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Zubov-Koopman Learning of Maximal Lyapunov Functions

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Abstract— **While there has been increasing interest in solving Zubov's equation to find the maximal Lyapunov function, it remains a challenge for dynamical systems with limited knowledge of system dynamics. In this paper, we present a Zubov-Koopman approach to learning a Lyapunov function that is nearly maximal for an unknown nonlinear system but has a known equilibrium point. The proposed approach is a lifting approach to map observable data into an infinite-dimensional function space, which generates a flow governed by our proposed '*Zubov-Koopman*' operator. By learning a Zubov-Koopman operator over a fixed time interval, we can indirectly approximate the solution to Zubov's Equation through iterative application of the learned operator on the identity function. We also demonstrate that a transformation of such an approximator can be readily utilized as a near-maximal Lyapunov function. We present an algorithm for learning Zubov-Koopman operators, asserting that this method not only decreases the necessary data volume but also achieves favorable outcomes in estimating regions of attraction, as illustrated by numerical examples.**

Index Terms— **Unknown systems, Zubov's Equation, Zubov-Koopman operators, maximal Lyapunov function**

I. INTRODUCTION

Lyapunov stability theory has been a cornerstone of automatic control. Lyapunov functions qualitatively characterize stability properties for various nonlinear systems. The existence of Lyapunov functions is guaranteed by converse Lyapunov theorems [2], [13], [24]. The same idea also forms the foundation of applying Lyapunov methods to control design for reachability and safety, which has achieved remarkable success in terms of reducing computational costs compared to formal methods [5], [12], [20].

The computation of Lyapunov functions has been developed [7] and gained increased attention with respect to data-driven methods [3]. On the other hand, Zubov's theorem characterizes the maximal Lyapunov function [25] defined on the domain of attraction. Zubov's construction of a Lyapunov function seems to address the issue by ensuring that the solution is always bounded. This approach can offer potential advantages in numerical approximations, particularly when solving a partial differential equation (PDE) to find a Lyapunov function [9], [15]. In this regard, recent investigations have focused on numerical solutions to Zubov's equation [8], [23]. In cases where system dynamics are known, the most recent work [14]–[16] introduced PINN algorithms for computing Lyapunov functions capable of approximating the entire region of attraction (ROA) for an asymptotically stable compact set with high accuracy. The Lyapunov candidate generated by the neural network was also formally verified.

In real-world applications, limited knowledge of the system dynamics can make the search for maximal Lyapunov functions more challenging. The recent work in [10] employed a purely data-driven approach to estimate the solution to Zubov's PDE. This method requires long-term observation of trajectory data and may have limited predictability of ROAs when the observation time is restricted.

Recent advances in system verification leverage Koopman operator-based approaches for analyzing unknown dynamical systems. Taking advantage of the spectral representation, in [1], [4], [17], [18], [26], the authors showed that a set of Lyapunov functions of nonlinear systems with global stability can be constructed based on the eigenfunctions of the learned Koopman operator. The current Koopman analysis requires the assumption of a forward-invariant compact subset within the state space. However, it sacrifices the ability to construct Lyapunov functions on a larger scale, given their unbounded nature near the boundary of the open ROA.

Considering the pros and cons of the Koopman approach and Zubov's PDE, we propose a Zubov-Koopman operator based data-driven technique, in line with trajectory data within a fixed observation span, to construct near-maximal Lyapunov functions of a known asymptotically stable compact set or equilibrium point for unknown dynamics.

The rest of the paper is organized as follows. Section II presents some preliminaries on the Koopman operator, Zubov's equation. In Section III, we extend Zubov's theorem and consider the solution restricted to a compact region of attraction. In Section IV, we formally introduce the Zubov-Koopman operator and demonstrate how it can effectively characterize the solution to Zubov's equation. Section V introduces the algorithms, with numerical experiments conducted in Section VI.

Due to page limitation and to enhance readability, this paper focuses on continuously differentiable vector fields and related auxiliary functions for a clearer illustration of the Zubov-Koopman approach. We kindly direct readers with further interest in this topic to [22] for detailed information and proofs.

Notation: We denote by $\mathbb{R}^n$ the Euclidean space of dimension. For $x \in \mathbb{R}^n$ and $r \geq 0$, we denote by $|\cdot|$ the Euclidean norm. For a closed set $A \subseteq \mathbb{R}^n$ and $x \in \mathbb{R}^n$, we denote the distance from x to A by $|x|_A = \inf_{y \in A} |x - y|$. For a set $A \subseteq \mathbb{R}^n$, $\mathrm{int}(A)$ denotes its interior, and ∂A denotes

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its boundary. For two sets $A, B \subseteq \mathbb{R}^n$, the set difference is defined by $A \setminus B = \{x : x \in A, x \notin B\}$.

