolvent, is introduced, along with its spectral characterization for three distinct types of nonlinear dynamics: ergodic evolution on an attractor, convergence towards a stable equilibrium point, and convergence towards a (quasi-)stable limit cycle. This investigation illuminates the Koopman resolvent’s role as a Laplace-domain representation for such nonlinear autonomous dynamics. The computational facet of the Laplace-domain representation is also explored, with particular emphasis on nonstationary Koopman modes.

In (Govindarajan et al., 2021), the method’s generalization for computing the Koopman operator’s spectral decomposition using periodic approximations is extended to the class of measure-preserving flows on compact metric spaces. The paper demonstrates the feasibility of approximating the spectral decomposition of the continuous one-parameter unitary group through an intermediate time discretization of the flow. A sufficient condition is established to ensure weak convergence of spectra in the limit, linking the temporal discretization of the flow to the spatial discretization of the periodic approximation. Specifically, this condition requires that spatial refinements progress faster than temporal refinements. This outcome is juxtaposed with the well-known CLF condition found in finite difference schemes for advection equations. The paper provides numerical results showcasing spectral computations for various benchmark examples of volume-preserving flows.

In (Lange et al., 2021), spectral methods are introduced for long-term forecasting of temporal signals originating from linear and nonlinear quasi-periodic dynamical systems. An algorithm is presented for linear signals, bearing similarities to the Fourier transform but devoid of reliance on periodicity assumptions. This approach enables forecasting with potentially arbitrary sampling intervals. Subsequently, an extension of this algorithm is devised to accommodate nonlinearities, utilizing Koopman’s theory. The resultant algorithm conducts a spectral decomposition within a nonlinear, data-dependent basis. It is imperative to note that the optimization objective for both algorithms exhibits a highly non-convex nature. Nevertheless, by expressing the objective in the frequency domain, the computation of global optima for the error surface is scalable and efficient. This is facilitated, in part, by exploiting the computational attributes of the Fast Fourier Transform. Moreover, owing to their close association with Bayesian Spectral Analysis, these spectral forecasting methods yield uncertainty quantification metrics as a natural byproduct. A comprehensive benchmarking evaluation of these algorithms is undertaken, encompassing a range of synthetic experiments and their application in real-world power systems and fluid flows.

In (Avila et al., 2021), a comprehensive endeavour unfolds, aiming to revolutionize game balancing through the judicious amalgamation of a balance criterion and Koopman operator methodologies. The central premise revolves around utilizing the Koopman model as a potent tool for disentangling the intricate dynamics within a game and optimizing its mechanics. The specific focus of this study is directed toward achieving equilibrium in DeepMind’s SC2 DefeatRoaches mini-game. Within this context, the narrative meticulously navigates through the intricate process of leveraging a Koopman model to orchestrate game balance. The crux lies in identifying the pivotal parameters that wield influence over game dynamics, all in pursuit of minimizing a balance criterion denoted as “J.” This endeavour entails modelling the game’s intricate dynamics and validating the model by harmonizing it with empirical game data. The fruits of this labour manifest in balanced games characterized by extended durations and players teetering on the precipice of near-zero health. However, they may not necessarily exhibit a 50-50 probability of winning. The framework orchestrates this achievement through the deft application of Koopman operator techniques and employing nonlinear programming solvers. While this study presents a groundbreaking paradigm for game balance in the context of the SC2 DefeatRoaches mini-game, its ramifications extend far beyond this singular application. As a precursor of innovation, it paves the way for the scalability of this framework, promising to tackle more intricate and complex games in the future. Additionally, future explorations will scrutinize the impact of initial conditions on the hallowed concept of game balance. Traditionally, the commercial gaming industry has relied upon trial-and-error methodologies and player feedback to navigate the labyrinth of game balance. However, this study ushers in a new era by showcasing the transformative potential of artificial intelligence algorithms. These algorithms are adeptly harnessed to automate the assessment of game balance, armed with the precision of a balance criterion that optimizes the very essence of game mechanics. The crux of this transformation hinges upon the quantitative unravelling of the temporal evolution of game dynamics, accomplished through the prism of the Koopman operator framework. This sophisticated framework lends itself to estimating governing equations, elucidating the intricate dance of game dynamics through spectral properties, eigenvalues, and eigenfunctions. The dynamics of a game are elegantly encapsulated through simplified equations within a closed-loop system, and the matrix M in the Koopman representation is effectively estimated through multiple game runs. Central to the quest for game balance is the minimization of a criterion meticulously designed to account for player score functions. The practical manifestation of this methodology finds expression in its application to the DeepMind SC2 mini-game, where a Koopman model, in harmony with game data gleaned from replays, strives to craft equilibrium. Sensitivity analysis complements this endeavour, illuminating the profound influence wielded by distinct parameters on the game’s outcomes. The authors of this study introduce a novel balance criterion, denoted as “J,” meticulously calibrated to measure the elusive concept of game balance. This criterion is the cornerstone for articulating parameters that culminate in attaining near-zero values for J, a hallmark of game equilibrium. The Koopman model, the linchpin of this pursuit, is entrusted with estimating balanced points, and the integrity of these results is firmly grounded in their alignment with empirical game data. In summary, this framework emerges as a trailblazer in-game balance,

showcasing its prowess by successfully balancing the intricate dynamics of a StarCraft II mini-game. As a precursor of possibilities, it offers scalability to address more complex games in future endeavours, heralding a seismic shift in the approach to game balancing, shunning traditional trial-and-error methods in favour of data-driven precision.

In (Hill et al., 2023), the text elucidates the realm of gait recognition to distinguish individuals based on their distinctive walking styles. This comprehensive exploration delves into the two primary paradigms of gait recognition, appearance-based and model-based approaches, shedding light on the intricate challenges of limited data availability. Moreover, it underscores the transformative impact of deep learning techniques, notably Convolutional *neural networks* (CNNs) and the Skinned Multi-Person Linear (SMPL) model, in enhancing the precision of gait recognition. The passage introduces a groundbreaking end-to-end model that amalgamates the VIBE model with a transformer network, thereby facilitating the fusion of temporal pose information and shape parameters. These innovations culminate in an advanced model, GaitVIBE + LDS, which represents a noteworthy advancement over earlier methodologies for gait recognition. This pioneering model harnesses the power of 3D human body models, achieving remarkable performance benchmarks when contrasted with previous approaches, particularly on specific datasets. Notably, integrating linear dynamical systems (LDS) constraints is a pivotal achievement, enhancing performance without necessitating additional data. Furthermore, the text explores the intricate details of various loss functions employed in gait recognition, encompassing reconstruction loss, identity loss, and motion loss. The proposed GaitVIBE model, bolstered by the LDS module, outperforms prior works in the domain of gait recognition, particularly in scenarios involving leg occlusion. Notably, the model's performance undergoes rigorous evaluation on the CASIA-B dataset, with the adversarial loss emerging as a particularly influential factor compared to the LDS loss. It is imperative to recognize the ethical and privacy considerations inherent in gait recognition, as this paper underscores. This research endeavour not only presents a formidable advancement in gait recognition through the utilization of 3D human body models and linear dynamical systems constraints but also contemplates potential real-world applications, including identifying individuals in contexts such as combating poaching or locating lost individuals.

5 Past Surveys in Applied Koopman Operator Theory

The focal points of (Budišić et al., 2012) revolve around the advancement and application of the Koopman operator to analyse and visualise high-dimensional dynamical systems. The potential for both academic and industrial applications is elucidated. The paper delves into theoretical concepts and numerical methods intrinsic to the Koopman operator while pinpointing areas necessitating further investigation. Noteworthy aspects of this work encompass the derivation of continuous indicators for ergodicity and mixing, which bear relevance in diverse domains such as path-planning for vehicles and micro-scale fluid mixing. The Koopman operator is thoroughly explored, elucidating its interplay with dynamical systems. The ambit extends to considering finite and infinite-dimensional spaces in the Koopman operator framework, encompassing its extension to handle continuous-time dynamics. The investigation of the spectral properties of the Koopman operator within the framework of a Banach space constitutes another pivotal dimension of this study. This paper's salient features encompass a comprehensive discussion of eigenfunctions and eigenvalues of the Koopman operator. The introduction of ergodic transformations and their interrelation with eigenfunctions unfolds, complemented by developing a computational approach to analyse the Koopman operator within specific sets. Establishing a linkage between periodic eigenvalues and eigenfunctions is a significant contribution. These concepts are applied through a particular instance involving the heat equation. Moreover, the paper broaches the topics of spectral decomposition and projection of observables onto eigenspaces, as well as the inclusion of physical measures in dynamical system evaluation. Exploring Koopman mode distribution and its current limitations in the literature augments the discourse. A pivotal contribution of this paper lies in introducing the Koopman mode decomposition concept and theorem, enabling the dissection of dynamical

systems into stable and unstable modes. This theorem’s application to the harmonic oscillator system is elucidated, albeit acknowledging the challenges of numerical implementation. Data-driven algorithms for computing Koopman modes, encompassing Krylov subspaces and the Arnoldi algorithm, are introduced. A variant of the Arnoldi algorithm, the Dynamic Mode Decomposition (DMD), is presented, along with its robust version for enhanced numerical stability. Koopman modes find application in model reduction and coherency analysis in power systems. This encompasses the identification of coherency in swing dynamics and precursors to coherent swing instability, illustrated through a case study involving the New England Test System. This paper highlights utilising Koopman modes to dissect nonlinear fluid flows, notably exemplified by a jet in crossflow configuration. The DMD algorithm is employed to compute a subset of Koopman modes for the flow field. Leveraging Koopman modes, relevant frequencies and corresponding flow structures are automatically identified. Computational intricacies of the Navier-Stokes equations, state space selection, and observables are expounded upon. This paper’s essential contribution lies in applying Koopman modes to analyse building energy efficiency. Invariant sets are identified through eigenfunctions, and a methodology to analyse level-set partitions independent of specific eigenfunctions is devised. A notable attribute of this paper is the application of the Sobolev space metric for ergodic quotient computation, resulting in the extraction of coherent layers in the state space. Weighted Euclidean norm and Fourier coefficient space are harnessed alongside distance computation between trajectories. The computational approach is instrumental in unveiling coherent structures. The paper traverses diverse dimensions, including temporal Fourier transforms of sequences and interpreting spatial Fourier coefficients as ergodic measures’ spatial Fourier transforms. Eigenquotient maps’ link to ergodic/Fourier average dichotomy is unveiled. The role of harmonic functions as observables to facilitate Sobolev norm evaluation is explored. Convergence errors in the Chirikov Standard Map are dissected, indicating slower convergence in chaotic regions than in regular domains. A proposal is posited to adapt simulated time based on relative convergence errors for enhanced efficiency. The extension of finite-time averages to approximate limiting measures of empirical distributions is broached, culminating in the formulation of continuous mixing and ergodicity indicators for feedback control in technical systems. Finally, this paper’s attributes employ the negative index Sobolev norm $\|\cdot\|_{2,-s}$ as a surrogate for ergodicity computation, applied to scenarios like search-and-rescue tasks and micro-mixer design. A juxtaposition of ergodicity and mixing criteria is presented, accompanied by an overview of the spectral theory of the Koopman operator within dynamical systems.

