Persistence of Excitation for Koopman Operator Represented Dynamical Systems

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Abstract—The increase in complexity of engineered systems and naturally occurring systems, coupled with increasingly data-driven representations of these systems motivates the need for design of experiment frameworks for nonlinear system identification. In the case of a general nonlinear autonomous system (without inputs or control), designing an experiment for identification relies on the selection of persistently exciting flows and their corresponding initial conditions. This work investigates persistence of excitation conditions for discrete-time nonlinear systems that can be represented using Koopman operators. The Koopman operator presents a linear lifted representation of the evolution of a nonlinear system over a space of observable functions. We use this framework to derive spectral conditions for persistence of excitation, relating classical notions of persistence of excitation to the spectral properties of initial conditions, seen through the lens of Koopman observable functions. We illustrate these concepts on a repressilator circuit, a classical biological system from the field of synthetic biology, to motivate the proper selection of initial conditions. We show that when the rank properties of the flow’s spectra are degenerate, the trained Koopman operator does not produce robust predictions on test data.

I. INTRODUCTION

Many physical systems exhibit phenomena with unknown governing dynamics. These systems can be high dimensional and partially modeled or completely unstudied. Emergent complex systems, biological networks, Internet of Things infrastructure models, smart-cities, and social networks are all examples of dynamically evolving systems that frequently require system identification. Discovering the governing equations for these systems has the potential to accelerate design and control to improve robustness of system performance, as well as to diagnose the source of faults or failure modes. The challenge is understanding how to design experiments, both observational and interventional, to ensure that data generated characterizing a system of interest is sufficiently informative.

Many algorithms have been proposed to address the problem of discovering governing equations for a system. Recently, an emerging set of operator-theoretic tools have gained traction, centered on discovering linear representations of nonlinear dynamical systems in a lifted space of coordinates. These tools are actually a rebirth of ideas from the early 1930s. Nearly 100 years ago, B. O. Koopman [1] proposed an operator theoretic framework for a class of nonlinear systems which provided a linear frame of reference for the evolution of a function of its state. The Koopman method was piloted by Mezic, Rowley, and Kutz, and has subsequently been a topic of research, both numerically and theoretically [2], [3], [4], [5], [5], [6], [7], [8], [9], [10].

Computational algorithms in Koopman operator theory center on discovering practical finite approximations to high dimensional or infinite dimensional coordinate spaces. With the increasing abundance in state-space data from myriad dynamical systems, recent years have seen resurgence of operator-theoretic methods alongside insurgence of data-driven methods like Dynamic Mode Decomposition (DMD) ([11], [12]). First introduced in [4] and [13], DMD gained popularity beyond fluids’ domain due to its purely data-driven nature. The Koopman operator was shown to be closely related to DMD by [14] and [15]. Ever since, numerous contributions have been made to data-driven derivations and approximations of Koopman theory ([10], [16], [17] and a variety of fields have seen applications of this ([18], [19], [20]) including control theory ([21], [22], [23], [7], [9]). Most recently, Deep-Learning based DMD (DeepDMD) discoveries of Koopman operators have been performed ([6], [24]) and demonstrated convergence with lesser data by wielding a wider variety of observables. The data-driven nature of Koopman operator theory brings up questions on how to maximize the quality of the system input to extract as much information as possible about global dynamics [10], [25].

The notion of informativity, or information gain, is a classical concept for formalizing how state or input parameters relate to the utility of a set of data for system identification. In biological network modeling and discovery, designing an informative set of experimental parameters are central to models of success. There is a growing effort to automate data collection and experimental workflows, using a combination of machine learning and system identification tools. Unfortunately, there are few measures relating the informativity of a particular experiment and the data it generates to the identifiability of the model class being used. This is especially true in nonlinear system identification, where the governing equations utilize hypothesis driven models, centered on assumptions regarding model class [17] and parametric priors.

