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REVIEW ARTICLE

Koopman operator theory and dynamic mode decomposition in data-driven science and engineering: A comprehensive review

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Abstract

Poincaré's geometric representation, while historically fundamental in dynamical system analysis, faces challenges with high-dimensional and uncertain systems in modern engineering and data analysis. This article extensively explores Koopman Operator Theory (KOT) and Dynamic Mode Decomposition (DMD) within data-driven science and engineering and advocates for a conceptual shift toward observable dynamics, emphasizing KOT's capacity to capture nonlinear dynamics in infinite-dimensional space. The potential practical applications of Koopman-based methods are highlighted. Leveraging Poincaré's framework, the limitations of traditional methods are discussed. The review also addresses the growing significance of data-driven methodologies for modelling, predicting, and controlling complex systems.

Keywords: Applied Koopman operator; data-driven dynamical systems and control; non-linear systems; data-driven estimation and prediction

AMS 2020 Classification: 37M10; 37C10; 47A35; 65P20

1 Introduction

Poincaré's geometric representation, which delves into the dynamics of states [1], 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 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 leaping academic theory to practical applications, demonstrating its versatility and effectiveness in real-world contexts.

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. However, geometric analysis has limitations when dealing with the full spectrum of behaviours in non-linear dynamical systems. Specifically, unstable manifolds in hyperbolic regimes can lead to trajectories that diverge exponentially, showcasing a complexity that requires more than just geometric insights to understand and predict fully. This complexity of real-world systems is both a challenge and an exciting opportunity, underscoring the need for advanced analytical, numerical, and computational methods to grasp their intricate behaviours.

Most of the real-world non-linear dynamical systems consist of noise and uncertainty. A single initial state does not deterministically lead to a unique trajectory for such a system-instead, it may give rise to various possible trajectories. Addressing inquiries about the behaviour of specific trajectories under such conditions can pose significant challenges. Many geometric arguments, such as Bendixson's criterion [2, 3] 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 without explicit 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. Koopman and Perron-Frobenius (PF) operators are the most commonly used among the operationalized systems for system analysis. 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 for a few seconds under each condition.

Extensive research has been dedicated to understanding system behaviour, driven by the necessity of prolonged run durations. However, the complexity of transient dynamics presents a significant challenge that requires further exploration and innovation.

Examining a few two-dimensional cross-sections in the state space can reveal overlapping invariant structures when visualizing nonlinear dynamical systems. However, employing the Perron-Frobenius operator complicates this approach, as it requires calculating the invariant density for the entire state space before deriving the densities on specific slices of interest.

The late 20th and early 21st centuries witnessed a dramatic increase in data availability, sparking a sensing revolution that spans diverse data acquisition methods. However, a significant portion of this data remains unprocessed and untapped, leading to missed opportunities in fields such as health, commerce, technology, and network security. This underscores the crucial importance of your work in data processing and utilization.

Various mathematical methodologies have emerged in response to this need, with Deep Neural Networks gaining particular prominence. Inspired by biological neurons, these networks have achieved remarkable success in areas such as image recognition, speech recognition, and natural language processing, grounded in supervised machine learning principles.

The introduction of convolutional neural networks, which mimic the hierarchical architecture of the animal visual cortex, has led to significant advances in image recognition and the creation of realistic images through Generative Adversarial Networks (GANs). While these accomplishments are notable, they mainly pertain to static pattern recognition or generation tasks. Deep learning methods face more significant challenges in dynamically evolving contexts, such as autonomous driving, where the intrinsic characteristics of the temporal variable must be accommodated.

On the other hand, the Koopman operator framework, with its inherent symmetry related to temporal translation, presents a promising avenue. It offers a robust approach to 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 to its contemporary focus on 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, aligning more closely with human cognition principles than previous machine learning paradigms. The potential of the Koopman operator framework is a beacon of hope for the future of unsupervised learning.

As this article emphasizes, 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 struggle with nonlinear systems due to the intricate nonlinear interactions at play. Introducing external forces adds another layer of complexity, further

complicating the solution process. This underscores the urgent need for new approaches that can effectively deal with the limitations of conventional methods.

In traditional practice, nonlinear systems are often linearized and use linearised 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 of which characterize 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 [4, 5]. Moreover, human intervention often amplifies model complexity [6]. 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 [7–10]. By their very nature, data-driven methodologies scrutinize the lens of data, making them especially well-suited for systems characteristics 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 [11], 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 [11, 12]. 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 [13, 14]. Mezic 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, [15] 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 [16]. 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 [16]. The symbiotic relationship between KMD and DMD, elucidated by [16] and [15], has emerged as a cornerstone in investigating nonlinear flows [17-20] and other interdisciplinary domains, as elaborated further Sections.

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 [18, 21]. Such systems are typically elucidated through continuous and discrete methodologies.

For a generalized continuous system represented by:

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

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:

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

where x_k represents an *n*-dimensional column vector of system states at time t_k , k = 1, 2, 3, ..., m, for *m* time steps, and x_{k+1} signifies the subsequent states following x_k . 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 $g : \mathbb{R}^n \to \mathbb{M}^p$, 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:

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

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

In continuous and discrete representations, respectively. Eq. (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 [17, 21–26]. Eqs. (3a) and (3b) enable the formulation of analogues for continuous and discrete-time dynamical systems, respectively, as depicted below:

$$\frac{d}{dt}g = \mathcal{K}g,\tag{4a}$$

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

However, as depicted in Figure 1, this operator facilitates the measurement of dynamic evolution



Figure 1. Schematic for illustrating the advancement of a dynamical system as defined by the Koopman operator on nonlinear dynamical systems [27]

over time [21, 23, 25]. Revisiting (2) where the rule *F* maps x_k from $F : \mathbb{R}^n \to \mathbb{R}^n$, 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:

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

The Koopman operator \mathcal{K} transforms a nonlinear dynamical system into a linear framework within the space \mathcal{H} , meaning it linearly advances observables:

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

This operator encapsulates the system's dynamics within the observable space \mathcal{H} , including *x* itself. The key characteristic of the Koopman operator is its linearity, which can be expressed as:

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

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

An eigenfunction-eigenvalue pair (ϕ_i , λ_i) of the Koopman operator is defined by the relation:

$$\mathcal{K}\phi_i = e^{\lambda_i t}\phi_i$$
 where $\lambda_i \in \mathbb{C}$.