In (Parmar et al., 2020), Koopman Mode Decomposition emerges as a flow analysis technique pioneered by (Mezić and Banaszuk, 2004), building upon the foundation laid by (Koopman, 1931; Koopman and v. Neumann, 1932) with the Koopman operator. Through Koopman decomposition, any well-sampled dynamic system, whether linear, nonlinear, laminar, or turbulent—chaotic or chaotic—can be dissected into its constituent single-frequency repetitive components, referred to as modes. This paper is a comprehensive survey, consolidating existing knowledge concerning data-driven Koopman analysis techniques. Its primary objective is to provide valuable insights for researchers contemplating utilising data-driven Koopman analysis as they embark on their modelling endeavours. The survey offers a fundamental mathematical elucidation of Koopman analysis, focusing on the data-driven dynamic mode decomposition (DMD) solution, which converges to the Koopman operator when applied to highly sampled datasets. The survey delves into the four primary domains where Koopman analysis finds application: flow analysis, power grid analysis, building thermal analysis, and biomedical analysis while referencing relevant publications. Furthermore, the paper is open to addressing the inherent weaknesses and challenges within Koopman analysis/DMD and presents potential solutions. Although computationally intricate, Koopman analysis is valuable for identifying periodic motion within highly sampled datasets. Compared to a similar analytical approach, *proper orthogonal decomposition*, *Koopman analysis* often offers additional insights into the structure of less prominent modes, albeit at the cost of increased computational complexity.

With ongoing developments in this field and numerous problems in intelligent mobility and vehicle engineering, a survey of Koopman operator techniques is warranted in (Manzoor et al., 2023). This review highlights various applications, particularly in mobility, and discusses theoretical aspects often overlooked but with

significant potential for addressing open problems in these domains.

6 Koopman Operator Theory in Non-linear system Identification

In (Mauroy and Goncalves, 2019), a novel lifting technique for nonlinear system identification within the framework of the Koopman operator is developed. The fundamental concept involves identifying the linear (infinite-dimensional) Koopman operator within the lifted space of observables instead of directly placing the nonlinear system within the state space. This approach results in a linear method for identifying nonlinear systems. The proposed lifting technique represents an indirect method that circumvents the need to compute time derivatives, making it particularly well-suited for low-sampling rate data sets. Two numerical schemes are introduced by considering various finite-dimensional subspaces to approximate and identify the Koopman operator: a primary and dual method. The primary method is a parametric identification technique capable of accurately reconstructing the vector field of a wide range of systems. In contrast, the dual method estimates the vector field at the data points and is especially suitable for identifying high-dimensional systems with limited datasets. This paper provides a comprehensive description of both methods, offers theoretical convergence results, and demonstrates the effectiveness of the lifting techniques through multiple illustrative examples.

In (Cibulka et al., 2019), this paper reveals the outcomes of identifying vehicle dynamics employing the Koopman operator. The core concept involves the transformation of the state space of a nonlinear system (in this case, a car) into a higher-dimensional space using basis functions. In this elevated space, the system dynamics assume a linear form. The critical aspect lies in selecting these basis functions, a topic that needs a universal approach; however, this paper delves into a discussion. Two distinct strategies for the selection of basis functions are presented. The first approach, grounded in Extended Dynamic Mode Decomposition, relies entirely on expert-driven basis selection and is purely data-driven. In contrast, the second approach leverages knowledge of the nonlinear dynamics to construct eigenfunctions of the Koopman operator. These eigenfunctions, by definition, evolve linearly along the trajectory of the nonlinear system and are subsequently employed as basis functions for prediction. These approaches are exemplified through numerical examples, and a discourse on their applicability to nonlinear vehicle systems is included.

In (Cibulka et al., 2020), this paper extends the work initiated by (Cibulka et al., 2019), wherein a nonlinear vehicle model was approximated exclusively through data-driven means, yielding a higher-order linear predictor—the Koopman operator. The vehicle system, characterized by numerous inherent nonlinearities encompassing rigid-body dynamics, coordinate system transformations, and tyre behaviour, presents a challenge. These nonlinearities are approximated within a predefined subset of the state space using the linear Koopman operator to address this. Subsequently, this linear approximation is utilized in designing a linear Model Predictive Control (MPC) framework, operating in the high-dimensional state space where the nonlinear system dynamics manifest as linear transformations. The outcome is a nonlinear MPC system derived through linear methodologies. The paper illustrates the efficacy of the Koopman-based controller, demonstrating its capacity to navigate the vehicle through highly unusual states where the nonlinearities, as mentioned earlier, exert significant influence. Furthermore, a comparative analysis with a controller relying on classical local linearization is presented, along with a discussion of the limitations associated with the latter approach.

In (Drmač et al., 2021), inferring the latent structure within complex nonlinear dynamical systems in a data-driven context emerges as a formidable mathematical challenge, encompassing an ever-expanding array of applications in science and engineering. The framework of Koopman operator-based linearization stands out as a potent tool suitable for identifying nonlinear systems across diverse scenarios. A method recently advanced by (Mauroy and Goncalves, 2019) hinges on elevating data snapshots into a well-suited finite-dimensional function space and subsequently identifying the infinitesimal generator of the Koopman semigroup. This approach,

characterized by its elegance and mathematical appeal, exhibits commendable analytical properties, including convergence guarantees. However, empirical evidence from numerical experiments highlights certain limitations in the software implementation of this method. Specifically, as the dimensionality increases—ensuring theoretically improved approximation and eventual convergence—the numerical implementation may encounter instability and, in some cases, even breakdown. The primary sources of these numerical challenges lie in the computations associated with the matrix representation of the compressed Koopman operator and its logarithm. This paper addresses these subtle numerical intricacies and proposes a novel implementation algorithm to mitigate these issues.

In (Mauroy, 2021), the Koopman operator theory is examined within the context of nonlinear infinite-dimensional systems, where the operator is defined over a space of bounded continuous functionals. The properties of the Koopman semigroup are elucidated, and a finite-dimensional projection of the semigroup is introduced. This projection offers a linear, finite-dimensional approximation of the underlying infinite-dimensional dynamics. This approximation is the foundation for extracting spectral properties from the data, representing a method that extends the Extended Dynamic Mode Decomposition principles to infinite-dimensional systems. The final analysis harnesses the proposed framework to identify a finite-dimensional approximation of the Lie generator associated with the Koopman semigroup. This innovative approach furnishes a linear method for identifying nonlinear partial differential equations (PDEs), accompanied by theoretical convergence results.

7 Koopman Operator Theory in Power Systems Research

In (Susuki and Mezić, 2011b), the utilisation of Koopman mode analysis is explored to extract spatial oscillation modes. The efficacy of Koopman modes is investigated for detecting coherent swings within power systems. A comparison between Koopman, linear global, and proper orthonormal modes is conducted. The capability of Koopman modes to capture the synchronised motion of generators is examined. The application of Koopman mode analysis to identify coherent swings within an extensive test system is demonstrated. The paper underscores identifying dominant components or modes within power system phenomena. It discusses the employment of Hilbert spectral analysis and proper orthonormal decomposition to identify these modes. Furthermore, the paper demonstrates the application of mode identification to determine coherency within transient stability analysis. Various techniques and algorithms developed by other researchers for coherency identification are also discussed.

On the other hand, in (Susuki and Mezić, 2011a), the Koopman Mode Analysis (KMA) is introduced and elucidated as a novel approach for analysing and controlling power systems. The application of KMA to the dynamics of swings in a multi-machine power system is presented. The theoretical foundation of Koopman operators and Koopman modes for nonlinear dynamical systems is introduced. Formulas for characterising dynamics using Koopman modes are provided, along with an explanation of their computation through a projection operation. The utilisation of KMA for investigating power system dynamics under varying conditions is addressed. Numerical outcomes and discoveries resulting from the application of KMA are presented. The authors also acknowledge the support of diverse funding sources in their work.

(Susuki and Mezić, 2012) presents a novel precursor to transient stability issues in multi-machine power systems. A key breakthrough lies in utilising Koopman Mode Analysis, a powerful technique grounded in a fully nonlinear spectral theory. This approach, extending beyond traditional linear methods, allows us to extract and understand intricate oscillatory modes from real-world sensor data and simulated power system oscillations. Crucially, the Koopman operator proves instrumental in identifying the Coherent Swing Instability (CSI) transmission path. They compute the action transfer operator by refining the mathematical model of transient stability through Koopman Mode Analysis. This operator is a pivotal tool, enabling the detection and monitoring of transient stability loss. Through this strategic integration of empirical

data, mathematical modelling, and computational insight, the Koopman operator emerges as the linchpin in comprehending the intricate dynamics of power system instability.

(Susuki and Mezić, 2015) introduce a novel technique for integrating measurements acquired from disparate sensors within nonlinear systems. This method capitalizes on the Koopman operator and its associated eigenfunctions, treated as inherent coordinates, which are approximated through an extended version of dynamic mode decomposition. The algorithm mandates time series data from each sensor and a modest quantity of shared measurements. Its applicability extends to systems featuring two distinct measurement sets, provided invertible mappings, and constant sampling intervals exist. The procedure entails the approximation of eigenfunctions through data-driven means and establishing mappings between observations via parameter values and principal-component analysis. By combining static and dynamic state estimation methodologies through interpolation, the method facilitates the creation of approximations for Koopman eigenfunctions and eigenvalues. These approximations are the foundation for parameterizing the data and characterizing the slow manifold. Moreover, the algorithm computes principal-component coefficients for new data points, effectively identifying minor numerical discrepancies in the reconstruction process. Notably, this approach empowers the generation of independent mappings connecting diverse measurement sets as long as each set possesses a mapping to the system state. The method aligns well with contemporary data-driven techniques like Extended DMD, enhancing its practical feasibility.

(Susuki and Mezić, 2014) discusses utilizing Koopman mode analysis to evaluate power system stability and detect dynamic power flow patterns. This method employs the eigenvalues and eigenfunctions of the Koopman operator for stability assessment. The study examines power exchange deviations and showcases a data-driven stability assessment approach based on the Koopman operator theory that does not require model development. Results highlight the presence of stable and unstable modes, with the latter persisting across various sample lengths. The Koopman operator theory adeptly captures global unstable trends, offering system operators valuable insights for preemptive actions. The computation of Koopman eigenvalues and modes employs the Arnoldi-like algorithm. The paper introduces a Koopman mode analysis (KMA) method based on physical power flow data for stability assessment in power systems. It delves into power flow dynamics, identifying stability patterns. This approach successfully analyzes data from significant power grid accidents, revealing unstable modes linked to disruptions. The method's data-driven nature eliminates the need for model development. Additionally, the paper proposes an approach for modelling cascading outages in power systems using Koopman mode analysis. This technique assesses stability and identifies short-term dynamic trends by analyzing power flow data. The method has been applied to significant grid accidents, uncovering unstable and stable dynamics tied to specific events. Using actual power flow data, Koopman mode analysis effectively scrutinizes power systems' dynamics and stability. This approach, known as KMA, can uncover instabilities that conventional model-based methods might overlook. This method identifies unstable modes by computing Koopman eigenvalues and modes, enabling monitoring and controlling large-scale, emergent events in power systems. For more on future problems and research direction, see (Susuki et al., 2016).

In (Korda et al., 2018), this seminal work addresses the challenging problem of transient stabilization within a power grid after a perturbing disturbance. The focal point of their investigation is the intricate cascade interconnection of seven New England test models, with the initial disturbance, exemplified by a powerline failure, manifesting in the primary grid and propagating through the network, emulating the onset of a widespread blackout scenario. Within this comprehensive study, the article embraces a data-centric control framework firmly rooted in the profound principles of Koopman operator theory. This innovative approach involves the construction of a linear predictor, which evolves within a higher-dimensional (embedded) state space. This predictor is meticulously constructed based on observed data and is subsequently harnessed within the model predictive control (MPC) framework. Notably, this integration of the Koopman operator theory with MPC offers the compelling advantage of deploying computationally efficient tools from the realm of linear MPC to govern the dynamics of this intrinsically nonlinear system effectively.