A control theoretic framework is currently lacking for certifying the identifiability of a Koopman model in terms of the persistence of excitation or sufficient richness of a dynamical system. Such a framework would be invaluable in designing an efficient yet substantial set of experiments to bootstrap models and governing equations from real-world
observations. Nonlinear systems lack a ubiquitous framework imposing excitation requirements on signals including that of their spectrum (absence of transfer functions) like the failure of applicability of a Pseudo-Random Binary Sequence [26]. However, the coordinate transformation to a linear space in the Koopman framework can be exploited to utilise the vast literature on system identifiability. "Informative" data is often understood by concepts of Sufficient Richness (SR) or Persistence of Excitation (PE). First introduced in [27], PE is "not (yet) consistently defined" ([28]) and often used interchangeably with SR ([29], [30]). In short, these concepts convey the ability of a signal to excite a system at frequencies besides its zeros and distinguish transfer functions unless they are the same. As shown later, the definition of PE adhered in [31] (and most recently in [32]) can be derived mathematically and ties this intuition with the definition of PE adhered in [31] (and most recently in [32]).

The present work aims to deduce the concept of richness, or persistence of excitation, in inputs for identifiability of certain nonlinear systems using a Koopman Operator approach. This is prescribed by a condition imposed on a control input in terms of its spectrum and is demonstrated by a design of experiments application in terms of initial conditions of a multi-dimensional system in synthetic biology. A repressilator is a genetic oscillatory circuit first reported by [33]. We consider the canonical three gene model, where each gene is expressing a protein that represses another downstream gene in the network. With the right feedback strengths, this system admits a limit cycle.

This paper is organised as follows: Section II introduces the Koopman operator framework and how a nonlinear dynamical system can be represented or approximated as a linear state space model defined on a function space of observables. Section IV states the motivation for this work and formulates the problem of nonlinear system identifiability in terms of persistence of excitation. Section V follows with a series of definitions and a proposition derived for nonlinear systems for computationally certifying the persistence of excitation of a designed (or fixed) input. Section VI illustrates the use of persistence of excitation results to inform the design of initial conditions for simulated experiments on two biological systems: a bi-stable genetic switch and a three node oscillator, the notable repressilator.

II. KOOPMAN OPERATOR THEORY

In 1931, Koopman showed the existence of a coordinate transformation \( \psi \in \mathbb{R}^{n_L} \) and a corresponding unitary operator \( \mathcal{K} : \mathbb{R}^{n_L} \to \mathbb{R}^{n_L} \) for any Hamiltonian (non-dissipative) dynamical systems. He showed that the operator \( \mathcal{K} \) and observable \( \psi \) could be used to represent the time evolution of the underlying Hamiltonian system as a linear time-invariant system. This idea has been developed and generalized to other classes of nonlinear systems in recent years ([2], [3], [5], etc.), in the effort to find global representations instead of local approximations.

A discrete-time nonlinear dynamical system with state \( x_t \in \mathbb{R}^n \) at time \( t \in \mathbb{N} \) under \( f : \mathcal{M} \to \mathcal{M} \) can be represented as:

\[
x_{t+1} = f(x_t)
\]

Then functions \( \psi \triangleq \{ \psi_i \}_{i=1}^{\infty} \in \mathcal{F}, i \in \mathbb{Z}_+ \) are called "observables," and represent a mapping from the state-space into a lifted set of coordinates. For example, \( \psi \) may be a scalar (or vector-valued) observable comprised of nonlinearities, weighted combinations of the state, such as \( \psi_1(x_t) = x_{1,t}, \psi_2(x_t) = x_{3,5,1}, \psi_3(x_t) = x_{2,t}x_{n,1}^2 \). The true Koopman observables are often approximated in numerical Koopman learning algorithms like extended DMD (eDMD), DeepDMD, and Hankel dynamic mode decomposition using functions which define a generic basis on a Hilbert function space, e.g. radial basis functions (RBFs), Hermite polynomials, or a combination of such basis functions in DeepDMD ([6], [24]).