II. PRELIMINARIES

A. Dynamical Systems

Given a state space $\mathcal{X} \subseteq \mathbb{R}^n$, we consider a continuous-time nonlinear dynamical system of the form

$$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t)), \ \ \mathbf{x}(0) = x \in \mathcal{X}, \ t \in [0, \infty), \tag{1}$$

where x denotes the initial condition, and the vector field $f : \mathcal{X} \to \mathcal{X}$ is assumed to be continuously differentiable. Throughout the paper, we will assume that the maximal interval of existence of the (unique) flow map $\phi : \mathcal{I} \times \mathcal{X} \to \mathcal{X}$ to the initial value problem (1) is $\mathcal{I} = [0, \infty)$. We also generally consider that the state space $\mathcal{X} = \mathbb{R}^n$.

Let us now consider a complete, but not necessarily Hilbert, function space $\mathcal{F}$ of the observable real-valued functions $h : \mathcal{X} \to \mathbb{R}$. The evolution of observables restricted on $\mathcal{F}$ is governed by the family of Koopman operators, which are defined as follows.

Definition 1 (Koopman Operator): The Koopman operator family $\{\mathcal{K}_t\}_{t \geq 0}$ of system (1) is a collection of maps $\mathcal{K}_t : \mathcal{F} \to \mathcal{F}$ defined by

$$\mathcal{K}_t h = h \circ \phi(t, \cdot), \quad h \in \mathcal{F} \tag{2}$$

for each $t \geq 0$, where $\circ$ is the composition operator. The (infinitesimal) generator $\mathcal{L}$ of $\{\mathcal{K}_t\}_{t \geq 0}$ is defined by $\mathcal{L}h(x) := \lim_{t \to 0} \frac{\mathcal{K}_t h(x) - h(x)}{t}$, where the observable functions should be within the domain of $\mathcal{L}$, defined as $\mathrm{dom}(\mathcal{L}) = \left\{ h \in \mathcal{F} : \lim_{t \to 0} \frac{\mathcal{K}_t h(x) - h(x)}{t} \text{ exists} \right\}$.

Suppose that the observable functions are bounded and continuously differentiable, the generator is such that $\mathcal{L}h = \nabla h \cdot f$ for all $h \in C_b^1(\mathcal{X})$.

Koopman operators form a linear C_0-semigroup that satisfies the following criteria. They allow us to study the nonlinear dynamics through the infinite-dimensional lifted space of observable functions with linear dynamics.

Definition 2 (Semigroup): A one parameter family $\{\mathcal{S}_t\}_{t \geq 0}$, of bounded linear operators from $\mathcal{F}$ into $\mathcal{F}$ is a semigroup of bounded linear operators on $\mathcal{F}$ if 1)$\mathcal{S}_0 = \mathrm{id}$, (id is the identity operator); 2) $\mathcal{S}_t \circ \mathcal{S}_s = \mathcal{S}_{t+s}$ for every $t, s \geq 0$. In addition, a semigroup $\{\mathcal{S}_t\}_{t \geq 0}$ is a C_0-semigroup if $\lim_{t \downarrow 0} \mathcal{S}_t h = h$ for all $h \in \mathcal{F}$.

B. Concept of Stability

We are interested in systems of the form (1) with an intrinsic asymptotically stable set $\mathcal{A} \subseteq \mathcal{X}$. We define the set stability as follows.

Definition 3 (Set stability): A closed invariant set $\mathcal{A} \subseteq \mathcal{X}$ is said to be asymptotically stable for (1) if 1) or every $\varepsilon > 0$, there exists a $\delta > 0$ such that $|x|_{\mathcal{A}} < \delta$ implies $|\phi_t(x)|_{\mathcal{A}} < \varepsilon$ for all $t \geq 0$, and 2) there exists a $\delta > 0$ such that $|x|_{\mathcal{A}} < \delta$ implies $\lim_{t \to \infty} |\phi_t(x)|_{\mathcal{A}} = 0$.

Furthermore, $\mathcal{A}$ is said to be locally exponentially stable, if there exists a $\delta > 0, M > 0$ and $c > 0$ such that $|\phi_t(x)|_{\mathcal{A}} \leq M|x|_{\mathcal{A}} e^{-ct}$, for all $t \geq 0$ and $x \in \{x \in \mathcal{X} : |x|_{\mathcal{A}} \leq \delta\}$.

We further define the region of attraction (ROA) of $\mathcal{A}$ given its asymptotic stability, which quantifies a region of the state space from which each absolutely continuous trajectory starts and eventually converges to the attractor itself.

Definition 4 (ROA): Suppose that $\mathcal{A}$ is asymptotically stable, the ROA of $\mathcal{A}$ is a set defined as

$$\mathcal{D}(\mathcal{A}) := \left\{ x \in \mathcal{X} : \lim_{t \to \infty} |\phi_t(x)|_{\mathcal{A}} = 0 \right\}.$$

Remark 5: It is a well-known result that the ROA is an open and forward invariant set. ◇

To better convey the idea, we propose the following hypothesis for unknown systems in the form of (1).

- (H1) We assume that there exists an equilibrium point x_{eq} of (1), i.e. a point such that $f(x_{\mathrm{eq}}) = \mathbf{0}$.
- (H2) We assume full knowledge of x_{eq}, and that $\{x_{\mathrm{eq}}\}$ is locally exponentially stable.

Based on Hypotheses (H1) and (H2), the purpose of this paper is to employ a data-driven approach to estimate the ROA of an equilibrium point of unknown systems.