In (Dylewsky et al., 2022), a data-driven approach for load forecasting emerges, seamlessly uniting dynamic mode decomposition (DMD) and Gaussian process regression (GPR) to enhance prediction accuracy and robustness in the realm of power grid load forecasting. This innovative method harnesses the intrinsic capabilities of DMD, excelling at uncovering linear intrinsic dynamics within time series data and deciphering anomalous events. The prowess of this technique is vividly demonstrated in its outperformance of alternative forecasting methods when applied to Duke Energy power company’s load data. The optimized DMD decomposition facilitates superior signal reconstruction and intriguingly offers the ability to constrain eigenvalues to a purely imaginary realm. This methodology ingeniously marries DMD with singular spectrum analysis (SSA), crafting a linear model grounded in a time-delay basis representation. This strategic fusion portrays system dynamics as a linear construct defined by periodic intrinsic solutions driven by a non-periodic external actuator. The magic of forecasting unfolds through fitting a stochastic model to this actuation signal, ushering in a vision of future evolution. Moreover, this data-driven paradigm integrates seamlessly with uncertainty quantification, underpinning its robustness and providing interpretability through astute analysis of the acquired forcing signal. The vision for the future lies in further enhancing this model by introducing additional input features and affording users greater control over the veil of uncertainty. In tandem, the text expounds on the formidable capabilities of Gaussian process regression (GPR) models, tailored explicitly for time series forecasting. These models, meticulously trained on data windows, are powerful tools for divining the future. The narrative also embraces the versatility of multiple-output/multivariate GPR models and illuminates input data projection onto its top SVD modes. The insightful evaluation of Delay-Coordinate Dynamic Mode Decomposition (DMD) models further enriches the forecasting landscape, gracefully capturing linear model intricacies grounded in eigenvalues and eigenvectors. A fascinating facet emerges as the text hints at the unsupervised learning of a forcing signal during the training window, elevating forecasting accuracy. When the rubber meets the road, this pioneering DMD forecasting method boldly stands its ground against the titans of forecasting, including LSTM, ARIMA, GPR, and ensemble GPR, reigning supreme as the method of choice. This data-driven marvel deftly constructs linear control models for time series forecasting, gracefully segregating noise and chaotic external forces from the prevailing quasiperiodic dynamics. The future promises refinement of the correlation between the learned forcing signal and real-world events and empowers users with greater control over the tapestry of uncertainty in ensemble forecasting. Having conquered the power grid load forecasting domain, this versatile methodology focuses on the intricate tapestries of other complex and stochastic systems.

8 Koopman Operator Theory in Control and Optimization

In (Mezić, 2015), Koopman operator theory finds application in the control systems analysis, delving into concepts like the Koopman expansion, elucidating stable and unstable subspaces, and the interrelation between spectral and geometric theories. This operator-theoretic methodology holds relevance within optimal control frameworks. The Koopman operator signifies the progression of observables over time and finds diverse utility in investigating geometric properties and high-dimensional evolution equations. The algebraic multiplicity of an eigenvalue is demonstrated to be greater than or equal to its geometric multiplicity through the Kato Decomposition. The discourse encompasses generalized eigenfunctions and their invariance under specific operations. The eigenfunctions of the Koopman operator serve as a basis for deriving stable and unstable subspaces. The spectral analysis of the Koopman operator imparts insights into the dynamics of nonlinear systems, with the expansion of states via Koopman eigenfunctions exhibiting an infinite nature in nonlinear contexts. This expansion is asymptotic, and the stable, central, and unstable subspaces can be delineated by examining the zero-level sets of Koopman eigenfunctions. The extension of Koopman operator theory into optimal control necessitates incorporating max-plus algebra.

In (Proctor et al., 2018), a novel extension of Koopman operator theory is unveiled, seamlessly integrating input and control influences. The Koopman spectral analysis is a foundational tool for delving into the

intricate analysis of nonlinear dynamical systems. This mathematical construct is inextricably linked to dynamic mode decomposition (DMD), a method revered for its ability to unearth coherent spatiotemporal modes from data. Significantly, DMD bridges the gap between local-linear analysis and nonlinear operator theory, providing an equation-free framework for dissecting complex systems. Standard Koopman analysis and DMD encounter limitations in scenarios involving actuated systems. They fail to generate input-output models, and the dynamics and modes inevitably undergo distortion due to external forcing. In response, this paper pioneers new theoretical advances that extend Koopman operator theory to encompass nonlinear input-output characteristics. This insightful development, in turn, finds a rigorous connection with a recent innovation termed dynamic mode decomposition with control. To tangibly illustrate the potency of this new theoretical landscape, a series of nonlinear dynamical systems are scrutinized. Among these, a conventional susceptible-infectious-recovered model takes centre stage, directly relevant to analyzing infectious disease data within the purview of mass vaccination (actuation). Through this intricate journey, the paper introduces groundbreaking concepts and substantiates their efficacy through comprehensive real-world applications.

In (Korda and Mezić, 2018b), a novel class of linear predictors for nonlinear controlled dynamical systems is presented. The fundamental concept involves elevating (or embedding) the nonlinear dynamics into a higher-dimensional space, wherein its evolution approximates linearity. Without control, this procedure corresponds to numerical approximations of the Koopman operator associated with the nonlinear dynamics. This research extends the applicability of the Koopman operator to controlled dynamical systems, employing the Extended Dynamic Mode Decomposition (EDMD) to compute a finite-dimensional approximation of the operator. Remarkably, this approximation assumes the form of a linear controlled dynamical system. Through numerical illustrations, the linear predictors derived from this methodology demonstrate superior performance compared to existing alternatives, such as those reliant on local linearization or the Carleman linearization approach. Constructing these linear predictors is entirely data-driven and straightforward, involving a nonlinear data transformation (the lifting) and a linear least squares problem in the lifted space. This problem can be easily solved, even for extensive datasets. These linear predictors offer practical utility in designing controllers for nonlinear dynamical systems using linear controller design methodologies, explicitly focusing on model predictive control (MPC). The research showcases that MPC controllers designed in this manner boast computational complexity similar to that of MPC for linear dynamical systems featuring the same number of control inputs and state-space dimensions. Crucially, the proposed MPC scheme allows for the linear imposition of constraints on state and control inputs, as well as handling nonlinear state-dependent cost functions. The study addresses both the scenarios of full-state measurements and input-output considerations while accommodating systems perturbed by disturbances or noise. Numerical examples serve to illustrate the effectiveness of this approach.

In (Korda and Mezić, 2018a), a framework is presented for data-driven learning of eigenfunctions associated with the Koopman operator, tailored explicitly for prediction and control purposes. The methodology capitalizes on the abundant spectrum of the Koopman operator in the transient, off-attractor regime. It leverages this richness to construct a substantial array of eigenfunctions, ensuring that the state (or any other observable of interest) resides within the span of these eigenfunctions, thereby enabling linear predictions. Once an uncontrolled system predictor is obtained through this approach, control is incorporated through a multi-step prediction error minimization process, executed via straightforward linear least-squares regression. The resulting predictor assumes the form of a linear controlled dynamical system, readily applicable within the Koopman model predictive control framework as outlined in (Korda and Mezić, 2018b), offering effective control strategies for nonlinear dynamical systems using linear model predictive control techniques. Importantly, this method is entirely data-driven and relies solely on convex optimization techniques, eschewing the need for neural networks or other non-convex machine learning tools. The innovative eigenfunction construction approach is subject to rigorous theoretical analysis, demonstrating conclusively that the family of eigenfunctions obtained is sufficiently comprehensive to span the entirety of continuous functions. Furthermore, the method is extended to encompass the creation of generalized eigenfunctions, yielding Koopman invariant subspaces and thereby facilitating linear prediction. The paper provides detailed

numerical examples illustrating the approach’s efficacy in prediction and feedback control.

In (Korda and Mezić, 2020), the presented work unveils a pioneering data-driven framework tailored to the derivation of Koopman operator eigenfunctions strategically oriented toward the domains of prediction and control. This methodology harnesses the intricate structure of the Koopman operator’s spectrum, particularly when it ventures away from attractors, as a foundational basis for constructing a comprehensive set of eigenfunctions. These eigenfunctions are meticulously crafted to ensure that the state variable (or any other observable quantity of interest) resides within the span of this eigenfunction ensemble, thereby rendering it amenable to linear prediction. The process of eigenfunction construction is inherently optimization-driven, obviating the need for any prior dictionary selection. Following the acquisition of a predictor for the uncontrolled facets of the system via this methodology, the integration of control mechanisms is executed through a multistep procedure that minimizes prediction errors. This is accomplished through a straightforward linear least-squares regression technique. The resulting predictor adopts a linear controlled dynamical system, ideally suited for seamless integration within the Koopman model predictive control (MPC) framework, as established in the seminal work of (Korda and Mezić, 2018b). This elegant synthesis facilitates the utilization of linear MPC tools to govern inherently nonlinear dynamical systems. It is worth emphasizing that this method is entirely data-driven and rooted predominantly in convex optimization. Furthermore, the novel eigenfunction construction method undergoes rigorous theoretical scrutiny, substantiating conclusively that the family of derived eigenfunctions possesses the requisite richness to span continuous functions. Moreover, this method extends its purview to encompass the construction of generalized eigenfunctions, which, in turn, engender Koopman invariant subspaces. These generalized eigenfunctions find utility in the realm of linear prediction. A comprehensive exposition of the methodology is provided through detailed numerical examples, exemplifying its efficacy in prediction and feedback control scenarios.

In (Arbabi et al., 2018), the focus shifts to a paper introducing a data-driven framework for controlling nonlinear partial differential equations (PDEs) using Koopman operator theory. This framework seamlessly integrates the extended dynamic mode decomposition algorithm (EDMD) with model predictive control (MPC), facilitating the construction of a linear approximation of system dynamics from empirical data. This linear approximation then serves as the foundation for real-time optimization. The underpinning essence of the Koopman operator theory lies in its capacity to expand observables utilizing Koopman eigenfunctions linearly. This theoretical construct finds extension into controlled systems by accommodating input sequences. The paper employs the Burgers equation as an illustrative example to illustrate this methodology. In this study, the Koopman-linear system is devised through full-state observations or sparse measurements. This engineered system proves effective in controlling unsteady fluid flows. Remarkably, the controllers based on Koopman linearization exhibit the ability to consistently diminish flow distances over time while showcasing enhanced suppression of travelling waves compared to standard techniques. Furthermore, the paper extends the Koopman operator model predictive control framework to encompass nonlinear PDE control. Notably, this extension performs better when juxtaposed with local linearization approaches. By venturing into this domain, the paper not only unveils an innovative approach but also effectively demonstrates its prowess through tangible examples and a wealth of controlled scenarios.