In the case of an analytical \( f(x_t) \), we know from [7] that there exists a countably infinite or finite dimensional Koopman operator \( \mathcal{K} \) that acts linearly on the observable \( \psi : \mathcal{M} \to \mathbb{R} \) under composition \( \circ \). Specifically, given two observable functions \( \psi_1, \psi_2 \) and constants \( \alpha, \beta \). This effectivity propagates any \( \psi(x_t) \) forward in time as:

\[
\mathcal{K}(\alpha \psi_1 + \beta \psi_2) = \alpha \psi_1 \circ f + \beta \psi_2 \circ f = \alpha \mathcal{K}(\psi_1) + \beta \mathcal{K}(\psi_2)
\]

Specifically, we have for \( \alpha = 1 \) and a given observable function \( \psi(x) \) the famous Koopman equation,

\[
\mathcal{K}\psi(x_t) = \psi \circ f(x) = \psi(f(x_t)) = \psi(x_{t+1}),
\]

which says that the action of the Koopman operator on an observable function is equivalent to the action of the observable function on the vector field of the state.

From the above transient behaviour, it can be seen that this itself is a dynamical system in the space of observables whose time-evolution is governed by an infinite-dimensional operator that preserves the essence of \( \mathcal{K} \). The transformation from \( \psi(f(x)) \) to \( \psi(x) \) is frequently referred to as "lifting" since the observable \( \psi(x) \in \mathbb{R}^{n_L} \) usually has dimension \( n_L \geq n \). This is not always the case, but [8] shows that the observables define an expansion of the nonlinearities in the governing equations.

In [3] it was shown that the spectra and eigenspace of the Koopman operator lend an alternative geometric perspective into the dynamics of the system. Specifically, let \( \{ \phi_j \}_{j=1}^{\infty} \in \mathcal{F}, j \in \mathbb{Z}_+ \), be the (Koopman) eigenfunctions and \( \{ \lambda_j \}_{j=1}^{\infty} \in \mathbb{R} \) be the respective (Koopman) eigenvalues:

\[
\mathcal{K}\phi_j = \lambda_j \phi_j
\]

The eigenfunctions define a basis for the observable space [3]; the observable \( \psi \) can expanded as

\[
\psi = \sum_{j=1}^{\infty} v_j \phi_j,
\]

where each \( v_j = \langle \psi, \phi_j \rangle \in \mathbb{R} \) is called (Koopman) eigen-mode of the observable \( \psi \) associated with the eigenfunction
\[ \phi_j \text{ and is a projection of } \psi \text{ onto } \phi_j. \] Using (3) in (2), we can now write
\[ \psi(x_{t+1}) = K\psi(x_t) = \sum_{j=1}^{\infty} \lambda_j \phi_j(x_t) = \sum_{j=1}^{\infty} \lambda_j \psi_j(x_t) \]

From the above, we see that flow map of the observable can be expressed in terms of the Koopman spectrum as:
\[ \psi(x_t) = \sum_{j=1}^{\infty} \lambda_j^{-t} \phi_j(x_t) \]  

When \( \lambda_j > 1 \), the eigenmode is unstable and represents a divergent mode in the flow map, away from the initial condition \( \psi(x_0) \). When \( \lambda_j \leq 1 \), the eigenmode is stable and the eigenfunction defines a forward and reverse invariant set.

### A. Finite Dimensional Approximations

It was shown in [3] that the spectrum for \( K \) can be continuous or discrete. Chaotic systems frequently have continuous spectra which are studied for the purposes of model reduction. Some systems demonstrate mixed spectra which can be separated out into discrete and continuous parts. Accordingly, reduced order approximations can be made ([34], [35]). If eigenfunctions are finite in number, then \( \{ \phi_j \}_{j=1}^{n_L} < \infty \) span a \( K \)-invariant subspace. Now, all \( \{ \phi_j \}_{j=1}^{n_L} : M \to \mathbb{R} \) can be stacked together as a vector \( \phi : M \to \mathbb{R}^{n_L} \), similar to a stack of Fourier or polynomial basis.

\[ D \triangleq \text{span}(\{ \phi_j(x_t) \}_{j=1}^{n_L}) \]

\[ \phi(x_t) := \begin{bmatrix} \phi_1(x_t) \\ \phi_2(x_t) \\ \vdots \\ \phi_p(x_t) \end{bmatrix} \quad (6) \]