C. Zubov's Theorem

The ROA can be characterized by a maximal Lyapunov function as described in the following theorem [15].

Theorem 6: Let $D \subseteq \mathbb{R}^n$ be an open set. Suppose that there exists a continuous function $V : D \to \mathbb{R}$ such that $\mathcal{A} \subseteq D$ and the following conditions hold: 1) V is positive definite on D with respect to $\mathcal{A}$; 2) the derivative of V along solutions of (1) is well-defined for all $x \in D$ and satisfies

$$\nabla V(x) \cdot f(x) = -q(x); \tag{3}$$

3) $V(x) \to \infty$ as $x \to \partial D$ or $|x| \to \infty$. Then $D = \mathcal{D}(\mathcal{A})$.

Theorem 6 is equivalent to Zubov's theorem stated below.

Theorem 7: Let $D \subseteq \mathbb{R}^n$ be an open set containing $\mathcal{A}$. Then $D = \mathcal{D}(\mathcal{A})$ if and only if there exists two continuous functions $W : D \to \mathbb{R}$ and $\eta : D \to \mathbb{R}$ such that the following conditions hold: 1) $0 < W(x) < 1$ for all $x \in D \setminus \mathcal{A}$ and $W(x) = 0$ for all $x \in \mathcal{A}$; 2) η is positive definite on D with respect to $\mathcal{A}$; 3) for any sufficiently small $c_3 > 0$, there exist $c_1, c_2 > 0$ such that $|x|_{\mathcal{A}} \geq c_3$ implies $W(x) > c_1$ and $\eta(x) > c_2$; 4) $W(x) \to 1$ as $x \to y$ for any $y \in \partial D$; 5) W and q satisfy

$$-\nabla W(x) \cdot f(x) + \eta(x)(1 - W(x)) = 0. \tag{4}$$

Remark 8: Based on Hypothesis (H1) and (H2), a typical choice for η is given by $\eta(x) = \alpha|x - x_{\mathrm{eq}}|$ for some $\alpha > 0$. In addition, Theorem 6 and Theorem 7 can be related by the following equation

$$W(x) = 1 - \exp(-\alpha V(x)), \ \ x \in \mathcal{D}(\mathcal{A}), \tag{5}$$

for some constant $\alpha > 0$. It is easy to verify that V satisfying (3) implies (4). ◇

III. AN EXTENSION OF ZUBOV'S THEOREM

For the rest of this paper, we will assume that Hypothesis (H1) and (H2) hold and denote $\mathcal{A} := \{x_{\mathrm{eq}}\}$.

Inspired by (4) and its connection with V through Eq. (5), to facilitate data-driven approximation, we explore the following dual form of Zubov's equation (4), namely Zubov's Dual Equation,

$$\nabla U(x)\cdot f(x)=\eta(x)U(x),\ U(x_{\text{eq}})=1. \tag{6}$$

Note that, on $\mathcal{D}(\mathcal{A})$, we always have $U(x)=1-W(x)$. We prefer this dual form of Zubov's equation because it allows us to potentially use a time series to approximate, as demonstrated in Section IV.

A. Zobov's Dual Equation

In this section, we construct the solution to the dual equation (6) of Zubov's equation. The settings adopted in this paper enable differentiable solutions to (6). However, in a broader context, solutions satisfy (6) in the viscosity sense, as discussed in [22].

Consider a positive definite $\eta\in C^1(\mathbb{R}^n)$. Define

$$V(x)=\int_0^\infty \eta(\phi(t,x))dt,\quad x\in\mathbb{R}^n, \tag{7}$$

where if the integral diverges, we let $V(x)=\infty$. Then, we have the following property [15, Proposition 1].

Lemma 9: The function $V:\mathbb{R}^n\to\mathbb{R}\cup\{\infty\}$ defined by (7) satisfies the following: 1) $V(x)<\infty$ if and only if $x\in\mathcal{D}(\mathcal{A})$; 2) $V(x)\to\infty$ as $x\to\partial\mathcal{D}(\mathcal{A})$; 3) V is positive definite with respect to $\mathcal{A}$.

Let $h\in C_b^1(\mathbb{R}^n)$. We further define

$$U_h(x)=\begin{cases}\exp\{-V(x)\}\,h(\phi_\infty(x)), & \text{if } V(x)<\infty,\\ 0, & \text{otherwise},\end{cases} \tag{8}$$

where $\phi_\infty(x):=\lim\limits_{t\to\infty}\phi(t,x)$. For test function $h(x)=\mathbb{1}(x)$, we denote $U:=U_{\mathbb{1}}$ for simplicity.

Remark 10: The notion of $h(\phi_\infty(x))$ seems redundant in that, given $V(x)<\infty$, by 1) of Lemma 9, we have $x\in\mathcal{D}(\mathcal{A})$ and $h(\phi_\infty(x))=h\circ\lim\limits_{t\to\infty}\phi(t,x)=h(x_{\text{eq}})$. However, we still keep it in (8) for consistency when using a time series to approximate in Section IV. ◇

The connection between (6) and (4) is stated as follows.

