Efficient Identification of Linear Evolutions in Nonlinear Vector Fields: Koopman Invariant Subspaces

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Abstract— **This paper presents a data-driven approach to identify finite-dimensional Koopman invariant subspaces and eigenfunctions of the Koopman operator. Given a dictionary of functions and a collection of data snapshots of the dynamical system, we rely on the Extended Dynamic Mode Decomposition (EDMD) method to approximate the Koopman operator. We start by establishing that, if a function in the space generated by the dictionary evolves linearly according to the dynamics, then it must correspond to an eigenvector of the matrix obtained by EDMD. A counterexample shows that this necessary condition is however not sufficient. We then propose a necessary and sufficient condition for the identification of linear evolutions according to the dynamics based on the application of EDMD forward and backward in time. Due to the complexity of checking this condition, we propose an alternative characterization based on the identification of the largest Koopman invariant subspace in the span of the dictionary. This leads us to introduce the Symmetric Subspace Decomposition strategy to identify linear evolutions using efficient linear algebraic methods. Various simulations illustrate our results.**

I. Introduction

Mathematical modeling of physical phenomena is at the heart of every problem considered in science and engineering. In particular, modeling of evolutions in time plays a crucial role in prediction and control. State-space models are one of the main ways to represent dynamical systems, usually leading to nonlinear models whose complexity grows with the dimension of the state space. Moreover, the nonlinear character makes the prediction of these dynamical systems difficult. This has spurred interest in finding alternative ways to describe dynamical behavior. The Koopman operator is a linear but generally infinite-dimensional operator that represents an autonomous dynamical system. Despite its linearity, the infinite-dimensional nature of the Koopman operator prevents one from implementing it using digital computers. To circumvent this issue one can find finite-dimensional subspaces that are invariant under the application of the Koopman operator and analyze the dynamical behavior on those subspaces. This is the problem considered here.

Literature Review: The eigenfunctions of the Koopman operator [1], [2] evolve linearly in time, and hence its eigendecomposition can be used to analyze and predict the behavior of dynamical systems [3]–[5]. This can simplify identification [6] and control [7]–[11] of nonlinear systems. Traditional roadblocks to the widespread use of the Koopman operator have been its infinite-dimensional nature and the lack of practical methods to find representations for it. One can circumvent these issues using data-driven methods such as Dynamic Mode Decomposition (DMD) [12] and Extended Dynamic Mode Decomposition (EDMD) [13] to approximate the projection of the Koopman operator onto a finite-dimensional subspace.

DMD was initially introduced as a method to extract dynamic information from time series data gathered from fluid flows under the assumption that the collected data are governed by a linear time-invariant mapping [12]. Later, it was generalized to work with non-sequential data snapshots, and its connection with the Koopman operator was further explained [14], including extensions [15], [16] that can work with noisy data. EDMD is a variation of DMD specifically designed to find finite-dimensional approximations of the Koopman operator [13]. In this method, the snapshots go through a dictionary of functions to form the dictionary snapshots. The EDMD algorithm finds a linear relationship between the dictionary snapshots by solving a least squares problem. The work [17] shows the convergence of the EDMD algorithm to the Koopman operator as the number of dictionary elements and data snapshots goes to infinity. In our recent work [18], we have proposed a noise-resilient counterpart of EDMD using element-wise weighted total least squares method to handle noisy data. Even though DMD and EDMD provide linear models for the original system, those linear models are not useful for long term prediction of the behavior of nonlinear systems since the models are not exact. As a result, finding dictionaries that span finite-dimensional Koopman invariant subspaces is of utmost importance. The works [19], [20] present methods to perform this task using neural networks. Moreover, since the eigenfunctions span a Koopman invariant subspace, one can find the eigenfunctions empirically using [21], [22] and form the dictionary using the calculated eigenfunctions. The aforementioned methods do not present theoretical guarantees for the calculated functions to be the eigenfunctions of the Koopman operator.