If \( D \subset F \), observables can be projected onto \( D \) as explained in [3]. Here, it is assumed that \( D = F \) and all observables \( \{ \psi_j \}_{j=1}^{n_L} \) can now be represented in eigen-basis (6), also stacked as a vector of the same dimension as:

\[ \psi(x_t) := \begin{bmatrix} \psi_1(x_t) \\ \psi_2(x_t) \\ \vdots \\ \psi_p(x_t) \end{bmatrix} = V \phi(x_t) \quad (7) \]

Then, \( D \) can be used for a finite-dimensional, representations of \( K \) as a matrix \( K \in \mathbb{R}^{n_L \times n_L} \) and the time-evolution in \( D \) based on (5) is presented:

\[ \psi(x_t) = V \begin{bmatrix} \lambda_1^{t-t_0} & 0 & \cdots & 0 \\ 0 & \lambda_2^{t-t_0} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_p^{t-t_0} \end{bmatrix} \phi(x_{t_0}) \quad (8) \]

Detailed mathematical formulations can be found in aforementioned literature. It can be seen that multiple initial-time and final-time pairs can be given as input-output in successive columns, this is how various computational implementations like that used in this paper are structured.

### III. KOOPMAN INPUT OUTPUT THEORY

Our study of the dynamical system (1), ultimately will require treating the initial condition as an input signal (via a Dirac delta function) to the system. For clarity, we introduce the notion of an input-Koopman operator here, as well as the notion of the Koopman transfer function of a nonlinear system. Given a discrete-time nonlinear system with analytic vector field \( f(x,u) \) and control input \( u_t \in \mathbb{R}^m \), we write the dynamics of the system as:

\[ x_{t+1} = f(x_t, u_t) \]

\[ y_t = h(x_t) \]

[23] showed that an observable \( \psi : \mathcal{M} \times \mathbb{R}^m \to \mathbb{R}^{n_L} \) can lift the above system to \( F \) such that:

\[ K\psi(x_t, u_t) = \psi(f(x_t, u_t), u_{t+1}) = \psi(x_{t+1}, u_{t+1}) \]

For an exogenous memoryless input, [9] demonstrated that the above can be modified by splitting \( \psi(x,u) \) into components \( \psi_x(x) \) and \( \psi_u(x,u) \), where \( \psi_x(x) \) is a stacked vector valued observable of all scalar valued observable functions from \( \psi(x,u) \) that do not depend on \( u \), and \( \psi_u(x,u) \) is a stacked vector valued observable of all remaining terms. This results in the decomposed representation

\[ \psi_x(x_{t+1}) = K_x \psi_x(x_t) + K_u \psi_u(z_t) \]

\[ y_t = W h \psi(x_t, u_t) \]

where \( \psi_u(z_t) \equiv \psi_u(x, u) \) and \( z_t \) is a stacked vector of all multivariate terms of \( u_t \) and \( x_t \). This is a representation of the nonlinear system dynamics that is linear in the lifted state observable \( \psi_x(x) \) and the lifted input-state mixture observable \( \psi_u(x,u) \). We thus can define the Koopman discrete time transfer function as:

\[ G_K(z) = W h(zI - K_x)^{-1} K_u \quad (10) \]

where we have assumed that \( y_t = \psi_x(x_t) \). The zeros and the poles of the transfer function are defined in the usual manner, but with respect to the transformations on the state \( \psi_x(x_t) \) and input \( \psi_u(z(u_t)) \). A continuous time analogue of the discrete-time Koopman operator is readily derived using the Koopman generator, rather than the Koopman operator. In this work, we primarily concern ourselves with the design of experiments and selection of conditions to
ensure identifiability of $G_K(z)$. What are the conditions under which it is possible to estimate a input-output transfer function model of the system given either 1) a fixed choice of data, or 2) the opportunity to design the collection of data to ensure identifiability?