Lemma 11: For any $h\in C_b^1(\mathbb{R}^n)$, let $W_h=1-U_h$, where U_h is defined in (8). Then, U_h is the unique solution to (6) and W_h is the unique solution to $\nabla W_h(x)\cdot f(x)=-\eta(x)(1-W_h(x))$ with $W_h(x_{\text{eq}})=1-h(x_{\text{eq}})$ on $\mathbb{R}^n$. This particularly holds for $h=\mathbb{1}$. In addition, $V=-\log(U)$ is continuously differentiable on $\mathcal{D}(\mathcal{A})$ and solves $\nabla V(x)\cdot f(x)=-\eta(x)$.

B. Reformulation on a Compact Domain of Interest

To facilitate data-driven techniques and prevent significant under-approximation of the ROA, we directly choose a sufficiently large compact region of interest $\mathcal{R}\subseteq\mathbb{R}^n$. This region can either contain the entire ROA, assuming it is bounded, or covers a significant portion of the ROA if it is unbounded. Our proposed method aims to recover the ROA relative to $\mathcal{R}$ using observable data.

To incorporate Zubov's Dual Equation, we need to recast the dynamics on $\mathcal{R}$. We first consider a first-hitting time of $\partial\mathcal{R}$ defined as follow, $\tau:=\tau(x)=\inf\{t\geq 0:\phi(t,x)\in\partial\mathcal{R}\},\ x\in\mathcal{R}$. It is clear that: 1) $\tau=0$ for all $x\in\partial\mathcal{R}$; 2) $\tau>0$ for all $x\in\text{int}(\mathcal{R})$; 3) $\tau=\infty$ for all $x\in\mathcal{D}(\mathcal{A})$ given that $\mathcal{D}(\mathcal{A})\subseteq\mathcal{R}$.

We further define stopped-flow maps so that one can observe the trajectories in $\mathcal{R}$.

Definition 12: Given the compact region of attraction $\mathcal{R}$, for each $x\in\mathcal{R}$, we define the stopped-flow maps $\hat{\phi}:[0,\infty)\times\mathcal{R}\to\mathcal{R}$ as $\hat{\phi}(t,x):=\phi(t\wedge\tau,x)$.

Note that in the above definition, the stopping time τ implicitly encodes the information of the starting position. It can also be verified that 1) $\hat{\phi}(0,x)=x$ and $\hat{\phi}(s,\phi(t,x))=\hat{\phi}(t+s,x)$ for all $x\in\mathcal{R}$, and 2) $\partial_t(\hat{\phi}(t,x))=f(\hat{\phi}(t,x))$ for all $x\in\text{int}(\mathcal{R})$.

We then consider a recast version of functions V and U_h (defined in (7) and (8)) accordingly, i.e.,

$$\hat{V}(x)=\int_0^\infty \eta(\hat{\phi}(t,x))dt,\quad x\in\mathcal{R}, \tag{9}$$

and, for any $h\in C^1(\mathcal{R})$,

$$\hat{U}_h(x)=\begin{cases}\exp\left\{-\hat{V}(x)\right\}h(\hat{\phi}_\infty(x)), & \text{if } \hat{V}(x)<\infty,\\ 0, & \text{otherwise},\end{cases}$$

where $\phi_\infty(x):=\lim_{t\to\infty}\phi(t,x)$. For test function $h(x)=\mathbb{1}(x)$, we denote $\hat{U}:=\hat{U}_{\mathbb{1}}$ for simplicity. In this notion, it can be verified that $\hat{V}(x)=\infty$ if and only if $\tau<\infty$ and $x\notin\mathcal{D}(\mathcal{A})$.

The following theorem collects nice properties of $\hat{V}$ and $\hat{U}$ on the refined region $\mathcal{R}$.

Theorem 13: For any $h\in C_b^1(\mathbb{R}^n)$, $\hat{U}_h$ is the unique solution to

$$\nabla\hat{U}_h(x)\cdot f(x)=\eta(x)\hat{U}_h(x),\ \hat{U}_h(x_{\text{eq}})=h(x_{\text{eq}}) \tag{10}$$

in $\mathcal{R}$. On any invariant set $\mathcal{I}\subseteq\mathcal{D}(\mathcal{A})\cap\text{int}(\mathcal{R})$, the function $\hat{V}(x)=-\log(\hat{U}(x))$ is the unique solution to $\nabla\hat{V}(x)\cdot f(x)=-\eta(x)$ with $\hat{V}(x_{\text{eq}})=0$. Additionally, $\hat{W}_h=1-\hat{U}_h$ is the unique solution to $\nabla\hat{W}_h(x)\cdot f(x)=-\eta(x)(1-\hat{W}_h(x))$ in $\mathcal{R}$ with $\hat{W}_h(x_{\text{eq}})=1-h(x_{\text{eq}})$, if and only if $\hat{U}_h$ solves (10).

By Theorem 13, suppose that $\mathcal{D}(\mathcal{A})\cap\text{int}(\mathcal{R})\neq\mathcal{D}(\mathcal{A})$, one can only recover a portion of $\mathcal{D}(\mathcal{A})$ that is not absorbed by the boundary by solving (10). This portion should be a sublevel set (relative to $\mathcal{D}(\mathcal{A})\cap\text{int}(\mathcal{R})$) of the $\hat{V}$. In view of [19]–[21], this sublevel set is a also subset of the refined open and invariant subregion of ROA, from which trajectories will satisfy the reach-avoid-stay property.