Statement of Contributions: We develop data-driven methods to identify finite-dimensional subspaces that are invariant under the application of the Koopman operator. The proposed methods are able to identify Koopman eigenfunctions, i.e., functions that evolve linearly in time according to the (generally nonlinear) vector field. We start by showing that being identified by the EDMD method is a necessary but not sufficient condition for a function to evolve linearly according to the dynamics. Motivated by this observation, we develop a necessary and sufficient condition for functions to evolve linearly based on the application of EDMD forward

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and backward in time. One can use this characterization as a tool to find the functions with linear evolution based on the available data. The identified functions are not necessarily Koopman eigenfunctions, since they are guaranteed to evolve linearly based on the available data snapshots, and might not do so over the whole state space. To circumvent this issue, we provide a necessary and almost sure sufficient condition to identify the Koopman eigenfunctions under the assumption that the dictionary functions are continuous and the set of sampled initial conditions converges to a dense subset of the compact state space with probability 1. The characterization based on the application of EDMD forward and backward in time requires the computation and comparison of the eigendecomposition of two potentially large matrices. This can be cumbersome for large dictionaries, since one needs to compare every eigenpair in the eigendecomposition of the matrices. To alleviate this issue, we propose the Symmetric Subspace Decomposition (SSD) algorithm, a strategy that uses the fact that any subdictionary in the span of the original dictionary of functions can be characterized by a matrix. Using this fact, we prune the dictionary at each iteration to remove the parts that do not correspond to linear evolutions. We prove that the SSD algorithm is equivalent to the method based on application of EDMD forward and backward in time. Simulations illustrate the versatility of the proposed approach. The proofs are omitted due to space constraints and will appear elsewhere[1].

II. Preliminaries

Here, we introduce the Koopman operator [5] and Extended Dynamic Mode Decomposition (EDMD) [13].

A. Koopman Operator

Consider a discrete-time autonomous dynamical system over a state space $\mathcal{M} \subseteq \mathbb{R}^n$ defined by a map $T : \mathcal{M} \to \mathcal{M}$,

$$x^+ = T(x), \tag{1}$$

The Koopman operator $\mathcal{K} : \mathcal{F} \to \mathcal{F}$ is defined as

$$\mathcal{K}(f) = f \circ T, \tag{2}$$

where $\mathcal{F}$ is a linear space of functions (also known as observables) defined on $\mathcal{M}$ which is closed under composition with T, i.e, $f \circ T \in \mathcal{F}$ for every $f \in \mathcal{F}$. Typically, $\mathcal{F} = L_2(\mu)$, where μ is a positive measure on $\mathcal{M}$. Linearity of $\mathcal{F}$ results in the linearity of the Koopman operator on the functional space $\mathcal{F}$, i.e., for functions $f_1, f_2 \in \mathcal{F}$ and c_1, c_2 in the field on which the linear space $\mathcal{F}$ is defined (typically $\mathbb{C}$), we have

$$\mathcal{K}(c_1 f_1 + c_2 f_2) = c_1 \mathcal{K}(f_1) + c_2 \mathcal{K}(f_2). \tag{3}$$

Since $\mathcal{K}$ is a linear operator, one can naturally define its eigendecomposition. The function $\phi \in \mathcal{F}$ is called an *eigenfunction* of $\mathcal{K}$ associated with *eigenvalue* λ if

$$\mathcal{K}(\phi) = \lambda\phi.$$

Since the states of the system are real, the complex eigenfunctions of the Koopman operator form a pair, i.e., if ϕ is a complex eigenfunction with eigenvalue λ, then $\bar{\phi}$ is an eigenfunction with eigenvalue $\bar{\lambda}$.

One can observe that the eigenfunctions of the Koopman operator evolve linearly in time. Formally,

$$\phi(x^+) = (\phi \circ T)(x) = \mathcal{K}(\phi)(x) = \lambda\phi(x).$$

The linear evolution of the eigenfunctions in conjunction with the spatial linearity of the operator (3) makes the Koopman operator a powerful tool in analyzing the behavior of the dynamical system (1), since one can use the spectral properties of the operator to predict the temporal behavior of the underlying system.

It is worth highlighting some difference between the operator-theoretic and conventional state-space viewpoints. The Koopman operator acts on functions in $\mathcal{F}$, as opposed to the dynamical system (1), which defines the evolution of states in $\mathcal{M}$. The Koopman operator is linear even if the dynamical system is nonlinear. In addition, despite its linearity, the Koopman operator captures the global characteristics of the underlying dynamical system as opposed to standard linearization techniques which are only valid locally.