A notable property of Koopman eigenfunctions is that if (ϕ_i, λ_i) and (ϕ_j, λ_j) are distinct pairs, then $(\phi_i\phi_j, \lambda_i + \lambda_j)$ is also an eigenfunction-eigenvalue pair. The spectral characteristics of the Koopman operator describe the state space dynamics. Specifically, the Koopman eigenvalues, the point spectra, allow for the evaluation of the system's stability. See [28–30] for more properties. Assuming that all system observables can be expressed as a linear combination, we have:

$$g(x) = \sum_{i=0}^{\infty} \nu_i \phi_i(x).$$
(5)

Where v_i 's are the coefficients in the Koopman expansion, known as Koopman modes associated

with the eigenfunction-eigenvalue pair (ϕ_i , λ_i). According to this equation, the Koopman modes are determined by projecting the observable onto the corresponding eigenfunction. The evolution of observables can then be described as:

$$\mathcal{K}g(x) = \sum_{i=0}^{\infty} \nu_i \phi_i(x) e^{\lambda_i t}.$$
(6)

The Koopman linear expansion in this equation applies to a broad class of nonlinear dynamical systems, including those with limit cycles and hyperbolic fixed points. For detailed examples, refer to [31].

Koopman operator for continuous-time system

Our focus has been on the Koopman operator formalism for discrete-time systems to align with measurement data from real-world experiments or simulations. However, to ensure a comprehensive discussion, we also consider continuous-time systems. Let us examine the continuous-time system described by:

$$\dot{x} = f(x). \tag{7}$$

For a continuous-time system, we can define a one-parameter semi-group of Koopman operators $\{\mathcal{K}^t\}_{t\geq 0}$, where each element of this group is expressed as:

$$\mathcal{K}^{t}g(x) = g(x) \circ F^{t}(x). \tag{8}$$

Here, g represents the observable of the system. Eq. (8) can also be written as:

$$\mathcal{K}^t g(x) = g(F^t(x)). \tag{9}$$

This system maintains the linearity of the composition operation, thus sharing the same properties as the Koopman operator for discrete systems. The evolution of observables in this context is given by:

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

Example of a Koopman embedding

Consider the following non-linear dynamical system with two variables x_1, x_2 :

$$\dot{x}_1 = \mu x_1, \tag{10a}$$

$$\dot{x}_2 = \lambda (x_2 - x_1^2).$$
 (10b)

For $\lambda < \mu < 0$, the system exhibits a slow attracting manifold defined by $x_2 = x_1^2$. It is possible to augment the state **x** with the nonlinear measurement $g = x_1^2$, thereby defining a three-dimensional Koopman-invariant subspace. In these coordinates, the dynamics presented by (10a)-(10b) become

linear:

$$\frac{d}{dt} \begin{bmatrix} y_1\\y_2\\y_3 \end{bmatrix} = \begin{bmatrix} \mu & 0 & 0\\0 & \lambda & -\lambda\\0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix} y_1\\y_2\\y_3 \end{bmatrix},$$
(11)

where

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_1^2 \end{bmatrix}$$

The entire three-dimensional Koopman observable vector space is visualized in Figure 2. Trajec-



Figure 2. Visualization of three-dimensional linear Koopman system from (11) along with projection of dynamics onto the $x_1 - x_2$ plane. The attracting slow manifold is red, the constraint $y_3 = y_1^2$ is blue, and the slow, unstable subspace of (11) is green. Black trajectories of the linear Koopman system in *y* project onto the full nonlinear system trajectories in *x* in the $y_1 - y_2$ plane. Here $\mu = -0.05$ and $\lambda = 1$. Reproduced from [27]

tories that start on the invariant manifold $y_3 = y_1^2$, visualized by the blue parabolic surface, are constrained to remain on this manifold.

A slow subspace exists, spanned by the eigenvectors corresponding to the slow eigenvalues μ and 2μ ; this subspace is visualized by the green planar surface. Finally, there is the original asymptotically attracting manifold of the original system, $y_2 = y_1^2$, which is visualized as the red parabolic surface. The blue and red parabolic surfaces always intersect in a parabola that is inclined at a 45° angle in the $y_2 - y_3$ direction. The green surface approaches this 45° inclination as the ratio of fast to slow dynamics becomes increasingly large. In the full three-dimensional Koopman observable space, the dynamics produce a single stable node, with trajectories rapidly attracting onto the green subspace and then slowly approaching the fixed point.

The left eigenvectors of the Koopman operator yield Koopman eigenfunctions (i.e., eigen-observables). The Koopman eigenfunctions of Eq. (11) corresponding to eigenvalues μ and λ are:

$$\varphi_{\mu} = x_1$$
 and $\varphi_{\lambda} = x_2 - bx_1^2$ with $b = \frac{\lambda}{\lambda - 2\mu}$

The constant *b* in φ_{λ} captures the fact that, for a finite ratio λ/μ , the dynamics only shadow the

asymptotically attracting slow manifold $x_2 = x_1^2$, but follow neighbouring parabolic trajectories. This is illustrated more clearly by the various surfaces in Figure 2 for different ratios λ/μ .

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

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

These eigen-observables define observable subspaces that remain invariant under the Koopman operator, even after coordinate transformations. They may be regarded as intrinsic coordinates [32] on the Koopman-invariant subspace.

Dynamic mode decomposition

The original Dynamic Mode Decomposition (DMD) algorithm, introduced by [16], was initially conceived using a Companion matrix framework. Later, [15] linked the DMD algorithm to the modified Arnoldi algorithm and Koopman operator theory. However, [20] argued that an algorithm based on Singular Value Decomposition (SVD) provides better numerical stability. Let us delve into this algorithm. Consider a scenario where sequential data arises from linear dynamics described by:

$$x_{k+1} = K x_k, \quad k = 0, 1, 2, \dots,$$
 (12)

with the matrix K being unknown. Even if the data originates from nonlinear dynamics, it is assumed that an operator K can approximate the underlying dynamics. The sequential data from the linear dynamics (12) can be represented as:

$$X_1 = \begin{bmatrix} x_0 & x_1 & x_2 & \dots & x_{N-1} \end{bmatrix},$$
 (13)

$$X_2 = \begin{bmatrix} x_1 & x_2 & x_3 & \dots & x_N \end{bmatrix}.$$
(14)

Next, we perform the Singular Value Decomposition (SVD) of X_1 :

$$X_1 = U\Sigma V^*, \tag{15}$$

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* represents the rank of X_1 . We then define the matrix \tilde{K} as:

$$\widetilde{K} = U X_2 V \Sigma^{-1}.$$
(16)

Next, we compute the eigenvalues and eigenvectors of \tilde{K} , given by:

$$\widetilde{K}w = \lambda w. \tag{17}$$

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

$$\widetilde{v} = Uw, \tag{18}$$

where \tilde{v} represents the projected DMD modes.