IV. ZUBOV-KOOPMAN OPERATORS AND SEMIGROUP PROPERTY

We have introduced Zubov's Dual Equation as well as its refined form on $\mathcal{R}$. The solution involves an improper integral up to ∞, which requires nearly the full knowledge of the trajectory [10]. To reduce the substantial amount of observation data, in this section, we derive an approximation approach using a time series. Specifically, this time series is governed by a convergent and time-homogeneous semigroup, which allows us to approximate the long-term behavior through a simple iterative process.

A. Introducing Zubov-Koopman Operators

Consider

$$v_t(x) := \int_0^t \eta(\phi(r,x))dr \tag{11}$$

and, for any $h \in C_b^1(\mathbb{R}^n)$ and $t > 0$, we define $\mathcal{T}_t : C_b^1(\mathbb{R}^n) \to C_b^1(\mathbb{R}^n)$ as

$$\mathcal{T}_t h(x) := \exp\{-v_t(x)\}\, h(\phi(t,x)). \tag{12}$$

Proposition 14: $\{\mathcal{T}_t\}_{t\geq 0}$ is a C_0-semigroup. In addition, for each $t \geq 0$ and for any $h \in C_b^1(\mathbb{R}^n)$, $\mathcal{T}_t U_h(x) = U_h(x)$ for all $x \in \mathbb{R}^n$.

The stochastic version of $\{\mathcal{T}_t\}_{t\geq 0}$ is the famous Feynman-Kac semigroup. For deterministic dynamical systems, we observe that $\mathcal{T}_t$ depicts a form of separation of variables and can be written as a multiplication of a contraction operator with the Koopman operator, i.e. $\mathcal{T}_t = \exp\{-v_t\}\,\mathcal{K}_t$. For the purpose of using the flow of h governed by $\mathcal{T}_t$ to approximate the solution of Zubov's Dual Equation, for any fixed t, we name $\mathcal{T}_t$ as the *Zubov-Koopman Operator*.

Theorem 15: Let the test function be $h \in C_b^1(\mathbb{R}^n)$. Suppose that $\eta \in C(\mathbb{R}^n)$ is nonnegative. Then

1) $u_h(t,x) = \mathcal{T}_t h(x)$ solves the following Cauchy problem, for all $t > 0$ and all $x \in \mathbb{R}^n$,

$$\begin{cases} \partial_t u_h(t,x) = \nabla_x u_h(t,x)\cdot f(x) - \eta(x) u_h(t,x), \\ u_h(0,x) = h(x). \end{cases} \tag{13}$$

2) Conversely, for any $u_h \in C^{1,1}([0,\infty), \mathbb{R}^n)$ that solves (13), the solution should be $u_h(t,x) = \mathcal{T}_t h(x)$.

We make a quick extension of the aforementioned results, further refining our observations on the compact region of interest $\mathcal{R}$.

Corollary 16: Recall the stopped-flow map $\hat{\phi}$ defined in Definition 12. Let $\hat{v}_t(x) := \int_0^t \eta(\hat{\phi}(r,x))dr$. For any $h \in C^1(\mathcal{R})$ and $t > 0$, we redefine $\mathcal{T}_t : C^1(\mathcal{R}) \to C^1(\mathcal{R})$ as

$$\mathcal{T}_t h(x) := \exp\{-\hat{v}_t(x)\}\, h(\hat{\phi}(t,x)). \tag{14}$$

Then, 1) $\{\mathcal{T}_t\}_{t\geq 0}$ is a C_0-semigroup. 2) For each $h \in C^1(\mathcal{R})$ and for each t, $\hat{U}_h$ is an eigenfunction such that $\mathcal{T}_t \hat{U}_h = \hat{U}_h$. 3) For any test function $h \in C^1(\mathcal{R})$, given that η is nonnegative, then $\hat{u}_h(t,x) := \mathcal{T}_t h(x)$ is the unique solution to (13) for all $t > 0$ and $x \in \mathcal{R}$.

B. A Time-Series and Data-Driven Approximation

By the definition of U_h in (8), for any $h \in C_b^1(\mathbb{R}^n)$, we have that $\lim_{t\to\infty} u_h(t,x) = \lim_{t\to\infty} \mathcal{T}_t h(x) = U_h(x)$ for all $x \in \mathbb{R}^n$. In particular, $\lim_{t\to\infty} \mathcal{T}_t \mathbb{1} = U$ uniformly, and U is also unique, up to a multiplicative constant, fixed point of $\{\mathcal{T}_t\}_{t\geq 0}$. To approximate U, one can pick a fixed time interval Δt, and define $\mathcal{T}_\Delta := \mathcal{T}_{\Delta t}$ as well as $\mathcal{T}_{k\Delta} := \mathcal{T}_\Delta \circ \mathcal{T}_\Delta \cdots \circ \mathcal{T}_\Delta$ with k iterations. Then, by (8) and the uniqueness (up to a multiplicative constant) of the fixed point, the composed operator $\mathcal{T}_{k\Delta} : C_b^1(\mathbb{R}^n) \to C_b^1(\mathbb{R}^n)$ for any $k \geq 1$, and $\lim_{k\to\infty} \mathcal{T}_{k\Delta} h = U$ for any h such that $h(x_{\text{eq}}) = 1$. Suppose that one can approximate $\mathcal{T}_\Delta$ properly, then $\mathcal{T}_{k\Delta} h$ for some large k should be a reasonably good approximation for U.

