Fitting an immersed submanifold to data via Sussmann’s orbit theorem

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Abstract—This paper describes an approach for fitting an immersed submanifold of a finite-dimensional Euclidean space to random samples. The reconstruction mapping from the ambient space to the desired submanifold is implemented as a composition of an encoder that maps each point to a tuple of (positive or negative) times and a decoder given by a composition of flows along finitely many vector fields starting from a fixed initial point. The encoder supplies the times for the flows. The encoder-decoder map is obtained by empirical risk minimization, and a high-probability bound is given on the excess risk relative to the minimum expected reconstruction error over a given class of encoder-decoder maps. The proposed approach makes fundamental use of Sussmann’s orbit theorem, which guarantees that the image of the reconstruction map is indeed contained in an immersed submanifold.

I. INTRODUCTION

The manifold learning problem can be stated as follows: A point cloud in $\mathbb{R}^d$ is given, and we wish to construct a smooth $m$-dimensional submanifold of $\mathbb{R}^d$ (where $m < d$) to approximate this point cloud. This problem has received a great deal of attention in the machine learning community, where such representations can serve as intermediate objects in multistage inference procedures, their lower dimensionality conferring computational advantages when the ambient dimension $d$ is high. Most existing approaches [1]–[6] attempt to construct a local description of the approximating manifold via an atlas of charts, and an additional step is needed to piece the charts together into a global description.

There have been several recent proposals for manifold learning relying on deep neural nets [7]–[10], which are currently the dominant modeling paradigm in machine learning. However, these approaches are also local in nature. In this work, we propose an alternative global procedure for fitting low-dimensional submanifolds to data via a deep and fundamental result in differential geometry — namely, Sussmann’s orbit theorem [11]. While we give the precise statement of the orbit theorem in the next section, the underlying idea is as follows: Given an arbitrary collection $\mathcal{F}$ of smooth vector fields on a smooth finite-dimensional manifold $M$, the orbit of $\mathcal{F}$ through a point $\xi$ of $M$, i.e., the set of all points attainable via successive forward and backward finite-time motions along a finite number of vector fields in $\mathcal{F}$ starting from $\xi$, has a natural structure of an immersed submanifold of $M$. The Chow-Rashevskii theorem [12], [13], which is fundamental in geometric control [14], is a corollary of this result.

This suggests the following natural recipe for fitting an immersed submanifold of $\mathbb{R}^d$ to a finite point cloud $S = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$:

1) Fix a family $\mathcal{F}$ of smooth vector fields on $\mathbb{R}^d$ and a family $\mathcal{A}$ of smooth functions from $\mathbb{R}^d$ into a finite interval $[T_0, T_1]$ containing 0.

2) Fix a positive integer $m < d$, which will serve as an upper bound on the dimension of the submanifold.

3) Find $m$-tuples $(f_1, \ldots, f_m) \in \mathcal{F}^m$ and $(a_1, \ldots, a_m) \in \mathcal{A}^m$ and a starting point $\xi$ in the convex hull of $S$ to minimize the average reconstruction error

$$\frac{1}{n} \sum_{i=1}^{n} |x_i - e^{a_m(x_i)f_1} \circ \cdots \circ e^{a_1(x_i)f_1}\xi|,$$

where $| \cdot |$ denotes the Euclidean norm on $\mathbb{R}^d$, and $e^{tf}$ denotes the flow map of $f$, i.e., the solution at time $t$ of the ODE $\dot{x} = f(x)$ starting from $x(0) = \xi$.

This procedure produces an explicit encoder map from $\mathbb{R}^d$ into $[T_0, T_1]^m$ given by $x \mapsto (a_1(x), \ldots, a_m(x))$ and an explicit decoder map from the $m$-cube $[T_0, T_1]^m$ into the orbit of $(f_1, \ldots, f_m)$ through $\xi$ given by $(t_1, \ldots, t_m) \mapsto e^{t_m f_m} \circ \cdots \circ e^{t_1 f_1}\xi$. Sussmann’s theorem then guarantees that the decoder maps the cube $[T_0, T_1]^m$ into an immersed submanifold of $\mathbb{R}^d$. Moreover, the reconstruction of a point $x$ as $e^{a_m(x)f_m} \circ \cdots \circ e^{a_1(x)f_1}\xi$ is realized as a composition of flow maps of $m$ time-homogeneous ODEs starting from $\xi$, where the duration and the direction (forward or backward) of each flow is determined by the target point $x$.