Exact dynamic mode decomposition

The Dynamic Mode Decomposition (DMD) algorithm was initially developed to analyze sequential and ordered data vectors $\{x_0, x_1, x_2, ..., x_n\}$ under the dynamics defined by:

$$x_{k+1} = K x_k, \quad k = 0, 1, 2, \dots,$$
 (19)

[20] extended this algorithm by relaxing the constraints on the data. They considered pairs

 $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\},\$

leading to the following definitions for the data matrices:

$$X_1 = \begin{bmatrix} x_1 & x_2 & \dots & x_N \end{bmatrix}; \quad X_2 = \begin{bmatrix} y_1 & y_2 & \dots & y_N \end{bmatrix}.$$
 (20)

Table 1 compares the data comparison for the standard DMD and the extended DMD. It shows that the data matrices for the DMD algorithm are a specific case for the exact DMD, where $y_k = x_{k+1}$.

Table 1. Comparison between data matrices

Data Matrix	DMD	Exact DMD
X_1	$\begin{bmatrix} x_0 & x_1 & \dots & x_{n-1} \end{bmatrix}$	$\begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}$
X_2	$\begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}$	$\begin{bmatrix} y_1 & y_2 & \dots & y_n \end{bmatrix}$

For the dataset given by (20), the operator *K* is defined as:

$$K = X_2 X_1^{\dagger}. \tag{21}$$

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 is as follows: arrange the data pairs { $(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)$ } into matrices X_1 and X_2 as defined in (20). Perform the reduced Singular Value Decomposition (SVD) of X_1 :

$$X_1 = U\Sigma V^*. \tag{22}$$

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

$$\widetilde{K} = U X_2 V \Sigma^{-1}.$$
(23)

Compute the eigenvalues and eigenvectors of K:

$$Kw = \lambda w.$$
 (24)

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

$$v = \frac{1}{\lambda} X_2 V \Sigma^{-1} w.$$
⁽²⁵⁾

For a more detailed exploration of the exact DMD, refer to [20].

Extended dynamic mode decomposition

The extended Dynamic Mode Decomposition (EDMD), initially introduced in [32], was further refined in [33]. In contrast to the original approach, [33] utilized left eigenvectors of the finitedimensional approximation of the Koopman operator for a similarity transformation, while [32] used right eigenvectors. This subtle distinction is crucial for the participation factors discussed in [34]. Following [33], consider a sequence of system state snapshots x_k . The matrices are defined as follows:

$$X_1 = \begin{bmatrix} x_1 & x_2 & \dots & x_N \end{bmatrix}; \quad X_2 = \begin{bmatrix} y_1 & y_2 & \dots & y_N \end{bmatrix},$$
 (26)

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

$$g(x_k) = \begin{bmatrix} g_1(x_k) & g_2(x_k) & \dots & g_q(x_k) \end{bmatrix}^{\top}$$
, (27)

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

$$O_{X_1} = [g(x_1) \ g(x_2) \ \dots \ g(x_N)],$$
 (28)

$$O_{X_2} = [g(y_1) \ g(y_2) \ \dots \ g(y_N)],$$
 (29)

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

$$K = O_{X_2} O_{X_1}^{\dagger}, (30)$$

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

$$\phi(x_k) = \Psi g(x_k),\tag{31}$$

where

$$\Psi = egin{bmatrix} \psi_1^ op & \psi_2^ op & \dots & \psi_q^ op \end{bmatrix}$$
 ,

contains the left eigenvectors of *K*, and

$$\phi(x_k) = \begin{bmatrix} \phi_1(x_k) & \phi_2(x_k) & \dots & \phi_q(x_k) \end{bmatrix}^{\top}.$$

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:

$$x_k = Bg(x_k). \tag{32}$$

From (31), we have $g(x_k) = \Psi^{-1} \phi(x_k)$, and:

$$x_k = Bg(x_k) = B\Psi^{-1}\phi(x_k), \tag{33}$$

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

$$x_{k} = \sum_{i=1}^{q} \phi_{i}(x_{k})v_{i} = \sum_{i=1}^{q} \phi_{i}(x_{0})v_{i}\lambda_{i}^{k}.$$
(34)

The convergence of EDMD to the Koopman operator was demonstrated in [35, 36].

3 Data-driven spectral analysis of dynamical systems using Koopman operator theory

[13, 14] uses the Koopman operator's spectral properties to compare dynamical systems with physical systems, incorporating a statistical Takens theorem [37] and an ergodic-theoretic approach for parameter identification and model validation. [38] addresses model reduction and validation, proposing a decomposition method based on the Koopman operator's spectral theory and the statistical Takens theorem [37]. [39] extends the Hartman–Grobman Theorem to the entire basin of attraction, linking the linearization with the Koopman operator's spectrum. [28] explores Lyapunov functions' connection to the Koopman and Perron-Frobenius operators, introducing a stability theory and a numerical technique for smooth eigenfunctions. [40] introduces isostables, extending isochrons for asymptotically periodic systems, with an algorithm for computing isostables using the Koopman operator's spectral properties. [29] leverages the Koopman operator's spectral characteristics to extend linear stability analysis to nonlinear systems, establishing a correlation between specific eigenfunctions and global stability. [41] applies the Koopman operator theory to non-smooth dynamical systems, focusing on a pendulum with state resets, linking geometric and operator-theoretic perspectives. [42] examines the interplay between Koopman operator eigenfunctions and the topological conjugacy in nonlinear systems, introducing the principle algebra for observables. [43] extends the Koopman operator framework to nonautonomous systems using time-paramtime-parameterized and *Floquet theory*.

[44] investigates Koopman's principal eigenfunctions in cascaded systems, establishing the asymptotic equivalence of the dynamics. [31] characterizes through Koopman operator spectral properties, defining the principal dimension of data and analyzing quasi-periodic attractors. [45] uses the Koopman operator framework for nonlinear control, connecting Dynamic Mode Decomposition (DMD) with Koopman Mode Decomposition (KMD) and character characterizing and isochrons. [46] derives convergence rates for Perron-Frobenius and Koopman operators, focusing on approximation spaces and sample-based operator estimates. [47] addresses nonautonomous dynamical systems, proposing algorithms to mitigate errors in computing nonautonomous Koopman eigenvalues using dynamic mode decomposition. [48] studies numerical approaches for Koopman Modes in Banach spaces using *generalized Laplace analysis*, investigating convergence in the finite section method and Krylov subspace approximations.