Similar to the approximation of Koopman operators, to obtain a discrete version $\mathbf{T}$ of the bounded linear operator $\mathcal{T}_\Delta$, it usually relies on the choice of a (discrete) dictionary of observable test functions, denoted by $\mathfrak{Z}_N(x) := [\mathfrak{z}_0(x), \mathfrak{z}_1(x), \cdots, \mathfrak{z}_{N-1}(x)]$ for $N \in \mathbb{N} \cup \{\infty\}$. Then, the approximation $\widetilde{\mathcal{T}} : \text{span}\{\mathfrak{z}_i\}_{i=0}^{N-1} \to \text{span}\{\mathfrak{z}_i\}_{i=0}^{N-1}$ is valid in the sense that, for each $h \in C_b^1(\mathbb{R}^n)$, there exists an $\mathfrak{h} \in \text{span}\{\mathfrak{z}_i\}_{i=0}^{N-1}$ and a uniformly continuous residual term $\vartheta \in C_b(\mathbb{R}^n)$ such that $\mathcal{T}_\Delta h = \widetilde{\mathcal{T}}\mathfrak{h} + \vartheta$. Possible choices of the dictionary $\mathfrak{Z}_N$ have been discussed in [4], [26].

V. DATA-DRIVEN ALGORITHMS

We modify the existing Koopman learning techniques for Zubov-Koopman operators $\mathcal{T}_\Delta$, as defined in Section IV-B, with a fixed training time interval Δt.

A. Generating Training Data

As we have briefly discussed the feasibility of using data-driven approaches to approximate the operator $\mathcal{T}_\Delta$ for each $\mathfrak{z}_i \in \mathfrak{Z}_N$ and each $x \in \mathcal{R}$, we consider $\mathfrak{z}_i(x)$ as the features and $\mathcal{T}_\Delta \mathfrak{z}_i(x) := \exp\left(-\int_0^{\Delta t} \eta(\hat{\phi}(s,x))ds\right) \mathfrak{z}_i(\hat{\phi}(\Delta t, x))$ as the labels. We inevitably need to acquire the stopped-flow map $\hat{\phi}$ and compute the integral. Drawing inspiration from [10], for each termination time, we can assess both the trajectory (without stopping) and the integral, i.e. the pair $\left(\phi(t,x), \int_0^t \eta(\phi(s,x))ds\right)$, by solving a single augmented ODE system

$$\begin{aligned} &\dot{\mathbf{x}}(t) = f(\mathbf{x}(t)), \;\; \mathbf{x}(0) = x \in \mathbb{R}^n, \\ &\dot{I}(t) = \eta(\mathbf{x}), \;\; I(0) = 0. \end{aligned} \tag{15}$$

The corresponding solutions related to $\hat{\phi}$ can be obtained in a similar manner, with a slight modification as introduced in [22, Algorithm 1]. Subsequently, we can calculate $\mathcal{T}_\Delta \mathfrak{z}_i(x)$ using (14). We summarize the algorithm for generating training data for one time period as in Algorithm 1.

