Introduction to Koopman operator theory of dynamical systems

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Koopman operator theory is an alternative formalism for study of dynamical systems which offers great utility in data-driven analysis and control of nonlinear and high-dimensional systems. This note gives a short and informal review of this theory, as well as a list of references that point to rigorous mathematical treatments and a variety of applications to physics and engineering problems.[1]

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[1] These notes are adapted from my PhD dissertation at UC Santa Barbara [1].

Contents

1 Classical theory of dynamical systems

A dynamical system, in the abstract sense, consists of two things: a set of *states* through which we can index the evolution of a system, and a *rule* for that evolution. Although this viewpoint is very general and may be applied to almost any system that evolves with time, often the fruitful and conclusive results are only achievable when we pose some mathematical structure on the dynamical system, for example, we often assume the set of states form a linear space with nice geometric properties and the rule of evolution has some order of regularity on that space. The prominent examples of such dynamical systems are amply found in physics, where we use differential equations to describe the evolution of physical variables in time. In this note, we specially focus on dynamical systems that can be represented as

$$\dot{x} = f(x), \tag{1}$$

where x is the state, an element of the state space $S \subset \mathbb{R}^n$, and $f : S \to \mathbb{R}^n$ is a vector field on that state space. Occasionally, we will specify some regularity conditions for f like being smooth or a few times differentiable.

We also consider dynamical systems given by the discrete-time map

$$x^{t+1} = T(x^t), \quad t \in \mathbb{Z} \tag{2}$$

where x belongs to the state space $S \subset \mathbb{R}^n$, t is the discrete time index and $T : S \to S$ is the *dynamic map*. Just like the continuous-time system in (1), we may need to make some extra assumptions on T. The discrete-time representation of dynamical system usually doesn't show up in representation of physical systems, but we can use it to represent discrete-time sampling of those systems. This representation is also more practical because the data collected from dynamical systems almost always comes in discrete-time samples.

The study of the dynamical systems in (1) and (2) was dominated by the geometric viewpoint in much of last century. In this viewpoint, originally due to Henri Poincaré, the qualitative properties of the solution curves in the state space are studied using geometric tools and the emphasis is put on the subsets of the state space that play a big role in the asymptotic behavior of the trajectories. We briefly describe some concepts from this theory here, but a more comprehensive exposition can be found in [22, 62, 64].

Assuming that the solution to (1) exists, we define the *flow map* $F^t : S \to S$ to be the map that takes the initial state to the state at time $t \in \mathbb{R}$, i.e.,

$$F^t(x_0) = x_0 + \int_{x_0, t'=0}^{t} f(x(t'))dt'. \tag{3}$$

The flow map satisfies the semi-group property, i.e., for every $s, t \geq 0$,

$$\begin{aligned} F^t \circ F^s(x_0) &= F^s(x_0) + \int_{F^s(x_0), t'=0}^{t} f(x(t'))dt', \\ &= \int_{x_0, t'=0}^{F^s(x_0), s} f(x(t'))dt' + \int_{F^s(x_0), t'=0}^{t} f(x(t'))dt', \\ &= \int_{x_0, t'=0}^{t+s} f(x(t'))dt', \\ &= F^{t+s}(x_0). \end{aligned} \tag{4}$$

where $\circ$ is the composition operator.

Some of the important geometric objects in the state space of continuous-time dynamical systems are as follows:

Fixed point: Any point x in the state space such that $f(x) = 0$ (or $F^t(x) = x$) is a fixed point. The fixed points correspond to the equilibria of physical systems. An important notion about fixed points is the stability, that is wether the trajectories starting in some neighborhood of fixed point stay in its neighborhood over time or not.

Limit cycle: Limit cycles are (isolated) closed curves in the state space which correspond to the time-periodic solutions of (1). The generalized version of limit cycles are tori (like Cartesian products of circles) which are associated with quasi-periodic motion.

Poincaré map: Consider a plane in the state space that is pierced by a limit cycle, and then define a discrete-time map as follows: take point x on the plane, move it with the continuous-time system until it pierces the plane again at the point $T(x)$. The Poincaré map is given by $x' = T(x)$ on that plane and can be used to study the properties of the limit cycle. The fixed point of the Poincarḿap occurs at the intersection of limit cycle and the plane. Stability of that fixed point indicates the stability of the limit cycle.