B. Extended Dynamic Mode Decomposition

The Koopman operator is generally infinite-dimensional, which impedes the use of conventional linear methods to compute the operator explicitly. To circumvent this issue, one can find finite-dimensional approximations for the Koopman operator using data-driven methods such as Extended Dynamic Mode Decomposition (EDMD). In this method, the data snapshots acquired from the system are lifted to a higher-dimensional space using a dictionary of functions and then the projection of the Koopman operator onto the span of the dictionary can be found by minimizing the sum of squares error. Formally, let $X, Y \in \mathbb{R}^{N \times n}$ be N data snapshots of the dynamical system (1): if x_i^T and y_i^T denote the ith rows of X and Y, respectively, this means that

$$y_i = T(x_i),\ i \in \{1, \ldots, N\}.$$

Furthermore, let $D : \mathbb{R}^n \to \mathbb{R}^{1 \times N_d}$ be a dictionary of N_d functions belonging to $\mathcal{F}$, with $D(x) = [d_1(x), \ldots, d_{N_d}(x)]$. Any function in the span of the dictionary can be written as $f(x) = D(x)v$, with $v \in \mathbb{C}^{N_d}$. Note that v fully characterizes f. We define the action of the dictionary on data matrices as

$$D(X) := [D(x_1)^T, \ldots, D(x_N)^T]^T,$$

[1]Throughout the paper, we employ the following notation. We denote the sets of natural, real, nonnegative real, and complex numbers by $\mathbb{N}$, $\mathbb{R}$, $\mathbb{R}_{\geq 0}$, and $\mathbb{C}$ respectively. For a matrix $A \in \mathbb{C}^{m \times n}$ we denote its transpose, complex conjugate, conjugate transpose, Frobenius norm, pseudo-inverse, and range space by A^T, $\bar{A}$, A^H, $\|A\|_F$, $A^\dagger$, $\mathcal{R}(A)$ respectively. Moreover, if $n = m$ we use A^{-1} to denote the inverse of A. For matrices $A \in \mathbb{C}^{m \times n}$ and $B \in \mathbb{C}^{m \times d}$, we denote by $[A, B] \in \mathbb{C}^{m \times (n+d)}$ the matrix created by concatenating A and B. For $v \in \mathbb{C}^n$, we use $\mathrm{Re}(v)$ and $\mathrm{Im}(v)$ to denote its real and imaginary parts, and define its 2-norm as $\|v\|_2 := \sqrt{v^H v}$. Given $v_1, \ldots, v_k \in \mathbb{C}^n$, $\mathrm{span}\{v_1, \ldots, v_k\}$ denotes the set comprised of all vectors in the form of $c_1 v_1 + \cdots + c_n v_n$, with $c_1, \ldots, c_n \in \mathbb{C}$. Given sets A and B, we use $A \cap B$ and $A \cup B$ to denote their intersection and union, respectively. Also, $A \subseteq B$ means that A is a subset of B. For functions $f : B \to A$ and $g : C \to B$, $f \circ g : C \to A$ represents their composition. We refer by class-$\mathcal{K}$ to the set consisting of all continuous strictly increasing functions $\alpha : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ with $\alpha(0) = 0$. Given a positive measure μ on $\mathcal{M}$, we use $L_2(\mu)$ to denote the set of all measurable functions $f : \mathcal{M} \to \mathbb{C}$ with $\int_{\mathcal{M}} f(x)^H f(x)\,\mathrm{d}\mu(x) < \infty$.

where $x_i^T, i \in \{1, \dots, N\}$ denotes the ith row of X.

The EDMD method approximates the projection of the Koopman operator on the span of the dictionary by minimizing the residual in sum of squares form $\|D(Y) - D(X)K\|_F^2$. This yields the matrix $K_{\mathrm{EDMD}}(D(X), D(Y))$ as a finite-dimensional approximation of $\mathcal{K}$. In closed form,

$$K_{\mathrm{EDMD}}(D(X), D(Y)) = D(X)^\dagger D(Y). \quad (4)$$

We simply use K_{EDMD} when the context is clear.

Inspecting (4) reveals that, due to the pseudo-inverse, the computational cost of EDMD grows as the number of data snapshots increases. The work [23] presents a kernel method approach to resolve this issue. A closer look at (4) reveals the dependence of EDMD on the choice of the dictionary. If $\|D(Y) - D(X)K_{\mathrm{EDMD}}\|_F \neq 0$, the EDMD algorithm loses some information about the operator. However, even under this circumstance, EDMD can capture important information regarding the operator if the dictionary is sufficiently rich.

III. Problem Statement

As mentioned in Section II-B, the approximation derived by the EDMD algorithm heavily relies on the choice of dictionary. Moreover, a larger dictionary is not necessarily better. For instance, the states of a linear dynamical system form a perfect dictionary for the system, i.e., $D(X) = X$, $D(Y) = Y$, and since the system is linear we have

$$\min_K \|D(Y) - D(X)K\|_F^2 = \min_K \|Y - XK\|_F^2 = 0.$$

This means that the error associated with the EDMD approximation is zero and the solution is exact. However, one can add a nonlinear function to the dictionary which leads to a nonzero approximation error and hence an inexact solution.