In this work, we consider the statistical learning setting, where the points of $S$ are independent samples from an unknown probability measure supported on a compact subset of $\mathbb{R}^d$. The encoders $(a_1, \ldots, a_m)$, the vector fields $(f_1, \ldots, f_m)$, and the starting point $\xi$ are obtained by minimizing the empirical risk on $S$, and we give a high-probability bound on the excess risk relative to the best expected reconstruction error. To accomplish this, we recruit control-theoretic techniques to quantify how the reconstruction error propagates forward through a composition of flow maps of vector fields. The bounds obtained from this analysis depend on the regularity conditions satisfied by the families of encoders and vector fields.

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This paper describes an approach for fitting an immersed submanifold of a finite-dimensional Euclidean space to random samples. The reconstruction mapping from the ambient space to the desired submanifold is implemented as a composition of an encoder that maps each point to a tuple of (positive or negative) times and a decoder given by a composition of flows along finitely many vector fields starting from a fixed initial point. The encoder supplies the times for the flows. The encoder-decoder map is obtained by empirical risk minimization, and a high-probability bound is given on the excess risk relative to the minimum expected reconstruction error over a given class of encoder-decoder maps. The proposed approach makes fundamental use of Sussmann’s orbit theorem, which guarantees that the image of the reconstruction map is indeed contained in an immersed submanifold.
II. Model description and problem statement

To motivate the encoder-decoder architecture, we review the setting and statement of Sussmann’s orbit theorem [11]. Let $\mathcal{F}$ be a family of smooth vector fields on a finite-dimensional smooth manifold $M$. We assume that, for each $f \in \mathcal{F}$, the flow map $e^t : M \rightarrow M$ is complete, i.e., defined for all times $t \in \mathbb{R}$. Consider the group $\mathbb{G}(\mathcal{F})$ of diffeomorphisms of $M$ generated by all such maps, i.e.,

$$\mathbb{G}(\mathcal{F}) := \{ e^{tk_1} \cdots e^{t_2} f \circ e^{t_1} f_1 : k \in \mathbb{N} \},$$

$$t_1, \ldots, t_k \in \mathbb{R}, \ f_1, \ldots, f_k \in \mathcal{F}.$$  

We define the orbit of $\mathcal{F}$ through a point $\xi \in M$ as the set $O_\xi = \{ g(\xi) : g \in \mathbb{G}(\mathcal{F}) \} \subseteq M$. The orbit theorem tells us that $O_\xi$ carries a canonical topological structure:

**Theorem 1** (Sussmann [11]). For each point $\xi \in M$, the orbit $O_\xi$ is a connected immersed submanifold of $M$. The tangent space to $O_\xi$ at the point $x$ is the linear subspace of $T_x M$ spanned by the vectors $g_* f(x)$, $f \in \mathcal{F}$, $g \in \mathbb{G}(\mathcal{F})$, where $g_*$, $f : M \rightarrow TM$ is the pushforward of $f$ by $g$.

One of the main applications of the orbit theorem is in geometric control [14]. Let $\dot{x} = f(x, u)$, $x \in M$, $u \in U$ be a smooth controlled system on $M$, where $U$ is some control set. Then one applies the orbit theorem to $\mathcal{F} = \{ f(\cdot, u) : M \rightarrow TM : u \in U \}$. Notice that $O_\xi$ is in general larger than the reachable set from $\xi$, because both forward- and backward-in-time motions are permitted, whereas the reachable set only allows forward motions.