IV. PROBLEM STATEMENT

As suggested by the exposition in the previous section, a primary application of Koopman operator theory is its use in data-driven applications to discover the governing equations or to learn a model to simulate dynamical system response. The use of Koopman operator theory to represent nonlinear systems has enabled new operator-theoretic approaches for nonlinear control [36]. The advent of data-driven algorithms for training Koopman operators [6], [24], [10], [37] raises the question of how to design experiments or the collection of data to ensure identifiability of the Koopman operator. In the absence of control, a system’s model identifiability is a Boolean property that is either satisfied or not [31]. However, when considering the design of experiments via the initial condition of a dynamical system $x_{t_0}$, or the design of a control perturbation $u_t$, identifiability can be viewed as a function of the design.

In classical system identification theory, the design of an input or initial condition to guarantee identifiability is framed in terms of PE. One of the merits of a Koopman operator representation is that it provides a representation of a nonlinear system in linear coordinates. This allows us to rigorously formulate the question of how to design an initial condition that guarantees identifiability of the model. Specifically, we consider two problems:

Problem 1 (Identifiability of a Nonlinear System with Fixed Initial Conditions). Given a discrete time-invariant autonomous nonlinear system of the form

$$x_{t+1} = f(x_t), \quad x_{t_0} \in X_0$$
$$y_t = h(x_t) \equiv x_t$$

(11)

determine if the model $f(x)$ can be uniquely identified from the continuously sampled data stream $x(t)$ and the set of initial conditions $X_0$.

This problem is generally difficult to solve, as it couples the problem of nonlinear function regression of $f(x)$ and $h(x)$ with the requirement of characterizing the richness of a set of fixed initial conditions. This problem is equivalent to the nonlinear state-space realization problem, given a single initial condition or set of initial conditions $X_0$. The other variant of this problem is where the initial conditions are design parameters in an experiment and can be set by the user.

Problem 2 (Identifiability of a Nonlinear System with Designed Initial Conditions). Given a continuous time-invariant autonomous nonlinear system of the form and the design choice of initial conditions $X_0$

$$x_{t+1} = f(x_t), \quad x_{t_0} \in X_0$$
$$y_t = h(x_t) \equiv x_t$$

(12)

Find $X_0$ that guarantees the model $f(x)$ can be uniquely identified from the continuously sampled data stream $x(t)$.

This variant of the problem presumably has more degrees of freedom, namely $\dim(x(t_0)|X_0) = n|X_0|$ to be precise. However, the challenge is to relate identifiability of the model to the initial condition, which for an unknown $f(x)$ is inherently difficult. We now use the input-Koopman framework derived in the previous sections to reformulate the problem with a linear Koopman representation. The recasting of the problem will permit extension of classical identifiability notions such as the design of sufficiently rich input signals or initial conditions, or persistence of excitation.

V. PERSISTENCE OF EXCITATION CONDITIONS FOR NONLINEAR SYSTEMS WITH KOOPMAN OPERATORS

Our contribution in this paper is to formulate the problem of identifiability with fixed and designed initial conditions using the method of Koopman. Once we have formulated the problem in the Koopman operator theoretic framework, we derive computational certificates for persistence of excitation for fixed or designed initial conditions. This leads to an algorithm for selection of the initial conditions of a dynamical system given $x_{t_0}$. In both scenarios, we treat the system’s initial condition as an input. Given a nonlinear discrete-time dynamic system of the form

$$x_{t+1} = f(x_t)$$
$$y_t = h(x_t)$$

(13)

where $x \in \mathbb{R}^n$ and $t \in \mathbb{Z}$, the Koopman equation for the corresponding system defines the action of an operator $K$ on a vector valued observable $\psi \in \mathbb{R}^{n_u}$ acting on the state $x_t \in \mathbb{R}^n$, namely

$$\psi(f(x)) = K\psi(x_t)$$

Then, (9) can be represented with initial state $\psi(x_{t_0})$ as an input:

$$\psi(x_{t+1}) = K\psi(x_t) + \psi(x_{t_0})\delta(t - t_0)$$

We thus model the initial condition as a Dirac delta input to the dynamical system. Accordingly, we will abuse notation slightly and define the input of the system as $\psi(x_{t_0})\delta(t - t_0) \equiv \varphi(u_t)$, which yields the classic input-state Koopman representation for a nonlinear system

$$\psi(x_{t+1}) = K\psi(x_t) + \varphi(u_t).$$

(14)

Notice that the state vector $\psi_x(x) \in \mathbb{R}^{n_u}$ is a vector observable function on which the Koopman operator acts as a linear operator to update the state. In essence, by defining an appropriate 'lifting' or 'observable' function, we can treat the problem as a classical linear identifiability problem, with additional caveats imposed by the presence of the nonlinearities in $\psi_x(x)$ and $\psi_{u}(x, u)$. As there are multiple definitions in the literature for persistence of excitation [31], [30], we chose a definition that enables relating identifiability to the initial condition of a transfer function. We pose an
extension of the definition from [31] which is that of SR from [30], but in the Koopman framework.