Invariant set: An invariant set B in the state space is any set that satisfies $F^t(B) \subseteq B$ for all t, i.e., the trajectories starting in B remain in B. Invariant sets are important because we can isolate the study of the dynamics on them from the rest of state space which simplifies the analysis task. Also they include important objects such as fixed points, limit cycles, attractors and invariant manifolds.

Attractor: An attractor is an attracting set with a dense orbit. An attracting set is an invariant subset of the state space to which many initial conditions converge. A dense orbit in a set is a trajectory that comes arbitrarily close to any point on that set. For example, a stable limit cycle is an attractor, because if a trajectory starts sufficiently close to it, it will come arbitrarily close to it, and, the limit cycle itself is a dense orbit. In contrast, the union of two separate stable limit cycles is an attracting set but not an attractor, because there is no trajectory that comes arbitrarily close to points on both cycles. Simple attractors include stable fixed points, limit cycles and tori. A more complicated example of attractor is the famous butterfly-shaped set in the chaotic Lorenz system which is called a strange attractor.

Attractors are the objects that determine the asymptotic (that is post-transient or long-term) dynamics of dissipative dynamical systems. In fact, the mere notion of dissipativity (we can think of it as shrinkage in the state space) is enough to guarantee the existence of an attractor in many systems [62]. In some cases, the state space contains more than one attractor, and the attractors divide the state space into *basins of attraction*; any point in the basin of attraction of an attractor will converge to it over infinite time.

Bifurcation: Bifurcation is any change in the qualitative behavior of all the trajectories due to the changes in vector field f or the map T. For example, if we add some forcing term to the vector field f, a stable fixed point might turn unstable or a limit cycle might appear out of *the blue sky.* A physical example is when we add damping to an otherwise frictionless unforced oscillator: without damping all trajectories are periodic orbits, but with damping they decay to some fixed point.

Here is the traditional approach to study of dynamical systems: We first discover or construct a model for the system in the form of (1) or (2). Sometimes, if we are very lucky, we can come up with analytical solutions and use them to analyze the dynamics, by which, we usually mean finding the attractors, invariant sets, imminent bifurcations and so on. A lot of times, this is not possible and we have to use various estimates or approximation techniques to evaluate the qualitative behavior of the system, for example, construct Lyapunov functions to prove the stability of a fixed point. But most of the times, if we want a quantitative analysis or prediction, we have to employ numerical computation and then extract information from a single or multiple simulated trajectories of the system.

The traditional approach has contributed a lot to our knowledge of dynamical and physical systems, but yet it is falling short in treating the high-dimensional systems that have arisen in various areas of science and technology. Some examples include turbulent flows around aircrafts, climate system of the earth, smart cars and buildings, power networks, and biological and social systems. For some of these systems like turbulent flows, we have fairly accurate state-space models but numerical modeling is very costly or impractical and we have to find a way to blend dynamical analysis with whatever amount of data we have from experiments, observations or simulations. Moreover, unlike the two- or three-dimensional system, the geometric objects and tools in the state space are difficult to realize and utilize and there is need to formulate the problems in a way which is more amenable to computation in large dimensions. For many of these systems like biological networks, there is a considerable amount of uncertainty in the state space models or there is even no model to start with. In this case, we have to use the available data to construct an explicit or implicit model to be utilized in design, control etc.

As a result of these demands, the field of dynamical analysis has started shifting toward a less model-based and more data-driven perspective. This shift is also boosted by the increasing amount of data that is produced by today's powerful computational resources and experimental apparatus. In the next section, we introduce the Koopman operator theory, which is the general framework for connecting data to the state space modeling of dynamical systems.

2 Data-driven viewpoint and the Koopman operator

In the context of dynamical systems, we interpret the data as knowledge of some variable(s) related to the state of the system. A natural way to put this into the mathematical form is to assume that *data is evaluation of functions of the state*. We call these functions *observables* of the system. Let's discuss an example: the unforced motion of an incompressible fluid inside a box constitutes a dynamical system; one way to realize the state space is to think of it as the set of all smooth velocity fields on the flow domain that satisfy the incompressibility condition. The state changes with time according to a rule of evolution which is the Euler equations. Some examples of observables on this system are pressure/vorticity at a given point in the flow domain, velocity at a set of points or the total kinetic energy of the flow. In all these examples, the knowledge of the state, i.e. the velocity field, uniquely determines the value of the observable. We see that this definition allows us to think of the data from most of the flow experiments and simulations as values of observables. We also note that there are some type of data that don't fit the above definition as an observable of the system. For example, the position of a Lagrangian tracer is not an observable of the above system, since it cannot be determined by mere knowledge of the instantaneous velocity field.