[32] presents a data-driven method for approximating Koopman operator eigenvalues and modes, extending dynamic mode decomposition (DMD). It also approximates Kolmogorov backward equation eigenfunctions for Markov processes. Examples demonstrate the method's performance on deterministic and stochastic data, with further results by [33, 36].

[49] introduces a technique using Koopman operator eigenfunctions for integrating sensor data in nonlinear systems. This method, requiring time series data and shared measurements, combines

static and dynamic state estimation to create Koopman eigenfunction approximations. [50] applies Koopman Mode Decomposition (KMD) to low-dimensional dynamic datasets, comparing DMD, Arnoldi KMD, and Prony algorithms. The study highlights Prony's superior performance in low frequencies and explores timeshifted time-series approaches for linear oscillation attenuation.

[51] proposes a framework using Koopman operators to compare dynamical systems or align them with empirical data, focusing on nonlinear behaviours and non-Gaussian noise. It combines ergodic partition theory with Hardy space theory, enriching the discourse on comparing dynamical systems and empirical data. [52] explores data-driven approaches for chaotic systems using the Takens embedding theorem and Koopman operator theory. The HAVOK model predicts lobeswitching events, while sparse regression techniques prevent overfitting, integrating machine learning with Koopman's theory for linear representations of chaotic dynamics. [53] introduces a methodology for modal decomposition using the Koopman operator, integrating parametric functions into neural networks. This method, leveraging LKIS-DMD, withstands observation noise and adapts to data uncertainties.

[54] employs KMD to analyze lid-driven flow dynamics, highlighting Koopman operator spectral properties. The study reveals KMD's superior performance over proper orthogonal decomposition in reconstructing flows with quasi-periodic components. [35] establishes the convergence of DMD algorithms for computing Koopman operator eigenvalues and eigenfunctions. Leveraging ergodicity, the article shows that DMD applied to Hankel data matrices accurately determines Koopman eigenfunctions and eigenvalues. [55] discusses an agent-based model to explore the impact of preferential gathering sites on urban insurgency. It finds a non-monotonic relationship: a moderate number of sites reduces large-scale outbursts compared to a few or numerous sites, which either concentrate or dilute insurgent activity. Koopman Mode Analysis reveals quasi-periodic spatial-temporal dynamics in insurgency and law enforcement interactions. Lattice size refers to the grid representing the simulation area, with larger lattices accommodating more agents and influencing visibility and interaction patterns.

In [56], the paper has two objectives: First, it introduces a robust computational tool for datadriven Koopman spectral analysis using Krylov decomposition and the Frobenius companion matrix, mitigating ill-conditioning via the discrete Fourier transform. This transforms the Vandermonde matrix into a generalized Cauchy matrix, enabling precise numerical computations. Second, it explores optimal reconstruction weights for snapshots using subsets of Koopman modes, demonstrating explicit reconstruction formulas that align with Koopman spectral theory, notably Generalized Laplace Analysis. In [57], a novel methodology combines compositional Koopman operators and graph networks for efficient dynamics modelling of complex systems. A linear approximation strategy overcomes neural network limitations. Scalability challenges are addressed by leveraging the system structure. The model, utilizing graph networks, excels in generalizing across environments, handling uncertainty, and enhancing control efficiency. Object-centric sub-embeddings and a block-wise Koopman matrix structure enable modelling and controlling multi-object systems. A least squares problem-solving approach identifies Koopman and control matrices, reducing parameter complexity. The model outperforms baselines in tasks involving ropes, soft materials, and swimming, making it advantageous in real-world scenarios with unknown parameters. Incorporating metric loss enhances prediction accuracy and distance preservation, particularly in novel environments with elusive physical parameters.

In [58], spectral properties of linear and nonlinear dynamical systems with globally stable attractors are explored. The Kato decomposition is used to formulate spectral expansions for linear systems, while generalized eigenfunctions linked to the Koopman operator elucidate stable, unstable, and centre subspaces. Open eigenfunctions and joint zero-level sets provide insights into centre manifolds for nonlinear systems. A novel class of Hilbert spaces is also introduced to capture

dissipative dynamics, with modulated Fock spaces facilitating spectral expansions for systems with stable limit cycles and tori.

In [59], a method for computing the fine structure of the Koopman operator's spectrum from measured data is presented. The approach partitions the spectrum into atomic and continuous components, with guaranteed convergence as the number of moments increases. It also identifies the singular continuous portion and offers two approaches for approximating the spectral measure, adaptable to large-scale systems. The method's simplicity and computational efficiency make it suitable for various applications, illustrated through numerical examples, including examining the spectrum in lid-driven cavity flow. [60] applies Koopman-operator analysis to partial differential equations describing relaxation to a stable state. It introduces Koopman eigenfunctions and analyzes analyzed nonlinear systems, including diffusion and phase-diffusion equations. [61] addresses rare event occurrence in dynamical systems using Koopman operators, identifying invariant subspaces through neural networks.

In [62], a Laplace-domain theory is developed for analyzing nonlinear dynamical systems, focusing on the Koopman semigroup and its generator. The Koopman resolvent is introduced and characterized spectrally for different types of nonlinear dynamics, shedding light on its role in Laplace-domain representation. Computational aspects, especially nonstationary Koopman modes, are explored. In [63], the method for computing the Koopman operator's spectral decomposition is extended to measure-preserving flows on compact metric spaces. Spectral decomposition is approximated through temporal discretization of the flow, with a condition ensuring weak convergence of spectra. Numerical results demonstrate spectral computations for volume-preserving flows using periodic approximations.

[64] introduces spectral methods for long-term forecasting of signals from quasi-periodic systems, utilizing theory for nonlinearities. The algorithms provide uncertainty quantification and demonstrate efficiency in synthetic and real-world applications. In [65], game balancing is advanced using a Koopman model to optimize in DeepMind's SC2 DefeatRoaches mini-game. The study identifies critical parameters to minimize criterion "J" by modelling game dynamics and validating with empirical data. This approach yields extended game durations with players near zero health, suggesting scalable applications for more complex games. Future research will focus on the impact of initial conditions, employing AI algorithms for precise game balancing beyond traditional methods. In [66], gait recognition distinguishes individuals by walking styles, utilizing techniques like CNNs and the SMPL model. The GaitVIBE + LDS model combines the VIBE model with a transformer network, enhancing performance on specific datasets without extra data. The study evaluates various loss functions and achieves notable results on the CASIA-B dataset, addressing ethical and privacy concerns while discussing real-world applications such as identifying individuals to combat poaching or locating missing persons.