Motivated by these observations, the goal of the paper is, given a dictionary, to find the largest invariant subspace of functions under the Koopman operator in the span of the dictionary. In other words, we seek to prune the dictionary in order to ensure that the remaining functions evolve linearly. Formally, we consider the dynamical system (1) where $T : \mathcal{M} \to \mathcal{M}$ is a continuous mapping, and we aim to find the maximal subspace in the span of the dictionary which is invariant under the application of the Koopman operator. In the other words, given a dictionary comprised of functions $d_1(x), \dots, d_{N_d}(x)$, we intend to find the functions $\tilde{d}_1(x), \dots, \tilde{d}_m(x)$ such that

$$\mathrm{span}\{\tilde{d}_1, \dots, \tilde{d}_m\} \subseteq \mathrm{span}\{d_1, \dots, d_{N_d}\}, \quad (5)$$

and, if $f \in \mathrm{span}\{\tilde{d}_1, \dots, \tilde{d}_m\}$ then

$$\mathcal{K}(f) \in \mathrm{span}\{\tilde{d}_1, \dots, \tilde{d}_m\}. \quad (6)$$

Moreover, $\mathrm{span}\{\tilde{d}_1, \dots, \tilde{d}_m\}$ must be maximal in the sense that for any dictionary of functions $\{\bar{d}_1, \dots, \bar{d}_k\}$ that satisfies properties presented in (5) and (6), we must have

$$\mathrm{span}\{\bar{d}_1, \dots, \bar{d}_k\} \subseteq \mathrm{span}\{\tilde{d}_1, \dots, \tilde{d}_m\}.$$

To tackle this task, we make the following assumption regarding the dictionary snapshots.

Assumption III.1: (Full Rank Dictionary Matrices): The matrices $D(X)$ and $D(Y)$ have full column rank. □

Assumption III.1 requires the dictionary functions to be linearly independent and the set of initial conditions to be rich enough to capture the characteristics of the vector field.

Since we rely on the EDMD algorithm throughout the paper and this method is not designed specifically to work with noisy data, we assume access to data with sufficiently high signal-to-noise ratio. Our results are indeed stated for the noise-free data case, which may require to preprocess the data before using the proposed algorithms.

IV. Capabilities and Limitations of EDMD

In this section, we study the advantages and disadvantages of the EDMD method regarding the identification of the eigenfunctions of the Koopman operator. The next result shows that the EDMD method captures the linear evolution of functions in the span of the dictionary even if this space is not invariant under the Koopman operator.

Lemma IV.1: (EDMD Captures the Linear Evolution of Functions in the Span of the Dictionary): Let $f(x) = D(x)v$, with $v \in \mathbb{C}^{N_d} \setminus \{0\}$, be a function with linear evolution based on the existing data, i.e., there exists $\lambda \in \mathbb{C}$ such that $D(Y)v = \lambda D(X)v$. Then under Assumption III.1, the vector v is an eigenvector of K_{EDMD} with eigenvalue λ. □

Based on the definition of the eigenfunctions of the Koopman operator, one can derive the following result.

Corollary IV.2: (EDMD Captures the Eigenfunctions of the Koopman operator in the Span of the Dictionary): Suppose that Assumption III.1 holds and $f(x) = D(x)v$, with $v \in \mathbb{C}^{N_d} \setminus \{0\}$, is an eigenfunction of the Koopman operator with eigenvalue $\lambda \in \mathbb{C}$. Then, v is an eigenvector of K_{EDMD} with eigenvalue λ. □

Lemma IV.1 and Corollary IV.2 provide a necessary condition for functions in the span of the dictionary to evolve linearly in time according to the dynamics. However, the aforementioned condition is not sufficient.

Example IV.3: Consider the scalar linear system $x^+ = 2x$ with state space $\mathcal{M} = [1, \infty)$ and dictionary $D(x) = [x, x^2 + x^3]$. Moreover, assume that we gather data in a way that Assumption III.1 holds. By Corollary IV.2, the EDMD algorithm identifies the true eigenfunction $f_1(x) = x$ with eigenvalue $\lambda_1 = 2$. Additionally, it identifies $f_2(x) = a_1 x + a_2(x^2 + x^3)$ as another eigenfunction with eigenvalue λ_2. Note that $a_2 \neq 0$ since the matrix K_{EDMD} defined in (4) must be full rank as a consequence of Assumption III.1. Now suppose that f_2 is an eigenfunction of the Koopman operator. Then, for every $x \in \mathcal{M}$ we have

$$\begin{aligned} &f_2(x^+) = \lambda_2 f_2(x) \\ &\Rightarrow 2a_1 x + a_2(4x^2 + 8x^3) = \lambda_2\big(a_1 x + a_2(x^2 + x^3)\big) \\ &\Rightarrow a_1(2 - \lambda_2) + a_2(4 - \lambda_2)x + a_2(8 - \lambda_2)x^2 = 0 \end{aligned}$$