For our purposes, though, Sussmann’s theorem provides a natural recipe for constructing immersed submanifolds in a global fashion, as opposed to a local description based on an atlas of charts: Given an ambient manifold $M$, we choose a finite family $\mathcal{F} = \{ f_1, \ldots, f_m \}$ of vector fields on $M$, an initial condition $\xi \in M$, and a finite interval $[T_0, T_1]$ of the real line containing 0, and then consider a map

$$[T_0, T_1]^m \ni (t_1, \ldots, t_m) \mapsto e^{t_m} f_m \circ \cdots \circ e^{t_2} f_2 \circ e^{t_1} f_1 \xi \in M.$$  

This map sends the $m$-cube $[T_0, T_1]^m$ into a subset of the orbit $O_\xi$ of $\mathcal{F}$ through $\xi$, which is an immersed submanifold of $M$. It should be emphasized, however, that the map $(t_1, \ldots, t_m) \mapsto e^{t_m} f_m \circ \cdots \circ e^{t_1} f_1 \xi$ is not an immersion, unless the vectors $f_1(\xi), \ldots, f_m(\xi)$ are linearly independent and the point $(t_1, \ldots, t_m)$ lies in a sufficiently small neighborhood of 0 in $\mathbb{R}^m$.

**A. The encoder-decoder architecture**

Inspired by this observation, we describe an encoder-decoder architecture for unsupervised learning of immersed submanifolds. Let $A$ be a family of smooth maps $a : M \rightarrow [T_0, T_1]$. Then, for any $a_1, \ldots, a_m \in A$, the product map

$$a := a_1 \times \cdots \times a_m : M \rightarrow [T_0, T_1]^m$$

$$x \mapsto a(x) = (a_1(x), \ldots, a_m(x)).$$

will be an encoder that “represents” a point $x \in M$ as a (possibly lower-dimensional) tuple of times $a(x) = (a_1(x), \ldots, a_m(x)) \in [T_0, T_1]^m$.

Now fix a family $\mathcal{F}$ of vector fields $f : M \rightarrow TM$ and an initial condition $\xi \in M$. Then any map of the form

$$g = g_f : \{ T_0, T_1 \}^m \rightarrow M$$

$$t = (t_1, \ldots, t_m) \mapsto e^{t_f} g := e^{t_m} f_m \circ \cdots \circ e^{t_1} f_1 \xi,$$

will be a decoder, which outputs the state obtained from starting at $\xi$ and iteratively flowing along each vector field $f_j$ for duration $t_j$, for $j = 1, \ldots, m$. Observe that $g(\mathbb{R}, \ldots, \mathbb{R}) \subseteq O_\xi$, i.e., the image of $g$ is (a subset of) the orbit of $\mathcal{F} = \{ f_1, \ldots, f_m \}$ through $\xi$, which is an immersed submanifold of $M$. We will refer to the composition $G_{a, f}(\xi) := g_f \circ a : M \rightarrow M$ as a reconstruction map. The main idea here is that, by choosing $a \in A^m$, $f \in \mathcal{F}$, and $\xi \in M$, we automatically choose an immersed submanifold of $M$, namely the orbit $O_\xi$ of $\{ f_1, \ldots, f_m \}$ through $\xi$, and the reconstruction map $G_{a, f}(\xi)$ then allows us to map any point $x \in M$ to a point $\tilde{x} = G_{a, f}(\xi)(x) \in O_\xi$.

**B. The learning problem and the basic excess risk bound**

Now we proceed to formulate the learning problem. Consider a probability measure $\mu$ that is compactly supported on $M = \mathbb{R}^d$, and a collection $S$ of independent and identically distributed samples $X_1, \ldots, X_n \sim \mu$. We denote the support by $K := supp(\mu) \subset \mathbb{R}^d$. We would like to fit an immersed submanifold of $M$ to the data $S$.

Suppose we have some families $A$ and $\mathcal{F}$ from which the encoders $a_1, \ldots, a_m$ and vector fields $f_1, \ldots, f_m$ will be drawn, where $m$ and $[T_0, T_1]$ are fixed in advance; the initial condition $\xi$ will be drawn from $K$. We will denote by $\mathcal{G}$ the set of all reconstruction maps $G_{a, f}(\xi) : M \rightarrow M$. We can then define the expected risk of $G \in \mathcal{G}$.

$$L_\mu(G) := E_{\mu}(|X - G(X)|) = \int_K |x - G(x)| \mu(dx),$$

as well as the minimum risk $L_\mu^*(\mathcal{G}) := \inf_{G \in \mathcal{G}} L_\mu(G)$.