In [67], a novel lifting technique is introduced for nonlinear system identification using the Koopman operator. This technique identifies the linear Koopman operator in a lifted space of observables, avoiding direct state space computations. Two numerical schemes are proposed: primary parametric and dual methods for high-dimensional systems with limited data. The effectiveness of these methods is demonstrated through various examples. [68] applies the Koopman operator to vehicle dynamics, transforming the state space into a higher-dimensional linear space using basis functions. Two strategies are discussed: one using Extended Dynamic Mode Decomposition and another constructing eigenfunctions from nonlinear dynamics. These approaches are exemplified through numerical examples. [69] extends [68] by approximating a nonlinear vehicle model with a higher-order linear predictor-the Koopman operator. This approximation is used in a linear Model Predictive Control framework, effectively handling the vehicle's nonlinearities-a comparison with classical local linearization provided.

[70] addresses the challenges of identifying latent structures in nonlinear systems using Koopman operator-based linearization proposed by [67] is enhanced to mitigate numerical instability in high-dimensional spaces. A novel implementation algorithm is introduced to address these issues. In [71], the Koopman operator theory is explored for nonlinear infinite-dimensional systems. A finite-dimensional projection of the Koopman semigroup is introduced, allowing for linear approximation and spectral property extraction from data. This method is applied to identify a finite-dimensional approximation of the Lie generator associated with the Koopman semigroup.

4 Past surveys in applied Koopman operator theory

In [72], the Koopman operator's advancement for analyzing and examining signal dynamical systems are explored emphasising academic and industrial applications. Key theoretical concepts, numerical methods, and areas for further research are detailed. Continuous indicators for ergodicity and mixing are derived, with applications in vehicle path-planning and micro-scale fluid mixing. The paper examines the Koopman operator's spectral properties in Banach spaces, including continuous-time dynamics, and discusses eigenfunctions, eigenvalues, and ergodic transformations. Practical applications include the heat equation and dynamical system evaluation using spectral decomposition and projection of observables. Koopman mode decomposition is introduced, illustrating its use in harmonic oscillators, model reduction, and coherency analysis in power systems. The Dynamic Mode Decomposition (DMD) algorithm, a robust variant of the Arnoldi algorithm, is presented, demonstrating its application in fluid flow analysis and building energy efficiency. The paper discusses temporal Fourier transforms, Sobolev space metrics, and eigen-quotient maps, highlighting convergence errors and proposing enhanced simulation time adjustments. Finally, ergodicity computation is applied to technical systems, proposing negative index Sobolev norm $\|\cdot\|_{2,-s}$ for scenarios like search-and-rescue and micro-mixer design. In [73], Koopman Mode Decomposition (KMD) is surveyed as a flow analysis technique based on [14] and [11, 12]. KMD dissects dynamic systems into single-frequency components or modes, providing insights for researchers using data-driven Koopman analysis. The survey covers mathematical foundations and applications in flow analysis, power grids, and building thermal and biomedical analysis. Challenges in Koopman analysis, including computational complexity and comparison with proper orthogonal decomposition, are addressed. [74] surveys Koopman operator techniques in intelligent mobility and vehicle engineering, highlighting various applications and theoretical aspects with the potential for addressing open problems in these domains.

Building on the foundational surveys by [72], which laid the groundwork for understanding the Koopman operator's theoretical constructs and applications, and [73], which explored the role of Koopman Mode Decomposition (KMD) in specific domains like flow analysis, this survey takes a broader and more integrative approach. Unlike [74], which focuses narrowly on intelligent mobility and vehicle engineering, our work systematically spans various disciplines, including power systems, robotics, aerodynamics, building energy management, and stochastic systems. Furthermore, this survey uniquely addresses challenges such as noisy, high-dimensional, and multiscale systems, emphasizing the Koopman operator's potential in data-driven discovery under uncertainty. In addition to cataloguing applications, our survey provides critical evaluations of algorithmic advancements like Extended Dynamic Mode Decomposition (EDMD) and neural network-based Koopman embeddings, offering a detailed analysis of their efficacy and limitations. Finally, this work highlights limitations and future research directions in KOT, such as its role in stochastic dynamics, multiscale interactions, and chaotic systems, proposing pathways for future research. This survey provides a comprehensive guide for researchers seeking to advance Koopman-based approaches in data-driven science and engineering by bridging theoretical developments with practical implementations and underscoring existing methodologies' strengths

and constraints.

5 Koopman operator of autonomous nonlinear system

Koopman operator exhibits unitary properties, meaning it bijects points in Hilbert space while preserving the inner product of any two observables [11]. This revelation opens up a new world of possibilities in studying nonlinear dynamical systems and control theory. Numerous studies have shown that classical attributes of dynamical systems can be seamlessly translated into the Koopman formalism. Notably, it has been demonstrated that the level sets of Koopman eigenfunctions can serve as invariant partitions within the state space of a dynamical system [75]. Furthermore, utilizing the Koopman operator, the local linearization rooted in the Hartman–Grobman theorem has been expanded to cover the entire basin of attraction of a stable equilibrium or limit cycle. This local linearization, a key concept in dynamical systems theory, involves approximating a nonlinear system by a linear one in a small neighbourhood of a fixed point, as per the Hartman–Grobman theorem. This linearization applies to both flows and maps [39].