**Definition 1** (Persistence of Excitation). A quasi-stationary discrete time observable \( \varphi(u_t) \in \mathbb{R}^{n_L} \) is said to be persistently exciting of order \( N \in \mathbb{Z}_+ \) if the covariance matrix \( \mathcal{R}_\varphi(N) \) is positive definite:

\[
\mathcal{R}_\varphi(N) := \begin{bmatrix}
R_\varphi(0) & \cdots & R_\varphi(N-1) \\
\vdots & \ddots & \vdots \\
R_\varphi(-(N-1)) & \cdots & R_\varphi(0)
\end{bmatrix}
\]  

(15)

where \( R_\varphi(k), k \in \mathbb{Z} \) is the auto-covariance of \( \varphi(u_t) \) formulated as:

\[
R_\varphi(k) := \mathbb{E}[\varphi(u_t)\varphi(u_{t+k})^T],
\]

(16)

and \( \mathbb{E} \) denotes the expectation operator. The above definition has been referred to as sufficient richness in [30] as well. Positive semi-definiteness of \( \mathcal{R}_\varphi(N) \) can easily be proved. By substituting the R.H.S. of (16) in (15) we obtain:

\[
\mathcal{R}_\varphi(N) = \mathbb{E}\left\{ \left[ \varphi(u_{t+1}) \right] \left[ \left[ \varphi(u_{t+1}) \right]^T, \cdots, \left[ \varphi(u_{t+N}) \right]^T \right] \right\}
\]

(17)

Defining \( v \triangleq \left[ \left[ \varphi(u_{t+1}) \right]^T, \cdots, \left[ \varphi(u_{t+N}) \right]^T \right]^T \), the above becomes:

\[
\mathcal{R}_\varphi(N) = \mathbb{E}[vv^T]
\]

\[
\forall q = [q_1^T, \ldots, q_k^T], q_k \in \mathbb{R}^{n_L} \setminus \{0\}
\]

\[
q^T \mathcal{R}_\varphi(N) q = \mathbb{E}[\|q^T v\|^2_2]
\]

(17)

Hence, \( \mathcal{R}_\varphi(N) \) is positive semi-definite. From the Herglotz Theorem, any function \( R_\varphi(k) \) defined on integers is positive semi-definite if and only if it has a Bochner representation (can be represented as the inverse Fourier transform of a unique Spectral Measure \( S_\varphi(\nu) \) on a circle:

\[
R_\varphi(k) = \int_{-\pi}^{\pi} e^{ik\nu} S_\varphi(\nu) d\nu
\]

(17)

If \( R_\varphi(k) \) is a scalar, \( S_\varphi(\nu) \) is its power spectrum as pointed out in [30] and [29]. Alternate definitions have been mentioned in literature but the following definition and result elucidates how persistence of excitation of an initial condition for a dynamical system can be related to the Koopman transfer function.

**Definition 2.** Given system (7), we say an initial condition \( x_0 \) treated as a Dirac delta signal \( \delta(x_0) \) is persistently exciting of Koopman-order \( n_L \) if it is persistently exciting for a state-inclusive Koopman operator \( \mathcal{K} \in \mathbb{R}^{n_L} \) of order \( n_L \) satisfying

\[
\psi(x_{t+1}) = \begin{bmatrix}
x_{t+1} \\
\varphi(x_{t+1})
\end{bmatrix} = \begin{bmatrix}
K_{xx} & K_{xf} \\
K_{fx} & K_{ff}
\end{bmatrix} \begin{bmatrix}
x_t \\
\varphi(x_t)
\end{bmatrix} + \delta_t \psi(x_0).
\]