Using the above notion, we formulate the data-driven analysis of dynamical systems as follows: Given the knowledge of an observable in the form of time series generated by experiment or simulation, what can we say about the evolution of the state?

Consider the continuous-time dynamical system given in (2). Let $g : S \to \mathbb{R}$ be a real-valued observable of this dynamical system. The collection of all such observables forms a linear vector space. The Koopman operator, denoted by U, is a linear transformation on this vector space given by

$$Ug(x) = g \circ T(x), \tag{5}$$

where $\circ$ denotes the composition operation. The linearity of the Koopman operator follows from the linearity of the composition operation, i.e.,

$$U[g_1 + g_2](x) = [g_1 + g_2] \circ T(x) = g_1 \circ T(x) + g_2 \circ T(x) = Ug_1(x) + Ug_2(x). \tag{6}$$

for any two observables g_1 and g_2. For continuous-time dynamical systems, the definition is slightly different: instead of a single operator, we define a one-parameter semi-group of Koopman operators, denoted by $\{U^t\}_{t\geq 0}$, where each element of this semi-group is given by

$$U^t g(x) = g \circ F^t(x), \tag{7}$$

and $F^t(x)$ is the flow map defined in (3). The linearity of U^t follows in the same way as the discrete-time case. The semi-group property of $\{U^t\}_{t\geq 0}$ follows from the semi-group property of the flow map for autonomous dynamical systems given in (4),

$$U^t U^s g(x) = U^t g \circ F^s(x) = g \circ F^t \circ F^s(x) = g \circ F^{t+s}(x) = U^{t+s} g(x). \tag{8}$$

An schematic representation of the Koopman operator is shown in fig. 1. We can think of the Koopman operator viewpoint as a *lifting* of the dynamics from the state space to the space of observables. The advantage of this lifting is that it provides a linear rule of evolution — given by Koopman operator — while the disadvantage is that the space of observables is infinite dimensional. In the next section, we discuss the spectral theory of the Koopman operator which leads to linear expansions for data generated by nonlinear dynamical systems.

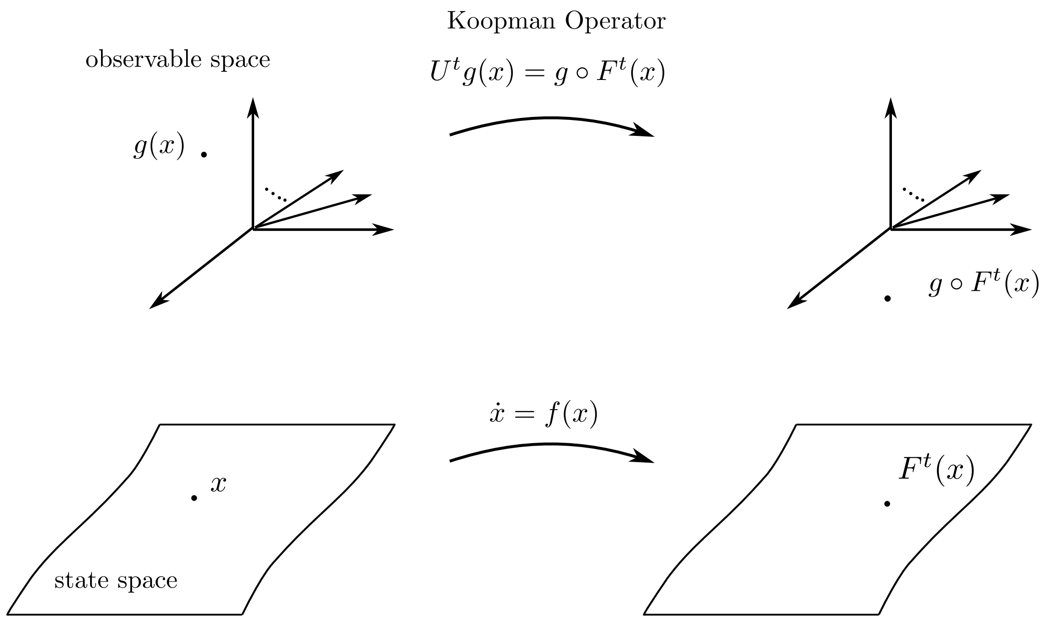

Figure 1: Koopman viewpoint lifts the dynamics from state space to the observable space, where the dynamics is linear but infinite-dimensional.