The minimum risk measures in some sense the inherent expressiveness of the model class $\mathcal{G}$. Given $\mu$, we can find some $G^* \in \mathcal{G}$ that (approximately) achieves $L_\mu^*(\mathcal{G})$. However, $\mu$ is in general unknown, so we attempt to learn $G^*$ from $S$ by minimizing the empirical risk $\frac{1}{n} \sum_{i=1}^n |X_i - G(X_i)|$ over $\mathcal{G}$. Observe that the empirical risk is a random variable, because the data $X_1, \ldots, X_n$ are random. We let $\tilde{G}$ be any minimizer of the empirical risk over $\mathcal{G}$ (of course, in practice one usually approximates $\tilde{G}$ using a numerical optimization routine such as gradient descent).

The generalization capacity of the model class $\mathcal{G}$ — which represents, roughly speaking, how well models tend to perform on data that are not seen during training but are drawn from the same distribution — is captured by its empirical Rademacher complexity

$$\mathbb{R}_n(\mathcal{G}) := E \left[ \sup_{G \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^n \varepsilon_i |X_i - G(X_i)| \right],$$

where $\varepsilon_1, \ldots, \varepsilon_n$ are independent Rademacher random variables, i.e., $\mathbb{P}(\varepsilon_i = \pm 1) = \frac{1}{2}$, that are independent of the training data $S$. This quantity measures how well the model
class is capable of fitting random noise — if the Rademacher complexity is large, then the learned model may generalize poorly to unseen data, whereas if the Rademacher complexity is small, then the model class is less able to exhibit high variability and perhaps generalizes better. The following excess risk bound is standard (see, e.g., [15]):

**Theorem 2.** Assume that $|x - G(x)|$ is bounded between 0 and $B < \infty$ for all $x \in K, G \in \mathcal{G}$. Then the following excess risk guarantee holds with probability at least $1 - \delta$:

$$L_\mu(\hat{G}) \leq L_\mu^*(\mathcal{G}) + 4 \mathbb{E} \mathcal{R}_n(\mathcal{G}) + B \sqrt{\frac{2 \log(\frac{1}{\delta})}{n}}.$$  

The main objective of this work is to bound the Rademacher complexity of the class $\mathcal{G}$ of encoder-decoder pairs with architecture as described previously. One can expect that the properties of and/or restrictions on the families $\mathcal{A}$ and $\mathcal{F}$, and the number of ‘layers’ $m$, will affect the Rademacher complexity. Namely, if $\mathcal{A}$ and $\mathcal{F}$ are themselves very expressive, then $\mathcal{R}_n(\mathcal{G})$ will tend to be larger, whereas if $\mathcal{A}$ and $\mathcal{F}$ are simple, then $\mathcal{R}_n(\mathcal{G})$ will tend to be smaller, and we wish to quantify this relationship. We will suppress absolute constants (i.e., ones that do not depend on any parameters of the problem) by writing $a \lesssim b$ as a shorthand for $a \leq Cb$ for some absolute constant $C > 0$.

### III. MAIN RESULT AND EXAMPLES

We impose the following assumptions on $\mathcal{A}$ and $\mathcal{F}$:

**Assumption 1.** $\mathcal{A}$ is equicontinuous on $K$.

**Assumption 2.** There exists a compact set $\tilde{K} \supseteq K$, such that $e^t f \xi \in \tilde{K}$ for all $t \in [T_0, T_1]^m, f \in \mathcal{F}^m, \xi \in K$. Moreover, $\mathcal{F}$ is uniformly bounded and equi-Lipschitz; there exist finite constants $L_0, L$, such that for every $f \in \mathcal{F}$

- $|f(x)| \leq L_0$ for all $x \in \mathbb{R}^d$
- $|f(x) - f(y)| \leq L|x - y|$ for all $x, y \in \mathbb{R}^d$.