The last equality can hold for at most two $x \in \mathcal{M}$ and hence f_2 cannot be an eigenfunction of the Koopman operator. □

Even though the necessary conditions in Lemma IV.1 and Corollary IV.2 identify N_d potential eigenfunctions, one still needs to check the effect of the dynamics on these functions to identify the ones that evolve linearly in time. This procedure is not practical for large N_d. As a result, finding necessary and sufficient conditions for a function to evolve linearly according the dynamics is desirable.

V. Identification of Koopman Invariant Subspaces

Here, we present two methods to identify linear evolutions in the data and consequently find Koopman invariant subspaces and eigenfunctions.

A. Forward and Backward EDMD

A simple observation reveals that if a function evolves linearly forward in time, then it also evolves linearly backward in time. The following result uses this observation to provide a necessary and sufficient condition for functions in the span of dictionary to evolve linearly according the available data.

Theorem V.1: (Identification of Linear Evolutions by Forward and Backward EDMD): Let Assumption III.1 hold. Then $v \in \mathbb{C}^{N_d} \setminus \{0\}$ is an eigenvector of $K_f = K_{\mathrm{EDMD}}(D(X), D(Y))$ with eigenvalue $\lambda \in \mathbb{C} \setminus \{0\}$, and an eigenvector for $K_b = K_{\mathrm{EDMD}}(D(Y), D(X))$ with eigenvalue λ^{-1} if and only if $D(Y)v = \lambda D(X)v$. □

According to Theorem V.1, one can find functions that evolve linearly in time *based on the available data* by performing the EDMD forward and backward in time, and comparing the eigenvectors and corresponding eigenvalues. However, this does not mean that they are eigenfunctions, as it is not guaranteed that they evolve linearly in time starting from anywhere in the state space. Before addressing this point, we make an assumption on the density of the sampling.

Given N data snapshots, we define S_N as the set comprised of the columns of X^T. Note that the size of X grows as we gather more data. Consequently, $S_N \subset S_{N+1}$ for every $N \in \mathbb{N}$. Next, we introduce an assumption regarding the state space and sampling procedure.

Assumption V.2: (Almost sure dense sampling): The state space $\mathcal{M}$ is compact and there exists a class-$\mathcal{K}$ function α such that, for every $N \in \mathbb{N}$,

$$\forall m \in \mathcal{M},\ \exists x \in S_N \text{ such that } \|m - x\|_2 \leq \alpha\Big(\frac{1}{N}\Big)$$

holds with probability p_N, where $\lim_{N\to\infty} p_N = 1$. □

The compactness of $\mathcal{M}$ holds in most practical cases (either because the state space is bounded itself or because attention is limited to a specific bounded range). Moreover, one is only able to gather data from bounded sets due to the limitation in the range of the sensors. In addition, most conventional random samplings satisfy Assumption V.2.

Theorem V.3: (Identification of Koopman Eigenfunctions by Forward and Backward EDMD): Suppose that Assumption III.1 holds and let $K_f^N = K_{\mathrm{EDMD}}(D(X), D(Y))$, $K_b^N = K_{\mathrm{EDMD}}(D(Y), D(X))$ for $X, Y \in \mathbb{R}^{N \times n}$. Given $v \in \mathbb{C}^{N_d} \setminus \{0\}$ and $\lambda \in \mathbb{C} \setminus \{0\}$, let $f(x) := D(x)v$. Then,

(a) If f is an eigenfunction of the Koopman operator with eigenvalue λ, then v is an eigenvector of K_f^N with eigenvalue λ and an eigenvector of K_b^N with eigenvalue λ^{-1}.

(b) Conversely, and assuming the dictionary functions are continuous and Assumption V.2 holds, if v is an eigenvector of K_f^N with eigenvalue λ and an eigenvector of K_b^N with eigenvalue λ^{-1} for every $N \geq N_d$, then f is an eigenfunction of the Koopman operator with probability 1. □

One can use Theorem V.1 to identify the functions that evolve linearly in time according to the available data. However, this procedure requires one to deal with potentially complex-valued eigenvectors and their corresponding eigenvalues, which can be cumbersome for large dictionaries. Since eigenfunctions come in complex-conjugate pairs, they can be described instead by their real and imaginary parts. We develop such methods next.