3 Koopman linear expansion

A naive but somewhat useful way of thinking about linear operators is to imagine them as infinite-dimensional matrices. Then, just like matrices, it is always good to look at the their eigenvalues and eigenvectors since they give a better understanding of how they act on the space of observables. Let $\phi_j : S \to \mathbb{C}$ be a complex-valued observable of the dynamical system in (1) and λ_j a complex number. We call the couple (ϕ_j, λ_j) an eigenfunction-eigenvalue pair of the Koopman operator if they satisfy

$$U^t \phi_j = e^{\lambda_j t} \phi_j. \tag{9}$$

An interesting property of the Koopman eigenfunctions, that we will use later, is that if (ϕ_i, λ_i) and (ϕ_j, λ_j) are eigenfunction-eigenvalue pairs, so is $(\phi_i \cdot \phi_j, \lambda_i + \lambda_j)$, because

$$U^t(\phi_i \cdot \phi_j) = (\phi_i \cdot \phi_j) \circ F^t = (\phi_i \circ F^t) \cdot (\phi_j \circ F^t) = U^t \phi_i \cdot U^t \phi_j = e^{(\lambda_i + \lambda_j)t} \phi_i \cdot \phi_j \ . \tag{10}$$

Let us assume for now that all the observables of the dynamical system lie in the linear span of such Koopman eigenfunctions, that is,

$$g(x) = \sum_{k=0}^{\infty} g_k \phi_k(x), \tag{11}$$

where g_j's are coefficients of expansion. Then we can describe the evolution of observables as

$$U^t g(x) = \sum_{k=0}^{\infty} g_k e^{\lambda_k t} \phi_k(x), \tag{12}$$

which says that the evolution of g has a linear expansion in terms of Koopman eigenfunctions. If we fix the initial state $x = x_0$, we see that the signal generated by measuring g

over a trajectory, which is given by $U^t g(x_0) = g \circ F^t(x_0)$, is sum of (infinite number of) sinusoids and exponentials. This might sound a bit odd for nonlinear systems since sinusoids and exponentials are usually generated by linear systems. But we keep in mind that this expansion has infinite number of terms.

It turns out that Koopman linear expansion in (12) holds for a large class of nonlinear systems, including the ones that have hyperbolic fixed points, limit cycles and tori as attractors. For these systems the spectrum of the Koopman operator consists of only eigenvalues, and their associated eigenfunctions span the space of observables. Now we consider some of these systems in more detail. We borrow these examples from [41] where more details on the regularity of the system and related proofs can be found.

3.1 Examples of linear Koopman expansion for nonlinear systems

1. Limit cycling is a nonlinear property in the sense that there is no linear system ($\dot{x} = Ax$) that can generate a limit cycle. If a limit cycle has time period T, then the signal generated by measuring $g(x)$ while x is moving around the limit cycle is going to be T-periodic. From Fourier analysis, we have

$$g(x(t)) = \sum_{k=0}^{\infty} g_j e^{ik(2\pi/T)t}$$

   where g_j's are the Fourier coefficients. We can construct the eigenfunctions by letting $\phi_k(x(t)) = e^{ik(2\pi/T)t}$, and eigenvalues by $\lambda_k = ik(2\pi/T)$. It is easy to check that (ϕ_k, λ_k) satisfy (9), and the above equation is the Koopman linear expansion of g.

2. Consider a nonlinear system with a *hyperbolic* fixed point, that is, the linearization around the fixed point yields a matrix whose eigenvalues don't lie on the imaginary

axis. There are a few well-known results in dynamical systems theory, such as Hartman-Grobman theorem [64], which state that the nonlinear system is conjugate to a linear system of the same dimension in a neighborhood of the fixed point. To be more precise, they say that there is an invertible coordinate transformation $y = h(x)$ such that the dynamics on y-coordinate is given by $\dot{y} = Ay$ (with the solution $y(t) = e^{At}y(0)$) and such that

$$F^t(x) = h^{-1}\big(e^{At}h(x)\big).$$

In other words, to solve the nonlinear system, we can lift it to y-coordinate, and solve the linear system, and then transform it back to the x-coordinates. We first show the Koopman linear expansion for the linear systems, and then use the conjugacy to derive the expansion for the nonlinear system.