(18)

**Proposition 1.** The initial condition \( x_0 \) is persistently exciting for the nonlinear dynamical system (7) if and only if the Fourier transform of the auto-covariance matrix \( R_\varphi(k) \)

\[
S_\varphi(\omega) = \sum_{k=-\infty}^{\infty} R_\varphi(k)e^{-ik\omega}
\]

has \( n_L \) distinct frequencies \( \omega_1, \ldots, \omega_{n_L} \) where \( S_\varphi(\omega) \) does not vanish, i.e. \( n_L \) positive spectral lines.

**Proof.** Let the dimension of the lifted space and corresponding Koopman vector valued observable \( \psi(x) \) be denoted as \( n_L \). We write the initial condition as an input to the nonlinear dynamical system (1), respectively. It suffices to demonstrate the equivalence of the persistence of excitation of \( \psi(x_0) \), up to order \( n_L \), to the linear independence of spectral lines for the power spectral density \( S_\varphi(\omega) \).

We know that the spectral measure \( S_\varphi(\omega) \) of \( R_\varphi(k) \) would be a positive semi-definite, symmetric matrix of bounded measures, symmetric over all \( \omega \) since the observable elements \( \varphi(x) \) are all real valued. We have by the definition of the spectral power measure that

\[
R_\varphi(k) = \int_{-\pi}^{\pi} e^{i\omega k} S_\varphi(\omega) d\omega
\]

(19)

Since the spectral measure is bounded almost everywhere, the monotone convergence theorem allows us to write

\[
\sum_{l,m=1}^{N} q_l^T \int_{-\pi}^{\pi} e^{i(m-l)\omega} S_\varphi(\omega) d\omega q_m \geq 0,
\]

after swapping the finite sum with limiting sums

\[
\int_{-\pi}^{\pi} \left( \sum_{l,m=1}^{N} q_l^T e^{-i\omega l} S_\varphi(\omega) e^{i\omega m} q_m \right) d\omega \geq 0
\]

and distributing sums across the integrand, we obtain

\[
\int_{-\pi}^{\pi} \left( \sum_{l=1}^{N} q_l^T e^{-i\omega l} S_\varphi(\omega) \left( \sum_{m=1}^{N} e^{i\omega m} q_m \right) \right) d\omega \geq 0
\]

(20)

Defining filters \( Q(e^{i\omega}) \triangleq \sum_{k=1}^{N} e^{ik\omega} q_k \), the above becomes:

\[
\int_{-\pi}^{\pi} \left( Q^*(e^{i\omega}) S_\varphi(\omega) Q(e^{i\omega}) \right) d\omega \geq 0
\]

Thus, positive definiteness of \( S_\varphi(\omega) \) only holds if and only if \( R_\varphi(k) \) is positive definite. But positive definiteness of \( S_\varphi(\omega) \) holds if and only if there are at least \( n_L \) frequencies in which the integrand does not vanish, namely \( n_L \) frequencies where

\[
\sum_{k=1}^{N} e^{ik\omega} q_k
\]
is in the orthogonal complement of the null space of $S_p(\omega)$. This proves the result.

From our simulation studies, we found that most initial conditions are persistently exciting up to order $n_L$, for their respective Koopman operator and dynamical system. If we consider the design problem of selecting an initial condition $x_0$ such that $\psi(x_0)$ is persistently exciting, or a set of $\Psi(x_0)$ are persistently exciting of Koopman-order $n_L$, we can express the problem in terms of the positive definiteness of $R_p(N)$, adjusting the signal $\psi(x_0)$ or more generally the timing of the input to ensure the positive definiteness of the auto-covariance matrix. Alternatively, when working the timing of the input to ensure the positive definiteness can express the problem in terms of the positive definiteness $x$ respective Koopman operator and dynamical system. If we $n$ is in the orthogonal complement of the null space of $S_p(\omega)$.