Algorithm 1 Generating Training Data

```
Require: $f$, $\eta$, $\mathcal{R}$, $\mathfrak{Z}_N$, $\Delta t$, and a set $\{x^{(m)}\}_{m=0}^{M-1} \subseteq \mathcal{R}$.
  for $m$ from 0 to $M-1$ do
      for $i$ from 0 to $N-1$ do
          Calculate $\mathfrak{z}_i(x^{(m)})$
          Calculate $\mathcal{T}_\Delta \mathfrak{z}_i(x^{(m)})$
      end for
      Stack
          $\mathcal{T}_\Delta \mathfrak{Z}_N(x^{(m)}) = [\mathcal{T}_\Delta \mathfrak{z}_0(x^{(m)}), \cdots, \mathcal{T}_\Delta \mathfrak{z}_{N-1}(x^{(m)})]$
  end for
  Stack $\mathfrak{X}, \mathfrak{Y} \in \mathbb{C}^{M\times N}$ such that $\mathfrak{X} = [\mathfrak{Z}_N(x^{(0)}), \mathfrak{Z}_N(x^{(1)}), \cdots, \mathfrak{Z}_N(x^{(M-1)})]^T$ and
  $\mathfrak{Y} = [\mathcal{T}_\Delta \mathfrak{Z}_N(x^{(0)}), \mathcal{T}_\Delta \mathfrak{Z}_N(x^{(1)}), \cdots, \mathcal{T}_\Delta \mathfrak{Z}_N(x^{(M-1)})]^T$
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B. EDMD Algorithm

We perform the EDMD algorithm to obtain the final approximation for $\mathcal{T}_\Delta$. EDMD algorithm provides an estimation of $\mathcal{T}_\Delta$ using one time period observation data. We use Algorithm 1 to obtain training data $(\mathfrak{X}, \mathfrak{Y})$, and to find $\mathbf{T} = \operatorname{argmin}_{A \in \mathbb{C}^{N\times N}} \|\mathfrak{Y} - \mathfrak{X}A\|_F$. For EDMD, the $\mathbf{T}$ is given in closed-form as $\mathbf{T} = \left(\mathfrak{X}^T\mathfrak{X}\right)^\dagger \mathfrak{X}^T\mathfrak{Y}$, where † is the pseudo inverse.

Similar to EDMD [26], the learned operator has the following sense of approximations. 1) Let $(\mu_i, \mathbf{e}_i)_{i=0}^N$ be the eigenvalues and eigenvectors of $\mathbf{T}$. Then, for each i, the learned eigenvalues μ_i can be used for approximate the true eigenvalues of $\mathcal{T}_\Delta$, and the learned eigenfunction $\widetilde{\zeta}_i$ satisfies $\widetilde{\zeta}_i(x) = \mathfrak{Z}_N(x)\mathbf{e}_i$. 2) For any $\mathfrak{h} \in \operatorname{span}\{\mathfrak{z}_0, \mathfrak{z}_1, \cdots, \mathfrak{z}_{N-1}\}$ such that $\mathfrak{h}(x) = \mathfrak{Z}_N(x)\mathbf{w}$ for some column vector $\mathbf{w}$, we have that $\mathcal{T}_t\mathfrak{h}(\cdot) \approx \mathcal{T}_t^N\mathfrak{h}(\cdot) \approx \mathfrak{Z}_N(\cdot)(\mathbf{T}\mathbf{w})$. By the universal approximation theorem, all of the function approximations from above should have uniform convergence.

C. Predicting ROA and Constructing Lyapunov Function

To predict U, we simply pick a tolerance and the largest number of iteration K, then iterate $\mathbf{T}$ until $\|\mathbf{T}^k - \mathbf{T}^{k-1}\|_F$ reaches the threshold or $k = K$, whichever comes first. For simplicity, we can also choose the dictionary $\mathfrak{Z}_N$ to include a real-valued $\mathfrak{z}_i$ such that $\mathfrak{z}_i(x_{\rm eq}) = 1$. Then, as a quick extension, we obtain a Zubov-Koopman approximation of U as follows

$$U_{\rm ZK}(\cdot) = \mathfrak{Z}_N(\cdot)(\mathbf{T}^k\mathbf{w}), \tag{16}$$

where $\mathbf{w}$ is the i-th standard basis vector. Since $U_{\rm ZK}$ and U are uniformly close, we can approximate the ROA by the largest connected positive level sets of $U_{\rm ZK}$.

We may not directly use the result $U_{\rm ZK}$ for constructing a Lyapunov function, since it only possesses a convergence with respect to the uniform norm. Fortunately, one can seek a smooth function that uniformly approximates U, and hence uniformly approximates $U_{\rm ZK}$, with its Lipschitz constant also converging to that of U [11]. We achieve this extra modification by neural networks (NN) using a new set of samples $\{x^{(m)}\}$ (could be different than the one used in Algorithm 1) and $\{U_{\rm ZK}(x^{(m)})\}$. This NN approximation will be named as $U_{\rm NN}$. We omit this algorithm as it follows the standard procedure. The formal verification of $U_{\rm NN}$ utilizes satisfiability modulo theories solvers such as dReal [6] and follows the exact procedures in [15, Section V].

VI. NUMERICAL EXAMPLE

In this section, we provide a numerical example to demonstrate the proposed Zubov-Koopman approach for predicting ROAs, as well as learning and verifying neural Lyapunov functions. More examples can be found in [22].

Consider the reversed Van der Pol oscillator $\dot{\mathbf{x}}_1(t) = -\mathbf{x}_2(t),\ \dot{\mathbf{x}}_2(t) = \mathbf{x}_1(t) - (1 - \mathbf{x}_1^2(t))\mathbf{x}_2(t)$ with $\mathbf{x}(0) := [\mathbf{x}_1(0), \mathbf{x}_2(0)] = [x_1, x_2]$. We use this example to compare the data efficiency of predicting the ROA of $\{\mathbf{0}\}$ as well as finding a Lyapunov function between the Zubov-Koopman approach and the data-driven approach presented in [10]. We set $\eta(x) = (x_1^2 + x_2^2)/10$, and pick the region of interest as $\mathcal{R} = [-3, 3]^2$. A total of $M = 100^2$, 200^2, and 300^2 uniformly spaced samples $\left\{x^{(m)}\right\}$ in $\mathcal{R}$ are generated respectively for three parallel experiments.