Let $\{v_j\}_{j=1}^n$ and $\{\lambda_j\}_{j=1}^n$ denote the eigenvectors and eigenvalues of A. The Koopman eigenfunctions for the linear system are simply the eigen-coordinates , that is

$$\tilde{\phi}_j(y) =< y, w_j >,$$

where w_j's are normalized eigenvectors of A^*. To see this note that

$$\begin{aligned} U^t\tilde{\phi}_j(y) &=< U^t y, w_j >=< e^{At}y, w_j >=< y, e^{A^*t}w_j > \\ &=< y, e^{\lambda_j^* t}w_j >= e^{\lambda_j t} < y, w_j >= e^{\lambda_j t}\tilde{\phi}_j(y). \end{aligned}$$

It is easy to show that $\phi_j(x) = \tilde{\phi}_j\big(h(x)\big)$ are eigenfunctions of the Koopman operator for the nonlinear system. Other Koopman eigenfunctions can be easily constructed using the algebraic structure noted in (10).

To find the Koopman expansion for the nonlinear system it is easier to further transform y into a decoupled linear system. If the matrix A is diagonalizable and V is the matrix of its eigenvectors, then the state variables of the diagonal system are, not surprisingly, the Koopman eigenfunctions, i.e.,

$$
\begin{aligned}
z &= [z_1, z_2, \ldots, z_n]^T = V^{-1}y = [\tilde{\phi}_1(y), \tilde{\phi}_2(y), \ldots, \tilde{\phi}_n(y)]^T \\
&= [\phi_1(x), \phi_2(x), \ldots, \phi_n(x)]^T.
\end{aligned}
$$

Now consider an observable of the nonlinear dynamical system $g(x) = g\big(h^{-1}(y)\big) = g\big(h^{-1}(Vz)\big) = \tilde{g}(z)$ where $\tilde{g}$ is real analytic in z (and therefore y as well). The Taylor expansion for of this observable in variable z reads

$$
\begin{aligned}
g(x) = \tilde{g}(z) &= \sum_{\{k_1,\ldots,k_n\}\in\mathbb{N}^n} \alpha_{k_1,\ldots,k_n} z_1^{k_1} z_2^{k_2} \ldots z_n^{k_n}, \\
&= \sum_{\{k_1,\ldots,k_n\}\in\mathbb{N}^n} \alpha_{k_1,\ldots,k_n}, \phi_1^{k_1}(x)\phi_2^{k_2}(x) \ldots \phi_n^{k_n}(x),
\end{aligned}
$$

Using the algebraic property of the Koopman eigenfunctions in (10), we can write the Koopman linear expansion of g as

$$
U^t g = \sum_{\{k_1,\ldots,k_n\}\in\mathbb{N}^n} \alpha_{k_1,\ldots,k_n} e^{(k_1\lambda_1+k_2\lambda_2+\ldots+k_n\lambda_n)t} \phi_1^{k_1}\phi_2^{k_2} \ldots \phi_n^{k_n}.
$$

Recall that the original Hartman-Grobman theorem for nonlinear systems is local [64], in the sense that we knew the conjugacy exists for some neighborhood of the fixed point. But the results in [40] has extended the conjugacy to the whole basin of attraction for stable fixed points using the properties of the Koopman eigenfunctions.

3. Now consider the motion in the basin of attraction of a (stable) limit cycle. The Koopman linear expansion for observables on such system can be constructed by, roughly

speaking, combining the above two examples. That is, observables are decomposed into Koopman eigenfunctions, and each Koopman eigenfunction is a product of a periodic component, corresponding to the limit cycling, and a linearly contracting component for the stable motion toward the limit cycle. The development of this expansion is lengthy and can be found in [41].

3.2 Koopman mode decomposition

A lot of times the data that is measured on a dynamical systems comes to us not from a single observable, but from multiple observables. For example, when we are monitoring a power network system, we may have access to the time series of power generation and consumption on several nodes, or in the study of climate dynamics there are recordings of atmospheric temperature at different stations around the globe. We can easily integrate these multiplicity of time-series data into the Koopman operator framework and Koopman linear expansion.