In (Bevanda et al., 2021), the Koopman operator emerges as a potent tool for managing nonlinear systems through a globally linear representation. This operator, however, inherently resides in infinite-dimensional spaces, necessitating finite approximations. Regrettably, there is a lack of a comprehensive framework to address this challenge, leading to a reliance on often ill-posed and unstructured methodologies. Furthermore, the Koopman operator theory boasts enduring ties to established system-theoretic and dynamical system concepts, yet these connections remain far from universally acknowledged. Given these dual circumstances, the present work endeavours to reconcile disparate aspects of both theory and practical realization. An exploration of data-driven representations for Koopman operator dynamical models is undertaken, categorizing these representations into unstructured and structured approaches. This categorization serves to underscore the distinctions between various existing methodologies. Additionally, concise insights are offered into the

paradigm’s relationship with system-theoretic principles, and the potential utility of this paradigm in the context of modelling control systems is scrutinized. Moreover, the challenges confronting researchers in this field are delineated, and reflections on prospective avenues for future research are provided.

In (Sinha et al., 2022), recent years have witnessed significant attention toward data-driven analysis of dynamical systems. Transfer operator techniques have assumed near-ubiquitous usage, specifically the Perron-Frobenius and Koopman operators. Since data is inherently discrete, this paper introduces an exclusively data-driven approach for crafting a stabilizing feedback control law applicable to a broad category of discrete-time control-affine nonlinear systems. The fundamental strategy involves the utilization of the Koopman operator, elevating a control-affine system into a higher-dimensional space, wherein the system’s evolution assumes a bilinear form. A comprehensive analysis ensues, probing the controllability of the elevated bilinear system and its relationship to the controllability of the underlying nonlinear system. Leveraging the framework of the Control Lyapunov Function (CLF), the paper proceeds to formulate a state feedback law precisely tailored to stabilize the system at its origin. Furthermore, the efficacy of this method is substantiated through practical demonstrations, showcasing its capability to stabilize the origin of both the Van der Pol oscillator and the chaotic Henon map, all solely from time-series data.

A strategic approach exists for nonlinear systems to discover data-driven coordinate transformations that render the system dynamics linear-like. These transformations are intricately linked to intrinsic coordinates delineated by eigenfunctions of the Koopman operator. Researchers have effectively employed Koopman analysis in nonlinear estimation (Surana (2016); Surana and Banaszuk (2016)) and control (Korda and Mezić, 2018b; Kaiser et al., 2021; Peitz and Klus, 2019) endeavours.

One can devise estimators and controllers directly from Dynamic Mode Decomposition (DMD) or extended DMD (eDMD) models. (Korda and Mezić, 2018b) employed model predictive control (MPC) to regulate nonlinear systems utilizing eDMD models. Remarkably, MPC performance with DMD models has proven effective, as demonstrated by (Kaiser et al., 2018). Furthermore, (Peitz and Klus, 2019) showcased MPC’s utility in switching control among a limited set of actuation values to pursue a target lift value in an unsteady fluid flow scenario. They characterized separate eDMD models for each constant actuation value.

(Surana, 2016; Surana and Banaszuk, 2016) have exhibited exemplary nonlinear estimators grounded on Koopman Kalman filters. Nevertheless, as previously discussed, eDMD models may encompass numerous extraneous eigenvalues and eigenvectors due to closure challenges associated with identifying a Koopman-invariant subspace. Alternatively, it could be advantageous to pinpoint a small set of pertinent Koopman eigenfunctions and conduct control directly within these coordinates (Kaiser et al., 2021). For more on the application of the Koopman operator in the control field, see Narasingam and Kwon (2020); Otto and Rowley (2021); Wang et al. (2022); Zhang et al. (2022); Dahdah and Forbes (2023); Zinage and Bakolas (2023); Eyuboglu et al. (2024); Rozwood et al. (2024).

9 Koopman Operator Theory in Fluid Dynamics

(Rowley et al., 2009) focuses on developing model-reduction techniques applied explicitly to fluid flows. The main objective is to derive simplified models that retain the essential physical characteristics of the flow while being computationally tractable for analysis and design of feedback control strategies. The authors provide an overview of various model reduction techniques, such as Proper Orthogonal Decomposition, balanced truncation, and the Eigensystem Realization Algorithm, discussing the strengths and weaknesses of each approach. Additionally, they introduce a novel method that utilises spectral analysis of the Koopman operator, a linear operator associated with nonlinear dynamical systems. The study demonstrates the effectiveness of the Koopman modes in decoupling the flow dynamics at different timescales and accurately capturing relevant frequencies, using the example of a jet in crossflow. This paper advances model-reduction techniques for fluid.

(Mezić, 2013) presents an in-depth exploration of Koopman modes within the context of fluid mechanics. The foundation of Koopman mode decomposition is built upon a remarkable revelation made by (Mezić, 2005) the natural counterparts of linear oscillation's normal modes, known as Koopman modes, emerge within the domain of nonlinear dynamics. To embark on this analogous journey, a transition becomes necessary. The representation of the system shifts from the state-space configuration to the dynamics governed by the linear Koopman operator, which encompasses an infinite-dimensional space of observables. While Koopman's original work concentrated on measure-preserving transformations, the discussion primarily centres around dissipative systems arising from Navier-Stokes evolution. The analysis's crux hinges on the Koopman operator's spectral attributes. Both the discrete and continuous components of the spectrum undergo scrutiny. The discrete segment corresponds to isolated oscillatory frequencies in the fluid flow and growth rates of stable and unstable modes. In contrast, the continuous spectrum aligns with the chaotic motion unfolding on the attractor. Investigation delves into methodological approaches for computing the spectrum and the associated Koopman modes, employing generalised Laplace analysis. When applied to generic observables, this technique unveils the complete point spectrum. Alternatively, they presented a computational avenue through Arnoldi-type methods, leading to dynamic mode decomposition. The interplay and distinctions between these two methods are elaborated upon. This survey has numerous applications in which such decompositions have been pursued. The theory of Koopman modes serves as a unifying framework, establishing a solid theoretical foundation for a host of fluid mechanics concepts, including global mode analysis, triple decomposition, and dynamic mode decomposition. This comprehensive study brings to the fore the intrinsic connections between Koopman modes and fluid dynamics concepts, enriching the understanding of complex fluid behaviours.

In a study published by (Sharma et al., 2016), the nexus between Koopman mode decomposition and resolvent mode decomposition manifests through each persistent solution of the Navier-Stokes equations, engenders an eigenvalue problem for a Koopman operator underpinned by analogous symmetries. This connection aligns resolvent modes as a foundational construct for expressing intricate turbulent flow patterns, proffering a viable surrogate for Koopman modes when direct computation becomes onerous or unfeasible. Notably, dynamic mode decomposition (DMD) modes approximate Koopman modes within specific contexts and can be transmuted into authentic Koopman modes by imposition of spatial and temporal shifts. The crux of this exposition illustrates the interplay between Koopman modes within a fluidic system's velocity and pressure fields. Central to this interplay is the role of time averaging. Even within fully nonlinear flow dynamics, the spectrum of the linear operator encompassing a designated state retains a lucid interpretation. An avenue for expanding and sequencing Koopman modes emerges through the prism of Schmidt decomposition, guided by an informed truncation criterion. The typical substantial separation of leading singular values facilitates an orderly expansion scheme. Notably, the primary Schmidt pair often yields a commendable approximation of the Koopman mode, regardless of the nuances of external forcing. Distinctive ways of response are discernible through various methodologies, contingent on the intricacies of the system at hand. The introduction of mean shear disrupts symmetry, instigating deviations of response modes from canonical Koopman modes. In this context, resolvent analysis furnishes insights rooted in spectral attributes. DMD modes and resolvent modes, while distinct - with the former being empirically ascertained and the latter analytically grounded - both approximate Koopman modes. In scenarios of low-dimensional systems, DMD modes emerge as practical approximations of Koopman modes. Moreover, the theoretical framework extends aptly to systems characterized by continuous spectra, such as turbulent phenomena. The discourse also alludes to the potential for extensions encompassing diverse group actions and spatial domains.

10 Koopman Operator: Stochastic Framework

The study of nonlinear dynamical systems through the lens of the Koopman operator has garnered significant interest across diverse fields. Dynamic Mode Decomposition (DMD) is a data-centric algorithm facilitating Koopman spectral analysis, offering numerous variants tailored to various applications. Nonetheless, conven-

tional implementations of DMD confront challenges when confronted with observational noise within random dynamical systems, leading to imprecise estimations of the spectra of the stochastic Koopman operator. (Takeishi et al., 2017b) introduces Subspace Dynamic Mode Decomposition (Subspace DMD) as a novel algorithm for addressing the complexities inherent in the Koopman analysis of random dynamical systems affected by observation noise. Subspace DMD operates by initially computing the orthogonal projection of forthcoming snapshots onto the space of past snapshots. Subsequently, it estimates the spectra of a linear model, with its output demonstrating convergence to the spectra of the stochastic Koopman operator, contingent upon standard assumptions. The article investigates the empirical performance of Subspace DMD across a spectrum of dynamical systems, showcasing its efficacy in facilitating the Koopman analysis of random dynamical systems. Through empirical validation, we elucidate the practical utility and robustness of Subspace DMD, underlining its potential as a valuable tool in advancing the study and understanding of complex nonlinear dynamical systems subjected to observational noise.

In (Koltai et al., 2018), various scenarios can lead to a stochastic system deviating from statistical equilibrium. Such deviations may occur due to time-varying forcing during a transient phase on its trajectory towards equilibrium, in cases where equilibrium is present but not readily discernible due to limited observations, or even in systems that do not admit an equilibrium distribution. This review explores different approaches that model the effective statistical behaviour of both equilibrium and non-equilibrium dynamical systems. Remarkably, these cases can be examined within a unified framework centred on optimal low-rank approximation techniques applied to transfer operators. The discussion places particular emphasis on the interconnections between these methods, Markov state models, and the concept of metastability. Additionally, attention is directed towards estimating reduced-order models based on finite simulation data. These topics hold significant importance, especially in fields like molecular dynamics, where Markov state models find frequent and successful applications, serving as a primary motivating application in this paper. The concepts discussed are illustrated through numerical examples to enhance clarity and understanding.

In (Črnjarić-Žic et al., 2020), this paper examines the Koopman operator linked to discrete and continuous-time random dynamical systems (RDS). The study presents outcomes that delineate the spectrum and eigenfunctions of the stochastic Koopman operator associated with diverse types of linear RDS. Furthermore, particular attention is devoted to RDS scenarios where the associated Koopman operator family forms a semigroup, especially those for which the generator can be ascertained. A stochastic Hankel- DMD algorithm is introduced to facilitate numerical approximations of the stochastic Koopman operator’s spectral entities (eigenvalues and eigenfunctions), and its convergence is rigorously proven. The methodology introduced in this paper is then applied to various examples. This application not only unveils critical elements within the spectral expansions of the stochastic Koopman operator but also paves the way for model reduction strategies.

In (Wu and Noé, 2020), the paper delves into inference, prediction, and control within complex dynamical systems, a pursuit with profound implications across diverse fields such as financial markets, power grid management, climate and weather modelling, and molecular dynamics. Central to this endeavour is the analysis of highly nonlinear dynamical systems, often facilitated by a notable observation: it is frequently possible to uncover a (typically nonlinear) transformation of the system coordinates, leading to features in which the system’s dynamics can be exceptionally well-approximated by a linear Markovian model. Furthermore, in many cases, many system variables undergo collective changes on extensive time and length scales, thereby enabling a low-dimensional analysis within this feature space. This paper introduces the *variational approach for Markov processes* (VAMP), a novel methodology that identifies optimal feature mappings and Markovian dynamics models based on provided time series data. The fundamental insight underpinning VAMP is that the finest linear model can be derived from the principal singular components of the Koopman operator. Consequently, a family of score functions, denominated as VAMP-, r emerges, and these scores can be computed directly from data. These scores, in turn, serve as invaluable tools for optimizing a Markovian model. Moreover, the paper introduces a novel metric by drawing upon the intricate

interplay between the variational scores and the approximation errors of Koopman operators. This VAMP-E score proves instrumental in cross-validation for hyper-parameter optimization and model selection within the VAMP framework. Notably, VAMP transcends the boundaries of reversible and nonreversible processes and applies to stationary and nonstationary processes or realizations.