1) Zubov-Koopman method: We simulate the trajectory up to $\Delta t = 1.5$. The dictionary $\mathfrak{Z} = [\mathfrak{z}_{0,0}, \mathfrak{z}_{0,1}, \mathfrak{z}_{1,0}, \cdots, \mathfrak{z}_{i,j}, \cdots, \mathfrak{z}_{2N-1,2N-1}]$ is selected in a similar manner as in the one-dimensional example with adjustments for two-dimensional inputs, i.e., we set $\mathfrak{z}_{i,j}(x_1, x_2) = \cos\left(\frac{2\pi(ix_1+jx_2)}{3}\right)\exp\left\{-\frac{x_1^2+x_2^2}{4}\right\}$ for each i and j. We set $N = 50$. To obtain $U_{\rm ZK}$ through iterations, we set the termination tolerance to 10^{-2} with a maximum of 8 iterations. The prediction of the ROA (or U) follows the same procedure as in Section V-C. For the verification of a Lyapunov function, we need to incorporate an additional NN modification. For all the experiments at this stage, we use 300^2 uniformly spaced samples, along with the evaluations of $U_{\rm ZK}$ at those points, to train $U_{\rm NN}$. We use a network with 2 hidden layers, each containing 15 neurons. We terminate training when the mean-square training loss was smaller than 10^{-8} or after 300 epochs.

2) Data-Driven method: As for the data-driven method in [10], for each experiment, we use the same samples as above and generate trajectory data up to a termination time $t = 10$, or until $\int_0^t \eta(\phi(s, x))ds \geq 200$. We then use $\left\{x^{(m)}\right\}$ and $\left\{\exp\{-\int_0^t \eta(\phi(s, x^{(m)}))ds\}\right\}$ to train a neural-network $U_{\rm DD}$. We use a network model with 2 hidden layers, each containing 15 neurons. We terminate training when the mean-square training loss is smaller than 10^{-8} or reaches 500 epochs. We predict the ROA as the largest connected positive level set of $U_{\rm DD}$. This neural solution $U_{\rm DD}$ is also ready to be verified as a Lyapunov function without extra modification.

3) Experiment results: The comparison results are reported in Table I. In the table, 'IVP solving' corresponds to solving (15), while 'stacking' involves preparing the data for learning. For the data-driven method, 'function learning' refers to the NN training, whereas for the Zubov-Koopman approach, it pertains to the iterative procedure to obtain $U_{\rm ZK}$ (see (16)). The formal verification of the Lyapunov functions is conducted using dReal. We visualize the predicted and verified boundaries of the ROA in Figure 1. The prediction using the Zubov-Koopman approach shows overall better accuracy, while the verified regions are similar for all the methods. On the other hand, with $M = 100^2$ initial samples, the region verified by the data-driven method is slightly smaller. This is because the verification relies on NN approximation for both methods, but the Zubov-Koopman approach's NN stage is based on an already good approximation of U, which is not constrained by the initial sample size. These phenomena also reflect that the learned $U_{\rm ZK}$ and the data generated for the data-driven method have similar quality in cases where $M = 200^2$ and 300^2.

VII. CONCLUSIONS

In this paper, we introduce a Zubov-Koopman approach to characterize the solution to Zubov's equation. The proposed

TABLE I: Verification of Neural Lyapunov Functions for Reversed Van der Pol Oscillator

Approaches	Sample size	IVP solving time	Stacking time	Operator learning time	Function U learning time	Modification (300^2 samples)	NN final loss	Verified Volume
Data-driven	100×100	10.13(s)	0.81 (s)	-	54.24(s)	-	8.48×10^{-5}	84.71%
ZK + NN	100×100	7.68(s)	5.40 (s)	89.26(s)	52.91(s)	482.10 (s)	1.25×10^{-6}	91.68%
Data-driven	200×200	40.83(s)	0.20(s)	-	366.90(s)	-	1.35×10^{-6}	88.87%
ZK + NN	200×200	31.24(s)	12.59(s)	128.57 (s)	53.18(s)	482.10 (s)	1.25×10^{-6}	90.32%
Data-driven	300×300	87.06(s)	0.32(s)	-	545.02(s)	-	9.37×10^{-7}	87.09%
ZK + NN	300×300	61.69(s)	16.82(s)	178.90(s)	51.10(s)	486.67(s)	1.05×10^{-5}	89.70%

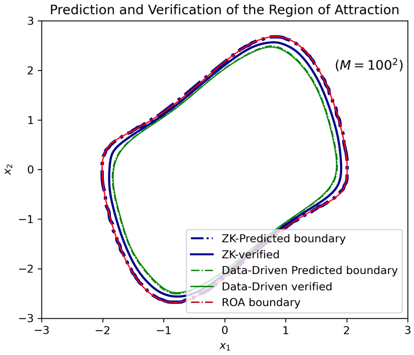

Fig. 1: Predictions and verification of the ROA for the reversed Van der Pol with Zubov-Koopman and Data-driven method using $M = 100^2$ samples.

operator exhibits a semigroup property, and the learning technique is similar to the conventional Koopman operator. We devise an iterative approach that employs the learned Zubov-Koopman operator to approximate the solution to Zubov's equation, achieving a high level of accuracy. Compared to the previous data-driven method, which requires long-term information of trajectories, our proposed technique can effectively address this issue with a short period of observation. Future directions will focus on the spectral analysis and dimension reduction of the Zubov-Koopman operator, with applications to high-dimensional physical systems.

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