We use $\mathbf{g} : S \to \mathbb{R}^m$ to denote a vector-valued observable, i.e.,

$$\mathbf{g} = \begin{bmatrix} g^1 \\ g^2 \\ \vdots \\ g^m \end{bmatrix}, \quad g^j : S \to \mathbb{R},\ 1 \leq j \leq m.$$

If we apply the linear Koopman expansion (12) to each g^j, we can collect all those expansions into a vector-valued linear expansion for $\mathbf{g}$,

$$U^t \mathbf{g}(x) = \sum_{k=0}^{\infty} \mathbf{g}_k e^{\lambda_k t} \phi_k(x). \tag{13}$$

The above expansion is the *Koopman Mode Decomposition (KMD)* of observable $\mathbf{g}$ and $\mathbf{g}_k$ is called the *Koopman mode* of observable $\mathbf{g}$ at the eigenvalue λ_k. Koopman modes are in fact the projection of observable onto the Koopman eigenfunctions. We can think of $\mathbf{g}_k$ as a structure (or shape) within the data that evolves as $e^{\lambda_k t}$ with time. Let us examine the concept of the Koopman modes in the examples mentioned above. In the context of power networks, we can associate the network instabilities with the Koopman eigenvalues that grow in time, that is $\lambda_k > 0$, and the entries of Koopman mode $\mathbf{g}_k$ give the relative amplitude of each node in unstable growth and hence predict which nodes are most susceptible to breakdown. In the example of climate time series, the Koopman modes of temperature recordings give us the spatial pattern (depending on the location of stations) of temperature change that is proportional to $e^{\lambda_k t}$, and therefore indicate the spots with extreme variations.

In some physical problems, we have a *field of observables*, i.e., an observable that assigns a physical field to each element of the state space. A prominent example is a fluid flow. The pressure field over a subdomain of the flow, or the whole vorticity field, are two examples of field of observable defined on a flow, since the knowledge of the flow state (e.g. instantaneous velocity field) unqiuely determines those fields. We can formalize the notion of a field of observable as a function $\mathbf{g} : (S, \Omega) \to \mathbb{R}$ where Ω is the flow domain and $g(x, z)$ determines the value of the field at point z in the flow domain when the flow is at state x. The Koopman linear expansion for $\mathbf{g}$ would be

$$U^t \mathbf{g}(x, z) = \sum_{k=0}^{\infty} \mathbf{g}_k(z) e^{\lambda_k t} \phi_k(x), \tag{14}$$

where the Koopman mode $\mathbf{g}_k(z)$ is a fixed field by itself, and similar to the Koopman mode vectors, determines a shape function on Ω which grows with the amplitude $e^{\lambda_k t}$ in time. In a fluid flow, the Koopman modes of vorticity, are steady vorticity fields, and the whole flow can be decomposed into such fields. with amplitudes that grow as $e^{\lambda_k t}$.

4 Koopman continuous spectrum and chaos

The major class of dynamical systems for which the Koopman linear expansion *does not hold* is the class of chaotic dynamical systems. It turns out that for these systems, the eigenfunctions of the Koopman operator (even if they exist) do not span the space of observables and we cannot decompose fluctuations of the system all into exponentials and sinusoids. In such cases the Koopman operator usually possesses a *continuous* spectrum. The continuous spectrum of the Koopman operator coincides with the concept of power spectrum for a stationary stochastic process if we think of evolving observables as stochastic processes [15]. Here we review this notion briefly and focus on connection with stochastic processes. Both discrete and continuous spectral forms are unified through the notion of Koopman spectral measure which we do not discuss here but it can be found in [4,38,39,44].

A remarkable property of many smooth dynamical systems is that in the asymptotic regime they naturally admit a probabilistic description. In a more precise statement, many attractors of dynamical systems support a measure which is invariant under the dynamics: Let A be the attractor of the dynamical system, and let μ be the invariant measure of the system. We also assume $\mu(A) = 1$ which means that we can think of (A, μ) as a sample space (with some suitable choice of events). The notion of dynamic invariance for measure μ means $\mu(B) = \mu\big(F^{-t}(B)\big)$ for any measurable $B \subset A$. Now under these conditions, a (measurable) observable $g : A \to \mathbb{R}$ becomes a *random variable*, that is, the values of g take a meaningful distribution on $\mathbb{R}$. The distribution function of this random variable is then given by

$$P_g(a) := P\bigg(g(x) < a\bigg) = \mu\bigg(g^{-1}\big((-\infty, a)\big)\bigg). \tag{15}$$

For such a random variable, the expected value can be computed as

$$\mathbb{E}[g] = \int_{\mathbb{R}} a \; dP_g(a) = \int_A g(x) \; d\mu(x) \tag{16}$$