In (Mardt et al., 2020), this study delves into the profound intricacies governing the long-term behaviour of intricate dynamical systems, which can be effectively elucidated through the lens of linear Markov or Koopman models, thoughtfully situated within a latent space tailored for the purpose. Recent advancements in variational methodologies have paved the way for optimizing the latent space representation and the linear dynamical model; all achieved through unsupervised machine learning techniques. Notably, this investigation endeavours to inject physical constraints into the fabric of the dynamical model, encompassing crucial considerations such as time-reversibility or stochasticity. While these constraints have been well-established within linear representations, their seamless integration into the domain of arbitrarily nonlinear (deep learning) latent space representations remains an open challenge. In this groundbreaking work, a comprehensive theoretical framework is meticulously constructed, accompanied by innovative methodologies, to imbue deep learning Markov and Koopman models that can gracefully accommodate such physical constraints. The rigorous mathematical proof affirms the model’s status as a universal approximator for reversible Markov processes. Furthermore, it is established that model optimization can be achieved through two distinct yet equally powerful techniques: maximum likelihood and the variational approach for Markov processes (VAMP). Empirical validation of the model’s prowess demonstrates its remarkable performance across equilibrium scenarios and, notably, its systematic improvement when confronted with biased data, thereby endowing researchers with an indispensable tool for dissecting the intricate long-timescale processes governing dynamical systems.

In (Bujorianu et al., 2021), the paper explores stochastic safety verification for random dynamical systems using barrier function. It introduces the concept of random sets and defines stochastic safety as a reach avoidance problem. To address the challenges of random obstacles, the paper extends barrier certificates and utilizes nonlinear integrals and probability distributions to establish crucial properties. The paper also defines random and stochastic Koopman operators and demonstrates that the safety function constitutes a solution for a nonstandard Dirichlet problem when the dynamical system is Markovian. When dealing with random obstacles, the paper addresses the challenges of defining barrier certificates in navigating the reach-avoidance problem within random dynamical systems. It introduces the innovative notion of random safety, employing occupation and hitting measures alongside Koopman operators. Additionally, the paper proposes data-driven approximations of barrier certificates using Koopman operator techniques, anticipating their application in an upcoming study on ship capsizing within the context of random dynamical systems.

In (Wanner and Mezić, 2022), the analysis centres on evaluating Dynamic Mode Decomposition (DMD)-based approximations of the stochastic Koopman operator within the context of random dynamical systems. In these systems, noise interference affects either the dynamics or observables. The noise within several DMD algorithms can introduce a consequential bias into the DMD operator, yielding less accurate approximations of the underlying dynamics. Notably, methods reliant on time-delayed observables, such as Hankel DMD, exhibit a predisposition toward bias when confronted with random dynamics. To address these challenges, the article introduces a novel and robust DMD algorithm, demonstrating its capacity to accurately approximate the stochastic Koopman operator even in the presence of noise. An essential feature of this algorithm lies in its adaptability to time-delayed observables, enabling the construction of a *Krylov subspace* utilizing a single observable source. This empowerment allows for the computation of a realization of the stochastic Koopman operator using a sole observable gathered from a single trajectory. To gauge the effectiveness of these algorithms, the article conducts comprehensive testing across various illustrative examples.

In (Kostic et al., 2022), the study revolves around a class of dynamical systems modelled as Markov chains, exhibiting an invariant distribution through the corresponding transfer, or Koopman, operator. Algorithms for reconstructing these operators from data are well-established, but their connection to statistical learning

remains relatively uncharted. A framework is formalized to acquire the Koopman operator from finite data trajectories of the dynamical system. The operator’s restriction to a reproducing kernel Hilbert space is considered, along with introducing a notion of risk, yielding different estimators as natural outcomes. The research establishes a link between the risk and the estimation of the spectral decomposition of the Koopman operator, motivating the development of a Reduced-Rank Operator Regression (RRR) estimator. Learning bounds for this estimator are derived and applicable in both i.i.d. and non-i.i.d. settings, the latter being expressed in terms of mixing coefficients. The results suggest the potential advantages of RRR over other commonly used estimators, as substantiated through numerical experiments for forecasting and mode decomposition.

In (Zhao and Jiang, 2023), this paper introduces a data-driven nonparametric methodology to forecast the evolutionary trajectory of probability densities within stochastic dynamical systems. This novel approach hinges upon utilizing the stochastic Koopman operator in conjunction with the extended dynamic mode decomposition (EDMD). To approximate the finite-dimensional eigendecomposition of the stochastic Koopman operator, EDMD is judiciously employed on the training data set, which is sampled from the stationary distribution characterizing the underlying stochastic dynamical system. Notably, the ensemble of Koopman operators forms a semigroup generated by the infinitesimal generator of the stochastic dynamical system. A profound association between this generator and the Fokker-Planck operator facilitates the construction of an orthonormal basis within a weighted Hilbert space. In this space, a spectral decomposition of the probability density function is systematically achieved. This method is inherently data-driven and serves the dual purpose of predicting the evolution of probability densities and real-time moment estimation. It is of paramount importance to underscore that in the asymptotic scenario characterized by a large number of snapshots and observables, the data-driven probability density approximation converges towards the Galerkin projection of the semigroup solution derived from the Fokker-Planck equation, with respect to a basis meticulously adapted to an invariant measure. The method proposed herein bears semblance to diffusion forecasting but distinguishes itself by offering a superior level of accuracy in probability density estimation, exceeding the capabilities of traditional diffusion forecasting. The paper substantiates these claims with numerical examples, effectively elucidating the performance and efficacy of the data-driven probability density forecasting approach.

11 Koopman Operator Theory in Building Energy Management

In (Georgescu and Mezić, 2014), an energy audit study was conducted on a university building with LEED Silver certification. The approach involved the decomposition of building data into spatial-temporal modes referred to as Koopman modes. These Koopman modes capture the influence of heat loads from internal and external sources, offering valuable insights into the building’s thermal performance. This framework was utilized to pinpoint instances of energy wastage. These inefficiencies included malfunctioning equipment, unnecessary equipment utilization, and suboptimal HVAC operating conditions that demanded high energy consumption to maintain thermal comfort. By addressing these identified issues, the article successfully achieved a 13% reduction in energy consumption for the building under study without any adverse effects on occupants’ comfort. It is worth noting that while Koopman mode analysis has previously been employed in examining thermal behaviours within building models, its practical application using accurate building data has been limited.

(Georgescu and Mezić, 2015) presents a method that employs the Koopman operator to create zoning approximations for building energy models. These approximations simplify building representations while retaining thermal characteristics. The process for generating zoning approximations from an EnergyPlus model using Koopman modes involves the following:

- Simulating the EnergyPlus model and extracting desired observables, like zone temperature.
- Calculating Koopman modes by projecting observables onto Koopman operator eigenfunctions.

This approach aims to simplify building energy models by focusing on zone temperature observations and maintaining accuracy. Simplifications, such as uniform space use and separating interior and perimeter rooms, minimally impact accuracy. An equilibrium point must be found to avoid excessive zone consolidation, varying based on the building layout. Using zoning approximations addresses the challenge of analyzing voluminous building energy data. The paper outlines a systematic Koopman operator-based procedure to generate simplified models with varied granularity. The accuracy of these models is analyzed as coarser building representations are developed. The paper employs the Koopman operator to analyze and visualize building behaviour, introducing a time-series method for creating zoning approximations. An analysis of building thermal behaviour using Koopman modes reveals coherent zones with spectral characteristics across modes. These modes relate to zone temperature influenced by model parameters and weather conditions. Accurate zoning approximations preserving the original model’s thermal dynamics can be formed by grouping zones with similar behaviour in Koopman modes. Accuracy assessment of zoning approximations within building models involves measuring HVAC energy consumption and comparing room temperature behaviour. Using Koopman modes retains building features, yet combining too many zones compromises accuracy. Zone reduction is based on temperature behaviour, allowing some exceptions for small zones. The overarching goal is to reduce model complexity without significant accuracy loss, potentially determined by building characteristics. Creating zoning approximations offers a promising solution to building energy model data analysis challenges.

In (Boskic et al., 2022), residential and office buildings’ existing thermal control and energy management methods often depend on intricate or high-dimensional thermal models. The approach offers an alternative avenue for deriving insights from in-office thermal data sensors without relying on conventional models. These data-driven methods are crafted through the utilization of Koopman operator theory. The resultant algorithms are validated by analyzing thermal data collected from a single thermal zone space. A notable advantage of this methodology is its ability to link the temporal characteristics of control mechanisms to the corresponding spatial zones of influence. This approach empowers the identification of spatial heating and cooling control modes directly from the data.

12 Koopman Operator Theory in Robotics

In (Kamenar et al., 2020), the primary objective is developing a data-driven model for effectively controlling the motion of a pneumatically driven soft robotic device, utilizing the principles of Koopman operator theory. This model derives its foundation from motion data collected during experiments and can notably predict the system’s behaviour accurately. Consequently, this approach helps streamline the design of controllers for soft robots while reducing computational complexity. This research capitalizes on a dimensional Extended Dynamic Mode Decomposition Koopman operator approximation, which has consistently demonstrated its aptitude in precise prediction of experimental data. The next phase of this endeavour entails extending the prediction window through rigorous testing with an expanded dataset of experimental information. Furthermore, the pursuit of advanced control methodologies is on the horizon, aiming to achieve precise tracking control for soft robotic devices. This work uses Koopman operator theory to create a data-driven model for pneumatically-driven soft robotic devices. This model, once realized, stands poised to facilitate the synthesis of motion control for these devices. The paper comprehensively examines the experimental setup, delineating the modelling procedure and presenting the obtained results. Importantly, it underscores the potential advantages inherent in this data-driven approach compared to traditional physically-based models. The creation of the data-driven model is predicated upon a nonlinear optimization process, with the

model’s accuracy rigorously affirmed through a series of experiments. Looking ahead, the research envisions an extension of the prediction window and the development of advanced control techniques to achieve precise tracking control. This development holds great promise for soft robotic devices.

In (Haggerty et al., 2020), the discussion revolves around the utilization of Koopman Operator Theory (KOT) in conjunction with Hankel Dynamic Mode Decomposition (HDMD) to approximate the dynamics of a soft robot arm and address the control problem aimed at achieving the desired poses. The current work is still in its preliminary stages and is accompanied by certain limitations, especially in capturing rapid dynamics and implementing closed-loop control strategies. A reasonable selection of dominant Koopman modes is essential to attaining the desired system behaviour. The authors employ the HDMD model to predict the evolution of observables for the soft robot. Through systematic experimentation, they explore various choices for observables and discern that time-delay observables offer superior performance. Subsequently, they integrate ten such observables into their analysis, employing them to reconstruct a twenty-second trajectory. This trajectory serves as a basis for evaluating the effectiveness of their modelling approach in controlling the system. The reduced-order model utilizing Koopman modes accomplishes static reference tracking and control in simulation and real-world robotic implementation. Notably, in specific scenarios, this model surpasses the performance of the full-state model. Nevertheless, the quest for more comprehensive capabilities remains ongoing, particularly in capturing rapid dynamics and implementing closed-loop control. The trajectory forward involves refining the model construction and further advancing the implementation of closed-loop control strategies.