B. Symmetric Subspace Decomposition

The eigenfunctions of the Koopman operator identified with the methods proposed in Section V-A can be employed to generate an invariant subspace. Here, we follow this path in the reverse order, i.e., we first find an invariant Koopman subspace using efficient linear algebraic methods and then use it to identify eigenfunctions of the Koopman operator.

We start with a dictionary $D : \mathbb{R}^n \to \mathbb{R}^{1 \times N_d}$ of N_d linearly independent functions and use it to construct a dictionary $\tilde{D} : \mathbb{R}^n \to \mathbb{R}^{1 \times \tilde{N}_d}$ with $\tilde{N}_d$ linearly independent functions in the span of D and defining a linear evolution based on available data. Formally, suppose that Assumption III.1 holds for D and data snapshots X, Y. Then the new dictionary $\tilde{D}$ must satisfy

$$\tilde{D}(Y) = \tilde{D}(X)K \tag{7}$$

for some $K \in \mathbb{R}^{\tilde{N}_d \times \tilde{N}_d}$. Moreover, since the elements of $\tilde{D}$ must lie in the span of the original dictionary, one can write $\tilde{D}(x) = D(x)C$, for all $x \in \mathcal{M}$, for some $C \in \mathbb{R}^{N_d \times \tilde{N}_d}$ with full column rank. Under Assumption III.1, this implies that $\tilde{D}(X)$, $\tilde{D}(Y)$, and K are also full rank. Consequently,

$$\mathcal{R}(D(X)C) = \mathcal{R}(D(Y)C).$$

Since one can fully obtain the new dictionary from the original one with the matrix C, our problem can be equivalently formulated as that of finding the matrix C with the maximum possible number of columns, full column rank, and such that $\mathcal{R}(D(X)C) = \mathcal{R}(D(Y)C)$. To tackle this task, we propose the "Symmetric Subspace Decomposition" strategy described in Algorithm 1. In this strategy, the function $\mathrm{null}([A_i, B_i])$ returns a basis for the null space of $[A_i, B_i]$, and if the null space only contains the zero vector, it returns $\emptyset$. Moreover, Z_i^A and Z_i^B have the same size.

The next result discusses the convergence of Algorithm 1 and the properties of its output.

Theorem V.4: (Symmetric Subspace Decomposition): Algorithm 1 has the following properties:

(a) Stops after a finite number of iterations[2];

[2] The most time-consuming calculation in Algorithm 1 is Step 4, which can be done via Singular Value Decomposition with complexity $O(NN_d^2)$, considering that $N \gg N_d$. Moreover, the algorithm terminates after at most N_d iterations. Consequently, the complexity is $O(NN_d^3)$, which is linear in the number of the dictionary snapshots N.

Algorithm 1 Symmetric Subspace Decomposition

Initialization
$i \leftarrow 1$, $A_1 \leftarrow D(X)$, $B_1 \leftarrow D(Y)$, $C \leftarrow I_{N_d}$
while 1 **do**
  $\begin{bmatrix} Z_i^A \\ Z_i^B \end{bmatrix} \leftarrow \text{null}([A_i, B_i])$ ▷ Basis for the null space
  if $\text{null}([A_i, B_i]) = \emptyset$ **then**
    return 0 ▷ The basis does not exist
    break
  end if
  $n_i^A \leftarrow$ number of rows of Z_i^A
  $m_i^A \leftarrow$ number of columns of Z_i^A
  if $n_i^A \leq m_i^A$ **then**
    return C ▷ The procedure is complete
    break
  end if
  $C \leftarrow C Z_i^A$ ▷ Reducing the subspace
  $A_{i+1} \leftarrow A_i Z_i^A$, $B_{i+1} \leftarrow B_i Z_i^A$, $i \leftarrow i+1$
end while

(b) Returns a matrix C which is either 0 or has full column rank and satisfies $\mathcal{R}(D(X)C) = \mathcal{R}(D(Y)C)$;

(c) The subspace $\mathcal{R}(D(X)C)$ is maximal, i.e., for any matrix E with $\mathcal{R}(D(X)E) = \mathcal{R}(D(Y)E)$, we have $\mathcal{R}(D(X)E) \subseteq \mathcal{R}(D(X)C)$ and $\mathcal{R}(E) \subseteq \mathcal{R}(C)$. □