Similar to above, one can show that $U^t g$ for any value of t is also a random variable with the same distribution, and therefore $\{U^t g\}_{t\in\mathbb{R}}$ is an identically distributed stochastic process. Moreover, the measure-preserving property also makes this process strongly stationary (proved by looking at joint probabilities of $(g, U^t g)$, then $(g, U^t g, U^s g)$ etc.). The spectral theory of stationary stochastic processes [15] provides a spectral expansion for the covariance of this stochastic process, that is,

$$\mathbb{E}\Big[(g - \mathbb{E}[g])(U^t g - \mathbb{E}[U^t g])\Big] = \int_{\mathbb{R}} e^{i\omega t} d\mathcal{P}_g(\omega). \tag{17}$$

The term $\mathcal{P}_g(\omega)$ is called the power spectral distribution of the stochastic process, and if we think of ω as frequency here (because of the complex exponential term which represents oscillatory motion), then $\mathcal{P}_g\big([\omega_1, \omega_2]\big)$ gives an idea of how much of the energy of the process is contained within the frequency interval $[\omega_1, \omega_2]$. It is often assumed that $\mathcal{P}_g$ is an absolutely continuous measure and therefore it can be represented by a density function, that is, $d\mathcal{P}_g(\omega) = \rho_g(\omega)d\omega$ with ρ_g being called the *the power spectral density* of the stochastic process. Another name for ρ_g is *Koopman spectral density of observable g*.

Note that unlike discrete spectrum there are no eigenfunctions associated with the continuous spectrum and therefore there are no Koopman modes — except the trivial mode associated with the zero Koopman eigenvalue. Nevertheless, the spectrum fully characterizes all that can be discovered about the dynamics of the system through the lens of observable g (see Theorem 1 and following remark in [33]). For more discussion on continuous spectrum and its computation see [4, 33, 38]. We also note that chaos in measure-preserving

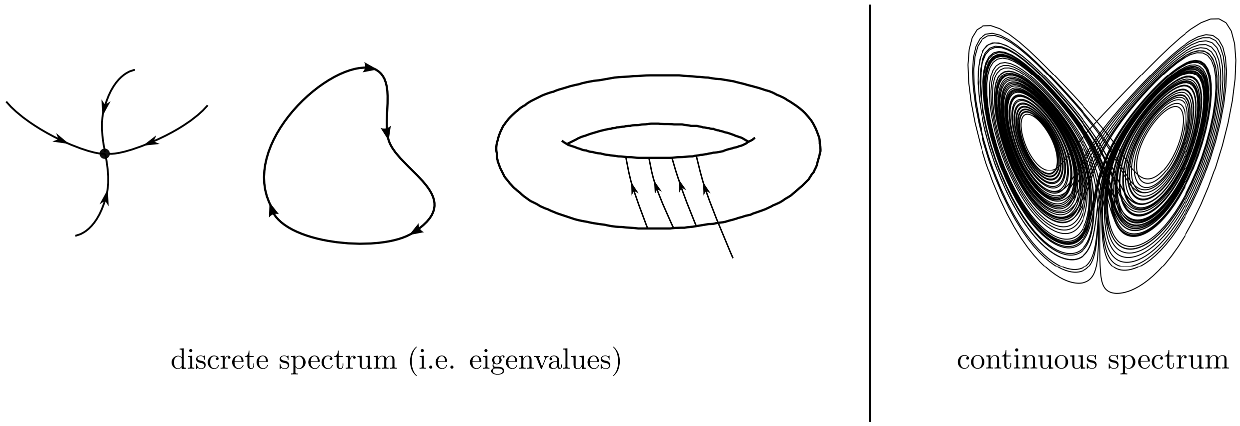

Figure 2: Koopman Mode Decomposition fully describes the evolution of observables on systems with Koopman discrete spectrum, but not for chaotic systems which have continuous spectrum.

system is associated with continuous spectrum, but continuous spectrum can also be seen in non-chaotic systems. See the cautionary tale in [41].

What is more interesting is that some systems possess *mixed spectra* which is a combination of eigenvalues and continuous spectrum. For these systems the evolution of a generic observable is composed of two parts: a quasi-periodic part associated with eigenvalues and eigenfunctions and a fully chaotic part corresponding to continuous spectrum. As such, the linear expansion and the Koopman modes docomposition apply to a part of the data. This is specially appealing for modeling real-world systems where strong periodic and quasi-periodic trends coexist with chaos and turbulence. Some classical examples of systems with mixed spectra are analyzed in [8, 43], and more applied examples from fluid mechanics and climate data are studied in [4, 5].