In (Folkestad et al., 2020), the authors advance a method for modelling and controlling robotic systems by utilizing Koopman-inspired techniques and Dynamic Mode Decomposition (DMD). The discourse grapples with the intricate challenges intrinsic to nonlinear systems modelling and advocates using Koopman eigenfunctions as a viable means of approximating their complicated dynamics. Central to their proposition is introducing a learning framework, KEEDMD, tailored for constructing Koopman eigenfunctions when the actual dynamics are unknown. Once derived, these eigenfunctions facilitate the development of a lifted linear state-space model, which proves helpful in conjunction with Model Predictive Control (MPC). The construction of Koopman eigenfunctions hinges on acquiring a diffeomorphism that bridges the gap between the linearized model and the actual underlying dynamics. Within this context, the passage expounds upon applying Koopman eigenfunctions to identify state space models and extend them to trajectory-tracking feedback controllers. It underscores the use of measurements and numerical differentiation techniques for deriving these eigenfunctions, complemented by regularization methodologies to counter overfitting. The discourse further engages in comparative analyses, highlighting the enhanced predictive capabilities and overall performance of the KEEDMD model. However, it is essential to acknowledge the method’s inherent limitations, notably its inability to account for state-dependent matrices in the system dynamics. The authors actively investigate issues related to stabilizing controllers and advocate exploring alternative control strategies, underscoring their commitment to advancing the field. In (Folkestad et al., 2020), the authors introduce an innovative approach to high-performance robotic applications, leveraging Koopman-inspired modelling and identification techniques, specifically the Dynamic Mode Decomposition (DMD) and extended DMD (EDMD) methods. The proposed methodology, known as KEEDMD, exhibits a remarkable capacity to learn a diffeomorphism from data and employs Koopman eigenfunctions to construct a linear model within a lifted space. Matrices A and B derivation rely on data collected from systems governed by Lagrangian dynamics, primarily utilizing position and velocity states. The KEEDMD algorithm adeptly learns the impact of actuation on the Koopman eigenfunctions, employing control perturbations as a means of exploration. To mitigate overfitting, the authors judiciously employ regularization techniques, including LASSO-regularization. The framework extends beyond modelling, enabling the estimation of state variables from the identified model and facilitating the development of linear trajectory-tracking controllers. A notable feature highlighted in the proof is that the derivatives of the eigenfunctions exhibit an affinity for external forcing signals, thereby effectively enabling KEEDMD to learn the impact of external forces with minimal modifications. Significantly, the method outperforms traditional linearization and classical EDMD in prediction and closed-loop control scenarios

while maintaining computational efficiency. Nevertheless, it is essential to acknowledge certain limitations, including the inability to accommodate state-dependent D matrices and the necessity to collect data using a linear stabilizing controller. The authors express their commitment to addressing these limitations and further exploring alternative control strategies, underscoring the ongoing evolution of this pioneering approach.

13 Koopman Operator in Climate Science

In (Hogg et al., 2020), the analysis focuses on sea ice concentration dynamics, applying the Koopman Mode Decomposition (KMD) method. The study reveals a declining trend in sea ice concentration over time, particularly notable in specific regions, with heightened annual variability near West Antarctica and within the Arctic marginal seas. Long-term decay patterns in both the Arctic and Antarctic regions are also identified. The predictive skill for future sea ice behaviour demonstrates a slightly positive performance for the Arctic and a roughly equivalent performance for the Antarctic. KMD-based forecasts exhibit a positive correlation and skill in sea ice prediction, with superior performance observed in the Northern hemisphere compared to the Southern hemisphere. Notably, KMD predictions display comparable errors to those of the input period mean model, surpassing the performance of linear fit models. The study further unravels potential physical significance within long-term exponentially decaying modes in sea ice concentration. The central aim of this investigation is to employ KMD as a predictive tool for sea ice concentration, drawing upon satellite image data for analysis. Five forecast models are enlisted to achieve this objective: KMD-based prediction, climatological and persistence models, and two additional models. The KMD methodology leverages eigenvalues and modes derived from the application of KMD to concentration values, enabling predictions of future behaviour. The low residuals in KMD forecasts result in superior predictions extending beyond the input data period. Specifically, utilizing Nrecon values around 16 out of 29 eigenpairs yields the highest skill values. Any discrepancies between KMD predictions and actual values are attributed to the finite dimensionality of KMD algorithms and the stochastic nature of climatological processes. The climatological and persistence models serve as reference benchmarks, and although the input data period is unspecified, permission is required to exceed the permitted use. Furthermore, sea ice, formed when ocean water freezes, is pivotal in various domains, including environmental preservation, economic considerations, and national security. The steady decline in Arctic sea ice, while presenting challenges for wildlife and local communities, concurrently opens up new avenues for maritime commerce and resource exploration. Predicting sea ice behaviour emerges as a critical endeavour with far-reaching implications. Koopman Mode Decomposition (KMD) is a valuable statistical tool for deciphering and anticipating the dynamics of sea ice concentration. KMD effectively captures nonstationary trends in data and has been effectively applied to satellite-based measurements in both the Arctic and Antarctic regions. The analysis reveals a pronounced reduction in sea ice concentration over time, particularly in regions such as the Beaufort Sea, Barents Sea, and West Antarctica. These findings signify prolonged decay patterns and a diminishing extent of sea ice coverage. Applying the KMD algorithm involves a comprehensive analysis of time series sea ice concentration data, enabling forecasting future concentration levels. These forecasts are then rigorously compared to reference models, shedding light on the skill and accuracy of the predictions. KMD-based predictions consistently outperform climatological and persistence models, prevailing in both the Northern and Southern hemispheres, albeit with slightly positive skill and accuracy values for most future months. While KMD facilitates a geographic overview of sea ice concentration changes across annual and multi-year timescales, it does not provide explicit physical explanations for the observed trends. The accuracy of future sea ice predictions hinges on the underlying dynamics of sea ice, with varying degrees of success in predictions discerned between the Northern and Southern hemispheres. Koopman Mode Decomposition (KMD) is pivotal in analyzing sea ice concentration data. KMD expands the dataset onto Koopman eigenfunctions, generating modes and eigenvalues that capture both temporal and spatial intricacies. The data preprocessing stage involves the conversion of image files into numerical arrays and the removal of land areas. KMD analysis is executed

through algorithms rooted in Arnoldi and DMD methods. Forecast skill evaluation is conducted by contrasting KMD-based predictions with four reference models. Throughout the KMD reconstruction process, the primary objective is to accurately portray the system dynamics while avoiding inappropriate growth in forecasted values. It is essential to acknowledge that KMD predictions may deviate from actual values due to the finite dimensionality of the algorithms and the stochastic nature of underlying processes. Critical metrics for evaluating prediction skills encompass mean square error (MSE) and the anomaly correlation coefficient (ACC). While MSE quantifies the disparity between forecasted and actual values, ACC gauges the correlation between predicted and valid anomaly values.

14 Koopman Operator Theory in Logistic Science

In (Hogg et al., 2019), the exploration focuses on modern logistics processes and systems characterized by intricate dynamics. Agent-based modelling is a potent tool for designing, analyzing, and controlling such logistics systems. However, the inherent complexity of these models can be overwhelming. *Koopman mode analysis* (KMA) has been introduced as a valuable tool for addressing this challenge. KMA excels in uncovering exponentially growing, decaying, or oscillating collective patterns within dynamic data. This methodology is applied to two problems, both exhibiting a bifurcation in their dynamical behaviour: *medical treatment facility* (MTF) logistics and *ship fueling* (SF) logistics. The MTF problem entails transitioning from efficient operation at low casualty rates to inefficient operation beyond a critical casualty rate. In contrast, the SF problem transitions from a short mission life at low initial fuel levels to sustained mission capability beyond a critical initial fuel level. The analysis effectively detects both of these bifurcations by scrutinizing the spectrum of the associated Koopman operator. Additionally, mathematical insights are provided justifying the Dynamic Mode Decomposition algorithm, particularly in scenarios characterized by punctuated linear decay dynamics, as exemplified in the SF problem.

15 Koopman Operator Theory in Intelligent Transport System

In (Avila and Mezić, 2020), the intricate facets of a vehicular traffic system, encompassing unpredictable elements such as human interaction and weather, give rise to a highly complicated, high-dimensional, nonlinear dynamical system. Consequently, formulating a mathematical or artificial intelligence model capable of describing the time evolution of traffic systems poses a formidable challenge. Concurrently, the escalating demands on transportation systems have placed traffic agencies in dire need of a robust method for analyzing and forecasting traffic. This discourse elucidates how the Koopman mode decomposition offers a model-free, data-driven approach to dissecting traffic dynamics. By performing a decomposition of datasets collected by the Federal Highway Administration and the California Department of Transportation, it becomes possible to reconstruct observed data, discriminate evolving or diminishing patterns, and extract a hierarchy of previously recognized and heretofore unidentified spatiotemporal patterns. Furthermore, the practical application of this methodology in forecasting highway network conditions is showcased.

16 Koopman Operator Theory in Non-linear Aerodynamics

In (Glaz et al., 2014), several key aspects are highlighted and discussed, shedding light on the complexities of dynamic stall phenomena. Firstly, the limitations of conventional methodologies in capturing the transient dynamics associated with the formation of dynamic stall vortex are addressed. The inherent shortcomings of existing approaches are examined, paving the way for a more effective analysis. A significant advancement in

the field emerges as modal decomposition methods based on the Koopman operator are introduced. These innovative techniques offer a novel perspective on the analysis of dynamic stalls. By employing modal decomposition, researchers gain the ability to delve deeper into the intricate dynamics of these phenomena. One notable feature explored in the paper is the potential of Koopman modes to serve as a fully nonlinear analogue to the global modes observed in linearized aerodynamic systems. This concept allows for a richer understanding of aerodynamic dynamics in linear and nonlinear contexts. The paper also underscores the need for further research, specifically on bifurcation and the transient stability loss encountered in dynamic stall scenarios. This call for deeper investigation signals the recognition of gaps in the current understanding and lays the groundwork for future explorations. The application of various methodologies is explored, including the utilization of dynamic mode decomposition (DMD) for calculating Koopman modes within dynamic stall systems. The integration of Fourier decomposition and Galerkin projection is highlighted as a means to model fluid flow dynamics effectively, providing insights into the intricate behaviour of the system. A critical contribution of this paper is introducing the Koopman operator in the context of continuous-time systems. This mathematical construct offers a fresh perspective on analyzing complex dynamic systems, enriching the understanding of their behaviour. Methodologically, the paper delves into the computation of Koopman modes, leveraging techniques such as the Generalized Laplace Analysis and an Arnoldi-like algorithm. These computational methods play a pivotal role in unravelling the intricate characteristics of dynamic stall dynamics. The paper explores the spectral properties and growth rates through Koopman spectral analysis. This analytical approach provides valuable insights into the underlying dynamics, contributing to a more comprehensive understanding of the complex behaviour exhibited by dynamic stall phenomena. Practical applications of the proposed methodologies are demonstrated through the analysis of two-dimensional computational fluid dynamics (CFD) simulations. The paper showcases the efficacy of employing Koopman eigenvalues and modes in the analysis, highlighting their relevance in understanding real-world phenomena. A significant contribution lies in the comparative study between Fourier analysis and DMD methodologies. The paper establishes a bridge between these approaches, demonstrating their alignment with experimental and computational results. The paper concludes by exploring specific cases, such as oscillating airfoils and cylinders. These cases offer valuable insights into behaviours like wake shedding, further enhancing the understanding of the intricate dynamics. Of particular note, the paper unveils intriguing findings on the behaviour of oscillating cylinders. The continuous spectrum observed in this context suggests the operation of the cylinder near a critical value of Hopf bifurcation. Moreover, the paper establishes intriguing connections between the spectral characteristics of pitch-oscillating airfoils and dynamic stalls. This analysis points towards a strong linkage between dynamic stall and oscillations, hinting at a critical bifurcation value. The paper leverages the Koopman spectral analysis technique to gain insights into complex and nuanced dynamics of dynamic stall phenomena. Through comprehensive analysis and exploration, the paper contributes significantly to advancing the understanding of this challenging field.