VI. PERSISTENCE OF EXCITATION OF DIFFERENT INITIAL CONDITIONS FOR A REPRESSILATOR GENETIC CIRCUIT MODEL

A. The Repressilator

The repressilator is a classical genetic circuit used in synthetic biology to implement circadian rhythms or synthetic oscillations. The architecture is that of a 3 node Goodwin oscillator, with three genes that produce proteins or mRNA that serve to repress the downstream or target gene’s function. Each gene represses its downstream target, with the final gene repressing the original gene to form a cycle of negative feedback. When the gain of the individual genes are balanced with respect to each other [38], the genetic circuit admits a limit cycle in the phase portrait and a single basin of attraction surrounding the origin.

There are many models of the repressilator, with varying degrees of complexity and intricacy to capture the underlying biophysical dynamics. We consider a simplified three dimensional model from the first experimental implementation of the repressilator [33], that captures the limit cycle and basin of attraction, to study the role of the initial condition in persistence of excitation of the nonlinear system. Consider the model:

$$m_{t+1,(i)} = \frac{-m_{t,(i)} + \alpha}{1 + p_{t,(j)}^I} + \alpha_0$$

$$p_{t+1,(i)} = -\beta(p_{t,(i)} - m_{t,(i)})$$

$$(i,j) = \{([lacI],[cI]),([tetR],[lacI]),([cI],[tetR])\}$$

$$n = 2, \ \alpha_0 = 0, \ \alpha = 100, \ \beta = 1$$

An example set of commonly used initial concentrations is $1, 0, 0, 0, 0, 0$ nM for LacI, $\lambda$-cI, TetR, mLacI, mLCI, and mTetR. We model the degradation and dilution rate of all proteins as a lump term with average kinetic rate $\delta = 0.5$. This model is a discrete time adaptation of the model presented in [33], [39], imposing a zero-order hold assumption on a modest sampling time-scale of every 15 minutes (the maturation time of a single protein). Fig. 1a and 1c shows simulations (solid lines) of the repressilator from different initial conditions. The repressilator exhibits a strongly attracting limit cycle and a single unstable equilibrium point at the origin. Several initial conditions in the phase space mapped through the observable function have low gain, specifically those within $B_1(0)$ (unit ball in $\mathbb{R}^6$). These observable functions have low gain power spectra with spectral lines on the magnitude of numerical noise. We noted that these initial conditions, when mapped through higher order polynomials lead to overfitting, due to the vanishing of the signal in higher-order terms.

We considered training the repressilator model with initial conditions drawn from two different regions of the phase.
Fig. 2: The repressilator trained from outside a unit ball centered at 0 and predicted from another basin of attraction using the Koopman operator with eDMD. (a) States oscillating with time as simulated (solid lines). Koopman operator trained up to \( t = 25 \) for prediction (dotted lines) then onward. (b) Simulated (solid) trajectories growing into limit cycles and prediction (dotted) of the limit cycles. (c) Simulated (solid) and predicted (dotted) trajectory form another basin of attraction. (d) Spectrum of initial conditions. (e) Spectrum of trajectories up-to \( t = 25 \) used to train the Koopman Operator space. First, initial conditions within the unit disc centered at the unstable equilibrium point (solid lines in fig. 1b) and secondly, initial conditions outside the unit disc centered at the same point (solid lines in fig. 2b). Interestingly, we found that the power spectrum of the flow of trajectories initiated from within the unit disc had degenerate power spectra, indicating a rank deficiency as illustrated in fig. 1c. In contrast, the power spectrum of the flow of trajectories initiated from outside the unit disc were full rank of order \( n_L = 19 \) as in fig. 2c. We simulated using 6 initial conditions from one basin of attraction and evaluated test predictions using initial conditions from another basin. For example, we would train within the unit disc (fig. 1b) or outside it (fig. 2b) and evaluate predictions of the Koopman operator for trajectories initiated outside that basin of attraction (fig. 1c and 2c respectively). In the case where the spectra of the flow trajectories had full rank (a Koopman operator trained on data initiated from outside the unit disc in fig. 2b), both the training and test predictions aligned with the ground truth data. When the spectra of the flow trajectories was degenerate, the Koopman operator predictions would diverge unstably from the ground truth data (dotted vs solid lines in fig. 1b and 1c).

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