The Koopman operator transforms a nonlinear system into a linear, high-dimensional space, presenting new and exciting challenges. In big data, the Koopman operator is particularly appealing because it relies on measurement data to linearly approximate nonlinear systems without traditional linearization around specific fixed points. This approach often expands the stability region around the equilibrium, as discussed in [34, Chapter 7]. However, a crucial question arises: Which data should be used? The variables essential for constructing the Koopman operator, known as observables, are paramount and deserve careful consideration. Observables are typically functions of system states that encapsulate the dynamics of interest. For instance, rotor speeds and angles are pivotal in determining system dynamics in a power system governed by the swing equation, a mathematical model used to simulate the behaviour of synchronous machines in an electric power system. Therefore, due to their correlation with system states, terminal bus voltages, generator electrical power, and system frequency are primary candidates for observables. Conversely, the reactive power of the generator is suboptimal as an observable due to its minimal dependence on rotor angle and speed. These practical implications make the Koopman operator a powerful tool in nonlinear dynamical systems and control theory, engaging researchers in its potential applications. However, the complexity of controlling the system depicted by [34, Chapter 1, Figure 4.1] precludes unfettered access to all system states or the straightforward determination of observables using conventional power system knowledge, as noted by [76]. This underscores the urgent need for a methodology to discern observables capable of accommodating partial states or functioning without state information. The forthcoming sections will elucidate a method for constructing the Koopman operator tailored to such systems, particularly those characterized by input-output dynamics. This research is of utmost importance in nonlinear dynamical systems and control theory.

6 Data-driven Koopman-based methodologies in power systems research

In [77], Koopman mode analysis is explored for detecting coherent swings in power systems, comparing it with other modal analysis methods. The paper demonstrates its effectiveness in identifying dominant components and coherency within transient stability analysis. Similarly, [78] introduces Koopman Mode Analysis (KMA) for analyzing and controlling power systems, presenting its theoretical foundation and application to multi-machine systems. Numerical outcomes from applying KMA and acknowledgment of diverse funding sources are discussed. [79] leverage Koopman Mode Analysis to address transient stability issues in multi-machine power systems. By identifying Coherent Swing Instability (CSI) transmission paths, they develop a data-driven approach for monitoring and mitigating transient stability loss.

[80] discuss a pragmatic application of Koopman mode analysis in a separate study. Their datadriven stability assessment method, based on Koopman operator theory, offers practical and valuable insights into system instabilities, particularly during grid accidents, thereby providing a sense of reassurance in critical situations. [81] introduces a groundbreaking method for integrating measurements from diverse sensors within nonlinear systems. This approach, which harnesses Koopman eigenfunctions and dynamic mode decomposition, allows for data parameterization and system dynamics characterization, thereby advancing the potential of modern data-driven techniques. [82] presents a data-centric control framework rooted in Koopman operator theory for transient stabilization in power grids. This approach constructs a linear predictor within a higher-dimensional state space, facilitating efficient control using model predictive control (MPC). [83] proposes a robust and interpretable data-driven approach for load forecasting in power grids. By combining dynamic mode decomposition and Gaussian process regression, their method not only outperforms alternative forecasting techniques but also instills a strong sense of confidence in its reliability and accuracy. These studies collectively demonstrate the efficacy of Koopman operator theory in addressing various challenges within power systems research, from transient stability analysis to load forecasting.

7 Koopman operator theory in control and optimization

Koopman operator theory, a crucial tool in control systems analysis and optimal control frameworks, plays a significant role in understanding the dynamics of high-dimensional systems. In [30], the theory analyses stable and unstable subspaces and explores the interplay between spectral and geometric theories. The Koopman operator, representing the time evolution of observables, is essential for understanding the dynamics of high-dimensional systems and optimal control, particularly when incorporating max-plus algebra. Koopman eigenfunctions enable the decomposition of state space into stable, central, and unstable subspaces. [26] push the boundaries of Koopman operator theory by extending it to include input and control effects. This novel approach addresses the limitations of traditional Dynamic Mode Decomposition (DMD) in actuated systems. This innovative method, dynamic mode decomposition with control, provides a robust framework for analyzing nonlinear systems, as demonstrated through applications such as infectious disease models.

[23] presents a method for developing linear predictors for nonlinear controlled dynamical systems. This technique approximates the Koopman operator by embedding nonlinear dynamics into a higher-dimensional space and employs Extended Dynamic Mode Decomposition (EDMD) to create linear models. These predictors facilitate efficient model predictive control (MPC) designs for nonlinear systems, effectively managing constraints and disturbances. Another contribution by [84] focuses on data-driven learning of Koopman eigenfunctions for prediction and control. This method constructs a comprehensive set of eigenfunctions from transient regimes, enabling linear predictions and integration within the Koopman MPC framework. This data-driven approach utilizes convex optimization to avoid non-convex machine learning tools.

[85] further refine the data-driven construction of Koopman eigenfunctions, emphasizing their utility for linear prediction and control. This work solidifies the theoretical foundations and demonstrates practical applications of Koopman-based control strategies, making the theory more engaging and relevant to the audience. [86] demonstrate the practical implications of their research by integrating Extended Dynamic Mode Decomposition (EDMD) with Model Predictive Control (MPC) to control nonlinear partial differential equations (PDEs). Using the Burgers equation as an example, they show how Koopman-linear systems can effectively control unsteady fluid flows and enhance the suppression of travelling waves compared to traditional methods.

[87] underscores the collaborative nature of academic research by highlighting the challenges in approximating the Koopman operator in finite dimensions and proposing structured approaches to reconcile theoretical and practical aspects. They discuss the paradigm's relationship with system-theoretic principles and suggest future research directions, inviting the audience to contribute to improving control system modelling. Using the Koopman operator, [88] propose a data-driven method for stabilizing discrete-time control-affine nonlinear systems. By transforming the system into a higher-dimensional bilinear form, they develop a state feedback law for stabilization, demonstrating its efficacy on systems like the Van der Pol oscillator and the chaotic Henon map. Koopman analysis has been effectively used in nonlinear estimation [89, 90] and control [17, 23, 91]. Estimators and controllers derived from DMD or eDMD models have proven effective, as shown in various applications, including fluid flow control [91, 92]. For more on comprehensive applications of Koopman operator in control theory and related areas, see [93–100].

8 Koopman operator theory in fluid dynamics

In [15], model-reduction techniques for fluid flows are explored, emphasizing the spectral analysis of the Koopman operator. The study demonstrates the efficacy of Koopman modes in capturing flow dynamics, exemplified by a jet in crossflow, advancing model-reduction techniques for fluid dynamics. [101] delves into Koopman modes in fluid mechanics, showcasing their emergence within nonlinear dynamics. The study investigates the spectral attributes of the Koopman operator, offering insights into various computational methods and applications and enriching the understanding of complex fluid behaviours. [102] discuss the connection between Koopman mode decomposition and resolvent mode decomposition in turbulent flow patterns. They highlight the role of time averaging and spatial shifts in approximating Koopman modes, extending the theoretical framework to systems with continuous spectra.