In the realm of rotorcraft air vehicles, both human-crewed and unmanned, there is a substantial surge of interest in exploring unsteady aerodynamics. The intricate flow patterns within these contexts manifest as unsteady separation, followed by the emergence of vortices akin to dynamic stalls. The progression and interaction of these vortices with flexible aerodynamic surfaces wield a substantial influence over flight stability and overall performance. The analysis of these flow phenomena is further complicated by their mixed character, encompassing elements of laminar, transitional, and turbulent behaviour, particularly at moderate Reynolds numbers. Moreover, the vast array of potential parameters, kinematic conditions, and configurations adds to the intricacy of the study. It is natural to seek methods that streamline the complexities by isolating individual modes to advance comprehension and predictive capabilities regarding the underlying fluid dynamic mechanisms. The widely adopted Proper Orthogonal Decomposition (POD) technique serves this purpose. However, it has been observed that while POD effectively extracts the energetically dominant aspects of the flow field, it needs to emphasize nuanced oscillatory phenomena that play a vital role in significant physical processes, such as shear layer separation. Within the domain of unsteady flows over airfoils undergoing substantial variations in the effective angle of attack, the phenomenon known as dynamic stall emerges. This

process is characterized by transient separation and prominent leading-edge and trailing-edge vortices. These vortices induce unpredictable fluctuations in aerodynamic loads. Early research hints at high-frequency effects during leading-edge vortex-shedding events absent in static stall scenarios. Building upon this foundation, (Fonoberova et al., 2014) aimed to advance these insights by applying Koopman operator mode decomposition techniques. The study commenced with an analysis of dynamic stall, employing the principles of Koopman operator theory. This endeavour yielded noteworthy findings, guided by dynamical systems methods and efficient numerical techniques for Koopman Mode Decomposition. In particular, the study delves into the impact of the oscillatory nature of the incoming velocity experienced by a wing due to pitching or plunging. By examining a model system involving a cylinder immersed in an oscillatory incoming flow, specific physical effects analogous to those observed in pitching airfoil scenarios were revealed. This sheds light on the dynamics of pitching airfoil behaviour as a nonlinear interplay between the forcing induced by the oscillating incoming flow frequency and the inherent natural frequency of vortex shedding dynamics.

Vehicle flight dynamics, inherently nonlinear, are typically approached by integrating system equations over small time steps. Methods like multiple-shooting and pseudo-spectral analysis are standard for understanding their behaviour. However, a generalized framework for explicitly characterizing and solving nonlinear systems still needs to be developed. In contrast, linear systems benefit from well-understood methods and efficient algorithms for characterization and prediction. Lock et al. (2022) showcases the application of analytically derived Koopman linearization for flight dynamics, structured into sections summarizing fundamental theory, past and future aerospace applications, implementation details, and performance demonstrations on specific systems, concluding with avenues for future research.

17 Application of DMD and EDMD Algorithm

In the context of the work presented in (Brunton et al., 2016a), Dynamic Mode Decomposition (DMD) is a powerful tool for analyzing extensive neural recordings. DMD facilitates the exploration of high-dimensional dynamic data by elucidating spatial-temporal modes. The essence of DMD is characterized by a fusion of principal components analysis and power spectral analysis, rendering it particularly suited for scrutinizing large-scale neural recordings. The method finds application in discerning sleep spindle networks and can be readily adapted to diverse forms of neural recordings. Crucial to the revelation of coherent structures within neural activity, DMD modes serve as discernible features within machine learning algorithms. An inherent robustness to noise and subsampling underscores the utility of DMD, affording insights into the intricate tapestry of thalamocortical connections and local cortical networks. At the core of calculating the pseudoinverse for large data matrices lies the Singular Value Decomposition (SVD). However, in scenarios where the matrix dimensions prove unwieldy, the computational burden of determining the eigendecomposition becomes pronounced. To alleviate this, a practical approach presupposes a low-dimensional spatial configuration within the data, permitting a streamlined procedure for estimating DMD modes and eigenvalues, thereby circumventing the direct computation of the matrix. Intrinsic to its essence, DMD represents a spatial-temporal decomposition methodology adept at discerning methods that encapsulate the foundational patterns and dynamics inherent to the dataset. A parallel mathematical foundation links DMD with Principal Component Regression (PCR), a methodology that similarly analyses data by capturing latent structures and dynamics. Notably significant, the stacking depth parameter fundamentally governs the fidelity with which DMD portrays data dynamics. The algorithmic core of DMD resides in its capacity to decompose matrices into eigenvalues and modes, which can be rescaled by the singular values originating from the SVD. The DMD spectrum is realized through a representation wherein mode power is plotted against its oscillation frequency. This analytical framework transcends challenges posed by subsampling and noise, manifesting its robustness. Significantly, its application is showcased in investigating brain activity during motor tasks and sleep states and in facilitating data clustering via Gaussian mixture modelling. As emphasized within this discourse, DMD is an instrumental methodology for the dissection and visualization of extensive neural recordings, including the domain of

Electrocorticography (ECoG) data. The ability of DMD to unveil coherent spatial patterns intertwined with diverse temporal frequencies holds profound significance. This methodological paradigm is judiciously deployed in delineating neural activity patterns during motor tasks and in the meticulous analysis of sleep spindle networks. Given its scalability, DMD holds the potential to scale up and accommodate the escalating demands of data recordings featuring numerous channels. In conclusion, the manuscript’s comprehensive engagement traverses diverse neural measurement techniques in the context of neural decoding tasks. Support from esteemed institutions, specifically the National Institutes of Health and the National Science Foundation, substantiates this scholarly endeavour’s scientific rigour and significance.

In (Alla and Kutz, 2017), the discourse centres on the utilization of reduced order models (ROMs) and dynamic mode decomposition (DMD) for model reduction within intricate systems. The study delves into the intricacies of projecting nonlinearity onto basis functions and conducts a comparative analysis between DMD and alternative techniques such as Proper Orthogonal Decomposition (POD) and Empirical Interpolation Method (EIM). Within this context, a proposition is put forth to synergistically combine POD and DMD methodologies, supported by the presentation of numerical tests that substantiate the efficacy of these integrated approaches. The DMD-Galerkin method emerges as a pivotal point of discussion, wherein system dynamics are approximated through the amalgamation of the DMD algorithm and Galerkin projection.

(Le Clainche and Vega, 2017a) introduces an extension of dynamic mode decomposition (DMD) tailored to address general periodic and quasi-periodic dynamics and transients that decay into periodic and quasi-periodic attractors. This includes scenarios—beyond the reach of standard DMD—exhibiting limited spatial complexity while involving a multitude of frequencies. Referred to as “higher order dynamic mode decomposition,” this extension employs time-lagged snapshots and can be conceptualized as a superimposed DMD conducted within a sliding window framework. The application and elucidation of this novel approach are demonstrated using simplified model dynamics, precisely the Stuart–Landau equation and the Lorenz system. Furthermore, this method’s efficacy and resilience are tested by applying it to both sustained and transient dynamics arising from the intricate *Ginzburg–Landau* equation (a paradigmatic example of pattern-forming systems). Here, standard DMD is revealed only to capture trivial dynamics. The approach is also employed to analyze thermal convection in a rotating spherical shell subject to a radial gravity field. For more applications of higher order dynamic mode decomposition, see more on (Le Clainche and Vega, 2017b; Le Clainche et al., 2017; Kou et al., 2018; Vega and Le Clainche, 2020; Zhou et al., 2021; Groun et al., 2022; Gutierrez-Castillo et al., 2022; Amor et al., 2023)

(Drmač et al., 2018) focus on the Dynamic Mode Decomposition (DMD) within the realm of computational data-driven analysis of fluid flows. An innovative data-driven formula for the residuals is introduced, enabling the selection of Ritz pairs. This augmentation leads to a more precise extraction of spectral information from the underlying Koopman operator. Furthermore, a well-established technique for refining Ritz vectors is adapted to suit data-driven scenarios. In addition, the article recast the DMD within a more comprehensive framework encompassing weighted inner product spaces. This generalized formulation prompts a thorough exploration of the ensuing numerical computation implications. Through a series of numerical experiments, the article showcases the tangible benefits of the proposed approach, which the article has designated as *DDMD R (Refined Rayleigh Ritz Data Driven Modal Decomposition)*.

In (Goswami et al., 2018), the operator-theoretic approach to dynamical systems takes centre stage, exploring measurable map evolution through the Koopman and Perron-Frobenius operators. These operators correspond to observables and uncertainties/densities, respectively. To approximate the PF operator, projection onto basis functions is necessary, achieved through Galerkin or Ulam’s methods. Ulam’s approach approximates the PF operator using Markov state transition matrices and Monte Carlo simulations. The paper introduces *Constrained Ulam Dynamic Mode Decomposition (CU-DMD)* as a novel method to approximate the PF operator. This technique addresses the challenge of long-time steps while maintaining accuracy. CU-DMD blends Ulam’s method and constrained EDMD, utilizing characteristic functions of state space grids as basis functions. A Markov chain is constructed by projecting the PF operator onto this basis, allowing

for eigenfunction approximation. The method solves a constrained optimization problem and incorporates multipass Monte Carlo data for density transport. Theoretical justification and performance results are presented in detail. The discretization of the PF operator involves fixing a time step size using Galerkin methods. Approximating the PF operator is akin to approximating a stochastic matrix. CU-DMD, the novel method introduced in the paper, combines the accuracy of Extended DMD with the Galerkin projection from Ulam’s method. CU-DMD surpasses Ulam’s method for smaller time steps, utilizing time-series data from Monte Carlo simulations and constrained quadratic programming to generate a Markov state-transition matrix. The algorithm’s effectiveness is showcased across several nonlinear systems, including those with and without diffusive Wiener noise. CU-DMD accurately approximates system modes. Future work aims to provide proof in the Hilbert space of transfer operators, further solidifying the method’s theoretical underpinnings.

In (Seenivasaharagavan et al., 2021), Koopman mode analysis emerges as a potent framework for examining nonlinear phenomena spanning many domains. Its practical implementation through Dynamic Mode Decomposition (DMD) has undergone extensive refinement and deployment throughout the past decade. Within this context, delving into the intricacies surrounding mean subtraction and DMD mode selection, all framed within the finite-dimensional Koopman invariant subspaces. The practice of preprocessing data by subtracting the temporal mean from a time series has stirred debate, particularly in companion matrix-based DMD. This debate stems from the potential for such preprocessing to render DMD equivalent to a temporal Discrete Fourier Transform (DFT). Here, establishing a fundamental insight: In the context of linearly consistent data, this equivalence remains unattainable when the order of the DMD-based representation of dynamics surpasses the system’s dimension. Furthermore, this parity between DMD and DFT predominantly signifies an insufficiency in the available data. This implies that the number of captured snapshots needs to be revised to represent the system’s actual dynamics. They subsequently advocated culling DMD eigenvalues based on the norm associated with their respective modes. Once a minimum number of time delays has been accounted for, DMD eigenvalues corresponding to modes exhibiting low norm are revealed to be spurious, necessitating their exclusion from the analysis. Notably, when confronting mean-subtracted data, the criterion above for detecting synthetic eigenvalues can be readily applied, especially when DMD is preceded by a time delay embedding step.