After finding C, one simply can find the dictionary by setting $\tilde{D}(x) = D(x)C$. Since $\mathcal{R}(D(X)C) = \mathcal{R}(D(Y)C)$, we have $\mathcal{R}(\tilde{D}(X)) = \mathcal{R}(\tilde{D}(Y))$, and consequently, one can find the matrix K satisfying (7). Given an eigenvector v of K with eigenvalue λ and using (7), we have $\tilde{D}(Y)v = \lambda \tilde{D}(X)v$ and consequently the function $f(x) := \tilde{D}(x)v$ evolves linearly according to the data snapshots. The eigendecomposition of K not only fully characterizes the linear evolutions in $\tilde{D}(X)$ and $\tilde{D}(Y)$ but also fully characterizes the linear evolutions in $D(X)$ and $D(Y)$ according to the next result.

Theorem V.5: (Identification of Linear Evolutions using Algorithm 1): Suppose that Assumption III.1 holds and let C be the output of the Symmetric Subspace Decomposition strategy. Let $\tilde{D} : \mathbb{R}^n \to \mathbb{R}^{1 \times \tilde{N}_d}$ the dictionary defined by $\tilde{D}(x) = D(x)C$, $x \in \mathcal{M}$. Then $\tilde{D}(Y)w = \lambda \tilde{D}(X)w$ for some $\lambda \in \mathbb{C}$ and $w \in \mathbb{C}^{\tilde{N}_d}$ if and only if there exists $v \in \mathbb{C}^{N_d}$ such that $D(Y)v = \lambda D(X)v$. In addition $v = Cw$. □

Theorem V.5 establishes an alternative necessary and sufficient condition to the one presented in Theorem V.1 for the identification of linear evolutions in data matrices. One can state a result similar to Theorem V.3 regarding the identification of eigenfunctions with the output provided by Algorithm 1, but we omit it here for reasons of space.

Remark V.6: (Approximation of Koopman Invariant Subspaces): One also can modify Algorithm 1 to approximate Koopman invariant subspaces when the span of the dictionary does not contain enough eigenfunctions to capture the behavior of the system. Specifically, at each iteration of Algorithm 1, the subspace reduction is performed based on the rank deficiency in $[A_i, B_i]$. In order to approximate the Koopman invariant subspaces, one can replace $[A_i, B_i]$ by a rank-deficient matrix. Let $\sigma_1 \geq \cdots \geq \sigma_{l_i} \geq 0$ be the singular values of $[A_i, B_i] \in \mathbb{R}^{N \times l_i}$. Also, let k_i be the minimum integer in $\{1, \dots, l_i\}$ such that

$$\frac{\sum_{j=k_i}^{l_i} \sigma_j}{\sum_{j=1}^{l_i} \sigma_j} \leq \epsilon, \quad (8)$$

where ϵ is a design parameter tuning the accuracy of the approximation. The modified algorithm employs a rank-deficient matrix close to $[A_i, B_i]$ by setting $\sigma_{k_i}, \dots, \sigma_{l_i}$ equal to zero in the singular value decomposition of $[A_i, B_i]$. □

VI. Simulation Results

Here we demonstrate the effectiveness of the Symmetric Subspace Decomposition strategy, cf. Algorithm 1, regarding the identification of Koopman invariant subspaces.

Example VI.1: (Linear System): Consider the second order-linear system $x^+ = Ax$, where $x = [x_1, x_2]^T$ and

$$A = \begin{bmatrix} 0.8 & 0.5 \\ -0.5 & 0.8 \end{bmatrix}.$$

We use $D(x) = [1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1x_2^2, x_1^2x_2, x_2^3]$ with $N_d = 9$. One can use direct calculation to verify that the dictionary $\tilde{D}(x) = [1, x_1, x_2, x_1^2, x_1x_2, x_2^2]$ spans the maximal subspace in the span of $D(x)$ that is invariant under application of the Koopman operator. We use $N = 10^4$ samples uniformly taken from $\mathcal{M} = [-2, 2] \times [-2, 2]$. After applying Algorithm 1, we find a new dictionary comprised of 6 functions which spans the same subspace as $\tilde{D}(x)$, i.e., the algorithm successfully identifies the maximal Koopman invariant subspace. The algorithm identifies the real-valued eigenfunctions $f_1(x) = 1$ and $f_2(x) = x_1^2 + x_2^2$ with eigenvalues $\lambda_1 = 1$ and $\lambda_2 = 0.89$. The algorithm also identifies two pairs of complex valued eigenfunctions. We illustrate one eigenfunction from each pair in Figs. 1 and 2.