9 Koopman operator: stochastic framework

[103] introduces Subspace Dynamic Mode Decomposition (Subspace DMD) for Koopman analysis in noisy random dynamical systems. Through empirical validation, Subspace DMD showcases robustness and utility, enhancing understanding of complex nonlinear systems affected by observation noise. [104] explores modelling equilibrium and non-equilibrium stochastic systems via optimal low-rank approximation techniques applied to transfer operators. The discussion emphasizes connections between methods, Markov state models, and metastability, with applications illustrated through numerical examples. [105] investigates the spectrum and eigenfunctions of stochastic Koopman operators for linear random dynamical systems, introducing a stochastic Hankel-DMD algorithm. Numerical examples demonstrate its applicability and potential for model reduction strategies. [106] presents the Variational Approach for Markov Processes (VAMP), a methodology for identifying optimal feature mappings and Markovian dynamics models based on provided time series data. VAMP leverages Koopman operator insights for model optimization and selection, which is applicable across reversible and nonreversible processes.

[107] develops deep learning Markov and Koopman models with physical constraints, leveraging variational methodologies for optimization. The approach yields a universal approximator for reversible Markov processes, offering systematic improvements in model performance, particularly with biased data. [108] addresses stochastic safety verification in random dynamical systems using barrier functions. The paper introduces random safety concepts and proposes data-driven approximations of barrier certificates using Koopman operator techniques. [109] introduces a robust DMD algorithm for approximating the stochastic Koopman operator in the presence of noise. The algorithm adapts to time-delayed observables, demonstrating effectiveness across various examples.

[110] formalizes a framework for acquiring the Koopman operator from finite data trajectories of Markov chains. The research establishes links between risk and spectral decomposition estimation, motivating the development of a Reduced-Rank Operator Regression (RRR) estimator. [111] proposes a data-driven nonparametric methodology for forecasting probability densities in stochastic dynamical systems, leveraging the stochastic Koopman operator and extended dynamic mode decomposition (EDMD). Numerical examples highlight its accuracy and efficacy in real-time moment estimation.

10 Koopman operator theory in building energy management

[112] conducts an energy audit on a LEED Silver-certified university building, utilizing Koopman mode analysis to identify energy wastage sources, such as malfunctioning equipment and suboptimal HVAC conditions. Addressing these issues leads to a 13% reduction in energy consumption without compromising occupant comfort. [113] proposes a method using the Koopman operator to create zoning approximations for building energy models. The method simplifies models while preserving accuracy, aiding energy data analysis and visualization by analysing building thermal behaviour with Koopman modes. [114] introduces data-driven methods for thermal control and energy management in buildings using Koopman operator theory. By analyzing thermal data from sensors, the approach identifies spatial heating and cooling control modes directly, offering insights without complex thermal models.

11 Koopman operator theory in robotics

[115] develops a data-driven model for motion control in soft robotic devices using Koopman operator theory. The model accurately predicts system behaviour, aiding controller design while reducing computational complexity. [116] employs Koopman Operator Theory (KOT) with Hankel Dynamic Mode Decomposition (HDMD) to approximate soft robot arm dynamics and address control challenges. Despite limitations, the method achieves static reference tracking and control, with ongoing efforts to capture rapid dynamics and implement closed-loop control. [117] proposes a method for modelling and controlling robotic systems using Koopman-inspired techniques and Dynamic Mode Decomposition (DMD). The KEEDMD framework constructs Koopman eigenfunctions from data, enabling the development of linear models and trajectory-tracking controllers. Ongoing research focuses on addressing limitations and exploring alternative control strategies.

12 Koopman operator theory in non-linear aerodynamics

In [118], Koopman operator mode decomposition techniques are applied to analyze dynamic stalls, revealing insights into oscillatory phenomena and shedding light on complex aerodynamic dynamics. [119] explores the impact of oscillatory incoming flow on wing dynamics using Koopman operator theory, unveiling insights into pitching airfoil behaviour and shedding light on the interplay between flow frequency and vortex shedding dynamics. [120] demonstrates the application of analytically derived Koopman linearization for flight dynamics, offering a structured overview of theory, applications, implementation, and performance demonstrations, with future research directions outlined.

13 Application of DMD and EDMD algorithm

In [121], Dynamic Mode Decomposition (DMD) is highlighted as a robust tool for analyzing extensive neural recordings, aiding in discerning sleep spindle networks and facilitating data clustering via Gaussian mixture modelling. [122] explores reduced order models (ROMs) and dynamic mode decomposition (DMD) for model reduction within intricate systems, proposing the

synergistic combination of POD and DMD methodologies. [123] introduces higher-order dynamic mode decomposition, extending DMD to address general periodic and quasi-periodic dynamics beyond standard DMD's reach, showcasing its efficacy in various applications.

[124] focuses on DDMD R (Refined Rayleigh Ritz Data Driven Modal Decomposition), enhancing DMD for computational data-driven analysis of fluid flows, showcasing tangible benefits through numerical experiments. [125] explores operator-theoretic approaches to dynamical systems using Koopman and Perron-Frobenius operators, introducing CU-DMD as a novel method to approximate the PF operator with accuracy and efficiency. In [126], Koopman mode analysis through DMD is discussed, addressing mean subtraction and DMD mode selection within finitedimensional Koopman invariant subspaces. [127] discusses stochastic parameterization coupled with DMD to represent unresolved small-scale dynamics and large-scale flow phenomena, introducing STO-DMD as an effective technique for enhancing variability in resolved flow dynamics. [128] demonstrates the Koopman operator's and DMD's efficacy in iterated function systems (IFS), showcasing their utility in analyzing and forecasting stochastic nonlinear dynamical systems.

14 In algorithm and neural network

In [129], the Koopman operator framework is applied to analyze and accelerate numerical algorithms, showcasing advantages in constructing reduced operator representations for prominent algorithms. In [130], the Koopman operator's spectrum is utilized to determine network depth, assess initialization, accelerate training, and enhance noise robustness in neural networks, offering insights into network architecture and convergence. In [131], algorithmic equivalence is explored through Koopman operator theory and spectra comparisons, showcasing the utility of Koopman mode decomposition in identifying equivalent algorithms without explicit equations. In [132], pruning algorithms motivated by Koopman operator theory are introduced, unifying magnitude and gradient-based pruning methodologies and shedding light on magnitude pruning's performance in early training stages. [100] proposes a framework integrating bilinear Koopman embedding and Control Lyapunov Function (CLF) to stabilize controllers for unknown nonlinear control systems, offering provable guarantees of asymptotic stability validated through numerical simulations.