In (Li et al., 2023), the discussion centres on applying stochastic parameterization coupled with dynamic mode decomposition (DMD) to address the intricate interplay between unresolved small-scale dynamics and large-scale flow phenomena. This inquiry primarily revolves around a quasi-geostrophic (QG) model and grapples with the formidable challenge of faithfully representing the inherent uncertainties of these unresolved small scales. The transformative impact of parameterization within the QG dynamical model is evident, as it yields enhancements in variability and eddy energy. A noteworthy outcome is the faithful reproduction of the eastward jet observed in wind-driven double-gyre circulation. This achievement is underpinned by the utilization of the DMD procedure, which adeptly captures the quasi-periodic dynamics characterizing the unresolved flow, ultimately resulting in the emergence of a stochastic model. This stochastic model, in turn, augments the variability inherent to the resolved flow dynamics. In a complementary vein, the paper introduces a novel modelling technique christened STO-DMD. This innovative approach demonstrates its mettle by significantly elevating the variability observed in large-scale resolved flow, surpassing the performance of alternative unresolved models. The STO-DMD technique integrates multiple noise components and incorporates an additional correction drift, attributes that contribute to its superior variability and eddy energy performance. The successful amalgamation of parameterization within a QG dynamical core, coupled with the judicious application of the DMD procedure, proves effective and leads to reduced computational and storage overheads, marking a substantial advancement in understanding large-scale flow dynamics.

(Ghosh et al., 2023) illustrate the efficacy of employing the Koopman operator and dynamic mode decomposition (DMD) within iterated function systems (IFS) (Ghosh and Marecek, 2022). More precisely, they elucidate how these methodologies can be utilized to analyze and forecast the behaviour exhibited by stochastic

nonlinear dynamical systems, as depicted by certain discrete-time Markov chains confined to compact state space.

18 In Computational Neuroscience

In (Kunert-Graf et al., 2019), the focus of attention revolves around Resting State Networks (RSNs) extracted from functional magnetic resonance imaging (fMRI) scans, which are widely regarded as reflections of the intrinsic organization and network architecture of brain regions. Traditional approaches for computing RSNs typically assume that these functional networks remain static throughout a scan, usually lasting between 5 to 15 minutes. However, it is well-established that these networks exhibit variations in timescales from seconds to years. Furthermore, the dynamic properties of RSNs are susceptible to alterations in various neurological disorders. Recent times have witnessed a proliferation of methods aimed at characterizing the dynamics of RSNs. Nevertheless, the extraction of reproducible time-resolved networks remains a formidable challenge. This paper introduces a novel methodology grounded in Dynamic Mode Decomposition (DMD) to extract networks from brief windows of noisy, high-dimensional fMRI data. This approach enables the robust resolution of RSNs from individual scans, offering a temporal resolution as fine as seconds. The method's efficacy is substantiated through validation on a synthetic dataset. Subsequently, an analysis is conducted using data from 120 individuals participating in the Human Connectome Project. The results demonstrate that unsupervised clustering of DMD modes facilitates the discovery of RSNs at the group level (gDMD) and the individual subject level (sDMD). The gDMD modes closely resemble canonical RSNs. Compared to established methods, the sDMD modes capture individualized RSN structures more faithfully and resemble the population RSN more closely while effectively encapsulating subject-level variations. The time-resolved sDMD analysis is also harnessed to deduce occupancy patterns and transitions among RSNs with high reproducibility. This automated DMD-based approach is a potent tool for characterizing the spatial and temporal structures of RSNs at the individual subject level.

19 In Algorithm and Neural Network

In (Dietrich et al., 2020), pursuing a systematic mathematical framework for examining numerical algorithms proves essential. Such a framework would serve multiple purposes, including facilitating comparisons, enabling conjugacy arguments, and fostering the discovery of enhanced, expedited, data-driven algorithms. Throughout the past century, the Koopman operator has emerged as a mathematical foundation for investigating dynamical systems. This operator facilitates conjugacy arguments and the development of efficiently reduced descriptions. More recently, this operator's advent of numerical approximations has empowered the analysis of numerous deterministic and stochastic dynamical systems within a wholly data-driven and essentially equation-free pipeline. It is crucial to recognize that discrete or continuous-time numerical algorithms, such as integrators, nonlinear equation solvers, and optimization algorithms, are dynamic systems. Leveraging this insight, this paper harnesses the Koopman operator framework to embark on a data-driven exploration of such algorithms. The ensuing discussion sheds light on this approach's advantages in terms of analysis and acceleration of numerical computation. For algorithms operating within high-dimensional spaces and swiftly contracting them towards low-dimensional manifolds, the paper illustrates how incorporating basis functions tailored to the data can aid in efficiently constructing reduced operator representations. The examples presented encompass prominent algorithms, including gradient descent, Nesterov optimization, and the Newton-Raphson algorithm.

In (Manojlović et al., 2020), the training process of a neural network takes on the role of a dynamic operation within the expansive weight space, notably characterized by its high dimensionality. At each epoch, the

optimization algorithm orchestrates a transformation via a mapping operation in conjunction with the loss function. This mapping, induced by the optimization algorithm and the loss function, facilitates the application of observables onto the weight space, thereby enabling the observation of their evolution over time. The dynamics governing the evolution of these observables exhibit intricate interplay with the Koopman operator linked to those above-induced dynamical systems. Employing the analysis of the Koopman operator’s spectrum and its modes, a comprehensive toolkit is devised to achieve the following objectives:

- **Network Depth Determination:** The methods provide a means to ascertain the optimal network architecture depth a priori.
- **Initialization Assessment:** Detection of unfavourable network weight initializations is enabled, permitting a restart before committing to extensive training time.
- **Training Acceleration:** Insights are offered to expedite the training process by monitoring the Koopman spectrum.
- **Noise Mitigation and Robustness Enhancement:** The techniques empower noise rejection and fortify the neural network’s robustness.

The subsequent elucidation highlights the Koopman spectrum’s pivotal role in determining the necessary network layers within the architecture. Furthermore, it unveils its utility in discerning the convergence or non-convergence of the training process. The presence of eigenvalues clustering around one within the spectrum is particularly noteworthy, serving as a crucial indicator for determining the optimal termination point for the learning process, thus enhancing efficiency. By leveraging Koopman modes, strategies for selective network pruning are devised, substantially accelerating the training procedure. Lastly, the demonstration underscores how incorporating loss functions grounded in adverse Sobolev norms equips us to reconstruct multi-scale signals, even in substantial noise contamination.

In (Redman et al., 2022a), the study is dedicated to identifying equivalent algorithms within the framework of Koopman operator theory and the spectra of the Koopman operator. It introduces the concept of (semi-)conjugacy and provides concrete examples of distinct algorithms found to be equivalent through this methodology. The study showcases the utility of principal eigenvalues of the Koopman operator for scrutinizing algorithmic behaviour and performs detailed comparisons of the spectra among different algorithms to establish their equivalence. Notably, Algorithm 7 exhibits striking similarities to Algorithm 6, primarily distinguished by a shift in their initial conditions. This close relationship between the two algorithms emerges from their respective Koopman spectra computations. This innovative approach facilitates the identification of algorithmic equivalences and offers clear advantages over conventional linear control-based methodologies. Moreover, the research in (Redman et al., 2022a) employs Koopman operator theory as a powerful tool for discerning algorithmic equivalence by carefully comparing the spectra associated with Koopman operators. It highlights the remarkable utility of the Koopman mode decomposition method, which excels in detecting instances of conjugacy and provides an overarching framework for probing algorithmic equivalency. Additionally, the study thoroughly investigates algorithmic behaviour and their interrelationships, particularly in the context of initial conditions, along with the *Wasserstein distance of their Koopman spectra*. One noteworthy aspect is that Koopman operator theory proves its mettle in identifying algorithmic equivalence without needing explicit underlying equations. It is equally adept at discriminating various congruency forms and is a valuable asset in proprietary software. However, it is essential to underscore that the efficacy of this method hinges on the availability of sufficient data, the implementation of an appropriate numerical scheme, and the attainment of precise approximations. This approach represents a distinctive departure from conventional linear control frameworks, offering new avenues for exploring algorithmic equivalences.

In (Redman et al., 2022b), the pursuit of sparse subnetworks capable of matching the performance of full models has garnered considerable applied and theoretical interest. Numerous pruning methods have

emerged to achieve this goal. Surprisingly, the straightforward approach of eliminating parameters based on their magnitudes has demonstrated robustness akin to more intricate state-of-the-art algorithms. Despite magnitude pruning’s empirical success, particularly in the pre-convergence phase, the lack of a comprehensive theoretical foundation and its relationship with other pruning techniques, such as gradient-based pruning, remain pivotal open questions within the field, demanding closer examination. To address these questions, the article leverages recent advancements in dynamical systems theory, specifically Koopman operator theory, to introduce a novel category of theoretically motivated pruning algorithms. The investigation reveals that these algorithms can be equivalent to magnitude and gradient-based pruning, thus unifying seemingly distinct methodologies. Moreover, these algorithms shed light on the performance of magnitude pruning in the early stages of training, providing valuable insights into its effectiveness. Study in (Zinage and Bakolas, 2023) uses Koopman operator theory to address the challenge of stabilizing controllers for unknown nonlinear control systems. The article proposes a framework that simultaneously constructs stabilizable bilinear models and identifies associated observables from data. By integrating a bilinear Koopman embedding and a Control Lyapunov Function (CLF), their approach offers provable guarantees of asymptotic stability for the Koopman-based representation of the system. Numerical simulations validate the effectiveness of the proposed stabilizing feedback controllers for these systems.

20 Conclusion

This survey thoroughly examined a wide range of literature, incorporating seminal contributions, innovative methodologies, and diverse applications across various domains. Scrutinizing over one hundred papers, numerous monographs, and a substantial array of doctoral dissertations (Bagheri, 2010; Tu, 2013; Mohr, 2014; Arbabi, 2017; Yang, 2017a; TAKEISHI, 2017; Johan, 2017; Netto, 2019; Zhang, 2019; Li, 2019; Pan, 2021; Seenivasaharagavan, 2023; Manzoor, 2023; Kim, 2024), we highlighted the profound influence and adaptability of Koopman Operator Theory and DMD in contemporary research. The amalgamation of theoretical rigour with practical applicability underscores the transformative potential inherent in these techniques. From revealing concealed patterns in high-dimensional datasets to enabling predictive modelling and control within dynamic systems, Koopman Operator Theory and DMD have emerged as pivotal pillars in the arsenal of data-driven methodologies.

The survey aims to encapsulate the essence of Koopman Operator Theory and DMD as isolated methodologies and catalysts driving innovation and discovery within Data-Driven Science and Engineering. As we navigate the era of big data and intricate systems, the insights gleaned from our review are poised to stimulate and propel future research endeavours, fostering a deeper understanding and harnessing of the dynamics inherent in our ever-evolving world.

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