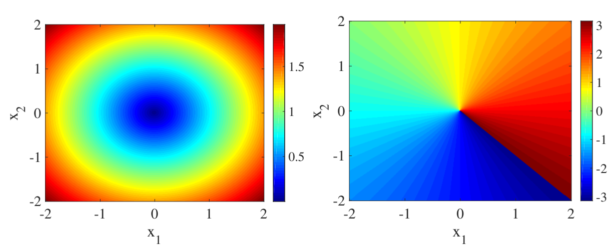

Fig. 1: Absolute value (left) and angle (right) of the eigenfunction corresponding to eigenvalue $\lambda = 0.39 + 0.8j$ on $[-2, 2] \times [-2, 2]$ for the system presented in Example VI.1.

Example VI.2: (Van der Pol Oscillator): Consider

$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = -x_1 + (1 - x_1^2)x_2. \quad (9)$$

We use Algorithm 1 to approximate Koopman invariant subspaces associated with the discretized version of (9). We use a dictionary consisting of all the $N_d = 36$ distinct monomials up to degree 7 of the form $\prod_{i=1}^{7} y_i$, where

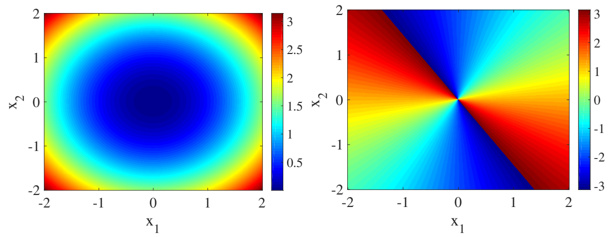

Fig. 2: Absolute value (left) and angle (right) of the eigenfunction corresponding to eigenvalue $\lambda = 0.8 + 0.5j$ on $[-2, 2] \times [-2, 2]$ for the system presented in Example VI.1.

$y_i \in \{1, x_1, x_2\}$ for $i \in \{1, \dots, 7\}$. We create our data snapshots using $N = 10^4$ points uniformly sampled from $\mathcal{M} = [-4, 4] \times [-4, 4]$ as initial conditions and finding the state of the system after $\Delta t = 5 \times 10^{-3} s$. Using Algorithm 1 on the dictionary snapshots results in the trivial dictionary $\tilde{D}_1(x) = [1]$, since $f(x) = 1$ is the only eigenfunction of the Koopman operator in the span of the dictionary.

One can resolve this issue by approximating Koopman invariant subspaces using the method presented in Remark V.6. Here we use $\epsilon = 10^{-4}$ and identify a dictionary $\tilde{D}(x)$ with $\tilde{N}_d = 24$. By computing $K_{\text{EDMD}} = K_{\text{EDMD}}(\tilde{D}(X), \tilde{D}(Y))$ and its eigendecomposition, one can approximate the Koopman eigenfunctions. We use the following relative error to measure the quality of the approximation

$$e_r = \frac{\|\tilde{D}(Y) - \tilde{D}(X) K_{\text{EDMD}}\|_F}{\min\{\|\tilde{D}(X)\|_F, \|\tilde{D}(Y)\|_F\}}.$$

By computing e_r using the available data, we get $e_r < 6 \times 10^{-4}$ which shows that the evolution of dictionary snapshots is close to linear. Fig. 3 shows a leading eigenfunction of the Koopman operator corresponding to system (9).

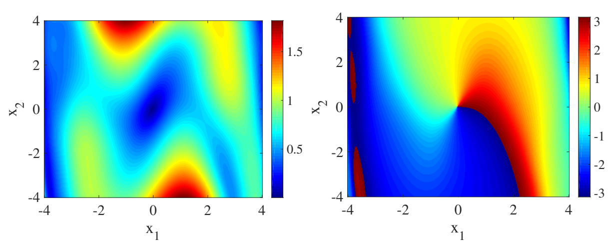

Fig. 3: Absolute value (left) and angle (right) of the eigenfunction corresponding to eigenvalue $\lambda = 0.9997 + 0.0048j$ on $[-4, 4] \times [-4, 4]$ for the Van der Pol oscillator.

VII. Conclusions

We have presented a necessary and sufficient condition for a function to evolve linearly according to the dynamics based on application of the EDMD method forward and backward in time. One can use the proposed condition to identify functions that evolve linearly according to the dynamics. Also, we have proposed an equivalent but more efficient algorithm to identify Koopman invariant subspace and linear evolutions according to the dynamics. For the future work, we plan on developing noise-resilient and distributed counterparts of the proposed algorithm. Moreover, we plan on modifying the proposed algorithm to work with streaming data sets.

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