15 Koopman operator in other branches of science

[133] employs Koopman Mode Decomposition (KMD) to predict sea ice concentration dynamics, revealing declining trends and heightened variability in specific regions. KMD-based forecasts demonstrate skill in predicting future sea ice behaviour, outperforming linear fit models and climatological benchmarks. [134] highlights how Koopman mode decomposition offers a data-driven approach to analyze and forecast traffic dynamics, aiding transportation agencies in managing highway network conditions. In [135], a novel methodology grounded in Dynamic Mode Decomposition (DMD) is introduced to extract Resting State Networks (RSNs) from high-dimensional fMRI data with acceptable temporal resolution, facilitating individualized RSN analysis and occupancy pattern deduction.

16 Limitations of Koopman operator and DMD algorithm

[136] explores ways to extend the use of Koopman's theory for analyzing PDEs commonly found in image and signal processing. These PDEs describe processes of gradual signal changes, which can sometimes include sudden shifts in behaviour (phase transitions). A key focus is understanding when the Koopman eigenfunctions (KEFs) can be used and how they help in tasks like breaking complex systems into simpler parts, reconstructing dynamics, and understanding the system's behaviour and control.

The study highlights DMD's weaknesses, which work well only under specific conditions, such as when the system's behaviour can be expressed as simple linear combinations of observations or when the system's behaviour has a consistent, predictable pattern (like exponential decay). DMD struggles when the system does not decay exponentially, and a single component corresponds to multiple patterns, the system has stable points (equilibrium), or specific patterns do not exist throughout the system's timeline. Additionally, some patterns may disappear entirely if the system's dynamics are not smooth everywhere. Koopman, EDMD and SDP-based methods were described in [59, 137] to approximate invariant measures purely from data. However, the method did not work well when trying to approximate invariant measures for the following two different random dynamical systems generated by the iterated function systems [138, Section 2.1] as follows:

$$\phi_u(x) = ux,\tag{35a}$$

$$\psi_u(x) = x + u(1 - x),$$
 (35b)

where *u* is chosen uniformly on (0, 1) and ϕ and ψ are chosen with probability $\frac{1}{2}$. The invariant density is

$$\rho_{\star}(x) = \frac{1}{\pi \sqrt{x(1-x)}},$$
(36)

$$f_1(x) = \frac{x}{2},\tag{37a}$$

$$f_2(x) = \frac{x}{2} + \frac{1}{2},\tag{37b}$$

where f_1 and f_2 are chosen with probability $\frac{1}{2}$. The invariant density is

$$U(0,1).$$
 (38)



Figure 3. (a) Histogram approximation (blue) of the density (36) of the stochastic dynamical system (35a)- (35b). (b) The approximated density using the Koopman, EDMD, and SDP-based method based on [137]



Figure 4. (a) Histogram approximation (blue) of the density (38) of the stochastic dynamical system (37a)- (37b). (b) The approximated density using the Koopman, EDMD, and SDP-based method based on [137]

This shows that the Koopman-EDMD-SDP-based methods may not work for data-driven discovery of invariant measures for random dynamical systems and, generally, for pice-wise continuous maps.

17 Future challenges and conclusion

The Koopman operator-theoretic approach, distinguished by its unique advantage, stands out from traditional linearization methods. It enables spectral analysis of nonlinear systems without sacrificing critical information, a feat not easily achieved by conventional spectral techniques that predict geometry locally in state space. This method's effectiveness in low and high-dimensional state spaces is a testament to its versatility. Transforming nonlinear dynamics into a linear framework shifts the analysis away from individual trajectories, making it especially suitable for studying noisy systems. Its reliance on data derived from simulations or experimental measurements to construct, approximate, or analyze operators makes it a flexible approach to understanding a system's underlying mechanisms, even when the system's dynamics are complex.

While the Koopman operator-theoretic approach offers unique advantages, it also presents significant challenges. These challenges include the demand for a departure from physical intuition, as the approach emphasizes functions over individual state-space points. Even in finite-dimensional state spaces, the technique fundamentally operates within an infinite-dimensional context, adding complexity to its conceptualization and implementation. While this trade-off enables the encapsulation of nonlinear dynamics within a linear system framework, it necessitates sophisticated numerical methods and approximations. Developing efficient numerical techniques, a critical area of focus remains a key aspect of these methodologies. This survey thoroughly examined a wide range of literature, incorporating seminal contributions, innovative methods, and diverse applications across various domains.

Often, a system's equations are unknown or partially known, or, in other words, there are situations where there are no governing fundamental physics equations that we can rely on. Discovering governing equations from data is crucial for the Koopman operator to show promising future research. Nonlinear dynamics still need to be better understood; even an epsilon non-linearity or a quadratic non-linearity confounds our understanding. We do not even know if solutions exist in closed form or topologically and are unique for some of these systems, and that is something Koopman's spectral analysis and linear embedding is going to help, as we have seen a toy example in Section 2. In nonlinear control theory, chaos, transients, intermittent and uncertain phenomena

are challenging.

Much of what we saw in the review here is still quite tricky for chaotic systems or systems with significant intermittent phenomena or non-stationary systems. Then, multiscale physics, one of the grand challenges of this kind of substantial data era, is in the past; a lot of what has been done has been applying analysis and computations and these dynamic systems models to uni-scale physics now. However, the need for multiscale analysis is urgent. These Koopman-based methods will help if we apply them to a multiscale problem like turbulence, climate, disease, or neuroscience. Data with noise and stochasticity is a foundational area to explore. Even computing derivatives from noisy data is a big challenge. However, there is optimism in the potential of Koopman and DMD techniques in dealing with noisy data, especially in scenarios with limited, irregularly sampled, or noisy data, which is common in real-world applications. The potential of extending Koopman operator frameworks to account for stochastic systems or systems with uncertainties, where the operator acts on probability distributions rather than deterministic states, is still a vast area to explore.

After scrutinizing over one hundred papers, numerous monographs, and a substantial array of doctoral dissertations [4, 8, 20, 34, 139–148], we can confidently assert 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 proven to be pivotal pillars in the arsenal of data-driven methodologies, reassuring their applicability in diverse research areas.

Declarations

Use of AI tools

The authors declare that they have not used Artificial Intelligence (AI) tools in the creation of this article.

Data availability statement

No Data associated with the manuscript.

Ethical approval

The authors declare that this research complies with ethical standards. This research does not involve human participants or animals.

Consent for publication

Not applicable

Conflicts of interest

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