5 History of Koopman operator theory

The Koopman operator formalism originated in the early work of Bernard Koopman in 1931 [29]. He introduced the the linear transformation that we now call the Koopman operator, and realized that this transformation is unitary for Hamiltonian dynamical systems (the "U" notation comes from unitary property). This observation by Koopman inspired John von Neumann to give the first proof for a precise formulation of ergodic hypothesis, known as *mean ergodic theorem* [24]. In the next year, Koopman and von Neumann wrote a paper together, in which they introduced the notion of the *spectrum of a dynamical system*, i.e. the spectrum of the associated Koopman operator, and noted the connection between chaotic behavior and the continuous part of the Koopman spectrum [30].

For several decades after the work of Koopman and Von Neumann, the notion of Koopman operator was mostly limited to the study of measure-preserving systems; you could find it as the unitary operator in the proof of the mean ergodic theorem or discussions on the spectrum of measure-preserving dynamical systems [36, 50]. It seldom appeared in other applied fields until it was brought back to the general scene of dynamical system by two articles in 2004 and 2005 [38, 43]. The first paper showed how we can construct important objects like the invariant sets in high-dimensional state spaces from data. It also emphasized the role of nontrivial eigenvalues of the Koopman operators to detect the periodic trends of dynamics amidst chaotic data. The second paper discussed the spectral properties of the Koopman operator further, and introduced the notion of Koopman modes.

In 2009, the idea of Koopman modes was applied to a complex fluid flow, namely, a jet in a cross flow [52]. This work showed the promise of KMD in capturing the dynamically relevant structures in the flow and their associated time scales. Unlike other decomposition techniques in flows, KMD combined two advantageous properties: it made a clear connection between the measurements in the physical domain and the dynamics of state space (unlike proper orthogonal decomposition), and it was completely data-driven (unlike the global mode analysis). The work in [52] also showed that KMD can be computed through a numerical decomposition technique known as *Dynamic Mode Decomposition (DMD)* [54]. Since then, KMD and DMD have become immensely popular in analyzing the nonlinear flows [7, 27, 46, 47, 53–57]. A review of the Koopman theory in the context of fluid flows can be found in [39].

The extent of KMD applications for data-driven analysis has enormously grown in other fields too. Some of these applications include model reduction and fault detection in energy systems for buildings [17, 18], coherency identification and stability assessment in power networks [60, 61], hybrid mechanical systems [19], extracting spatio-temporal patterns of brain activity [9], background detection and object tracking in videos [16, 35], design of algorithmic trade strategies in finance [37], analysis of numerical algorithms [14] and traffic data [6].

Parallel to the applications, the computation of Koopman spectral properties (modes, eigenfunctions and eigenvalues) has also seen a lot of major advancements. For post-transient systems, the Koopman eigenvalues lie on the unit circle and Fourier analysis techniques can be used to find the Koopman spectrum and modes [4, 43]. There is also another rigorous route to approximate the Koopman operator of measure-preserving systems through the classical periodic approximation [20, 21]. For dissipative systems, the Koopman spectral properties can be computed using a theoretical algorithm known as *Generalized Laplace Analysis* [44, 45].

In applications involving transient beahvior, DMD is the popular technique for computation of Koopman spectrum from data. In [65], the idea of Extended DMD was introduced for general computation of Koopman spectrum by sampling the state space and using a dictionary of observables. The works in [12] and [63] discussed the linear algebraic properties of the algorithm and suggested new variations for better performance and wider applications. New variants of DMD were also introduced in [34] to unravel multi-time-scale phenomena and in [51] to account for linear input to the dynamical system. Due to constant growth in the size of the available data, new alterations or improvements of DMD are also devised to handle larger data sets [23,26], different sampling techniques [11,23,63] and noise [13,25]. The convergence of DMD-type algorithms for computation of Koopman spectrum was discussed in [3,31,42].

The ultimate goal of many data analysis techniques is to provide information that can be used to predict and manipulate a system to our benefit. Application of the Koopman operator techniques to data-driven prediction and control are just being developed, with a few-year lag behind the above work. This lag is perhaps due to the need to account for the effect of input in the formalism, but promising results have already appeared in this line of research. The work in [10] showed an example of optimal controller which was designed based on a finite-dimensional Koopman linear expansion of nonlinear dynamics. The works in [58,59] have developed a framework to build state estimators for nonlinear systems based on Koopman expansions. More recent works, have shown successful examples of Koopman linear predictors for nonlinear systems [32], and optimal controllers of Hamiltonian systems designed based on Koopman eigenfunctions [28]. More recent applications include feedback control of fluid flows via using Koopman linear models computed from data in a model-predictive control framework [2, 48, 49].

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