**Remark 1.** If $\mathcal{F}$ is uniformly bounded and equi-Lipschitz on $\tilde{K}$ but not necessarily on $\mathbb{R}^d$, we can always ensure global boundedness and Lipschitz continuity by multiplying each $f \in \mathcal{F}$ by a $C^\infty$ bump function $\rho$ satisfying $\rho(\tilde{K}) \equiv 1$ and $\rho(\mathbb{R}^d \setminus \tilde{K}) \equiv 0$ for some compact set $\tilde{K}$ containing $K$, so that the flows $e^{\rho f(t)} \xi$ are unaffected on $\tilde{K}$ provided that $\xi \in K$.

Assumption 2 suffices to guarantee the existence and uniqueness of flow maps and the existence of a continuous comparison function $\beta : [0, \infty) \times \mathbb{R} \rightarrow [0, \infty)$ such that for every $f \in \mathcal{F}$ and every $\xi, \xi' \in \mathbb{R}^d$, we have

- $|e^{t f} \xi - e^{tf} \xi'| \leq \beta(|\xi - \xi'|, t)$
- $\beta(r, 0) = r$ and $\beta(0, t) = 0$ for all $r \geq 0$ and $t \in \mathbb{R}$
- $r \mapsto \beta(r, t)$ is monotonically increasing for each $t \in \mathbb{R}$

The second condition actually follows from the first by setting $t = 0$ or $\xi = \xi'$, respectively, and the last one follows from properties of ODEs given that the bound must hold for all initial conditions and times. We will also assume that $\beta$ is right-differentiable at zero in the first argument, which is without loss of generality as can be seen from the following.

Assuming nothing more about $\mathcal{F}$, we can form a worst-case estimate of $\beta$. A standard argument using Grönwall’s inequality [16] shows that if $f$ is globally $L$-Lipschitz and $x, x'$ are solutions to the initial value problems

$$\dot{x} = f(x), x(s) = \xi; \quad \dot{x}' = f(x'), x'(s) = \xi',$$

then we have $|x(t) - x'(t)| \leq \beta(|\xi - \xi'| e^{-Lt}, t)$ where $\beta(r, t) = r e^{L|t-s|}$ is a suitable comparison function. In fact, since every vector field in $\mathcal{F}$ is bounded in magnitude by $L_0$, $\beta(r, t) = \min\{r e^{L|t|}, r + 2L_0 |t|\}$ also works. However, it may be possible to improve upon this estimate depending on other properties of $\mathcal{F}$. This is explored further in the examples at the end of this section.

We will equip the sets $A_{|K}$ and $\mathcal{F}|_K$ with the corresponding $C^0$ metrics, i.e., for the restrictions of $a, a' \in A$ and $f, f' \in \mathcal{F}$ to $K$ and $\tilde{K}$ respectively, we let

$$\|a - a'||_{C^0} := \max_{x \in K} |a(x) - a'(x)|$$

and similarly for $\|f - f'||_{C^0}$ on $\tilde{K}$. The set $\tilde{K}$ will be equipped with the usual Euclidean ($\ell^2$) metric. For any metric space $(\Theta, \delta)$, we will write $N(\Theta, \delta, \delta)$ for its covering numbers.

Before stating our main result on the Rademacher complexity of $\mathcal{G}$, we introduce some additional notation:

- $D := \max_{x, x' \in K} |x - x'|$ is the Euclidean diameter of $\tilde{K}$, also giving the constant $B$ in Theorem 2;
- for $j = 0, 1, \ldots, \beta^j : [0, \infty) \rightarrow [0, \infty)$ are defined by
  - $\beta^0(r) := r$,
  - $\beta^j(r) := \max_{t \in [T_0, T_1]} \beta(r, t)$,
  - $\beta^{j+1}(r) := \beta(\beta^j(r))$, $j = 1, 2, \ldots$

since $r \mapsto \beta(r, t)$ is continuous and monotone increasing in $r$ for each $t$, the functions $r \mapsto \beta^j(r)$ are lower semicontinuous and monotone increasing;
- given the comparison function $\beta$, we define

$$\tilde{B} := \max_{t \in [T_0, T_1]} \left| \int_0^t \frac{\partial \beta}{\partial r}(0, t - s) \, ds \right|,$$

where $\frac{\partial \beta}{\partial r}(t)$ is the right partial derivative of $\beta$ with respect to $r$;
- for an arbitrary $\delta \geq 0$, let $\rho_1(\delta), \rho_2(\delta), \rho_3(\delta)$ be the largest nonnegative solutions $\delta_1, \delta_2, \delta_3$ to

$$\delta \geq \sum_{j=0}^{m-1} \beta^j(L_0 \tilde{B} \delta_1)$$

$$\delta \geq \sum_{j=0}^{m-1} \beta^j(\tilde{B} \delta_2)$$

$$\delta \geq \tilde{B}^m(\delta_3)$$

respectively (these solutions exist due to monotonicity and lower semicontinuity of $r \mapsto \beta^j(r)$).
Theorem 3. The Rademacher complexity (conditioned on the data $S$) of the class of reconstruction maps $G$ satisfies

$$R_n(G) \lesssim \frac{1}{\sqrt{n}} \inf \left\{ m \log N(A|K, \| \cdot \|_{C^0, \rho_1(\gamma_1)}) + m \log N(\mathcal{F}|K, \| \cdot \|_{C^0, \rho_2(\gamma_2)}) + \log N(K, \| \cdot \|_{C_\beta(\gamma_3)})^{1/2} \bigg\} \delta$$

where the infimum is over all positive $\gamma_1, \gamma_2, \gamma_3$ satisfying $\gamma_1 + \gamma_2 + \gamma_3 = 1$.

Theorem 3 gives a general recipe for upper-bounding the Rademacher complexity of $G$, and we can instantiate the bounds in some specific cases. To that end, we first assume that both $A$ and $\mathcal{F}$ admit finite-dimensional parameterizations, i.e., there exist positive integers $p, q$ and positive real constants $C_{A,K}$ and $C_{\mathcal{F},K}$, such that

$$N(A|K, \| \cdot \|_{C^0, \delta}) \lesssim \left( \frac{C_{A,K}}{\delta} \right)^p,$$

$$N(\mathcal{F}|K, \| \cdot \|_{C^0, \rho_2(\gamma_2)}) \lesssim \left( \frac{C_{\mathcal{F},K}}{\delta} \right)^{q'}.$$ 

This would be the case if, for instance, the elements of $\mathcal{F}$ are of the form $x \mapsto f(x; \theta)$, where the vector of parameters $\theta$ takes values in a bounded subset $\Theta$ of $\mathbb{R}^q$, and the parameterization is Lipschitz in $\theta$. Using these facts together with the fact that $N(K, \| \cdot \|_{\delta}) \lesssim (C_K/\delta)^d$ for some $C_K > 0$ and choosing (say) $\gamma_1 = \gamma_2 = \gamma_3 = \frac{1}{3}$ in Theorem 3, we get

$$R_n(G) \lesssim \frac{1}{\sqrt{n}} \int_0^D \left( m \log \left( \frac{C_{A,K}}{\rho_1(\delta/3)} \right) + m \log \left( \frac{C_{\mathcal{F},K}}{\rho_2(\delta/3)} \right) + d \log \left( \frac{C_K}{\rho_3(\delta/3)} \right) \right)^{1/2} \delta,$$

which is the best one can do without further assumptions on $\mathcal{F}$. We now consider some specific examples.

Example 1. Suppose we only allow positive times — that is, for all $\lambda > 0$, $\beta(r, t) = e^{-\lambda t}$, $\tilde{\beta}(r) = r$, $j = 0, 1, 2, \ldots$

\[ \hat{B} = \max_{t \in [0, T]} \left| \int_0^t e^{-\lambda (t-s)} ds \right| = \frac{1}{\lambda}. \]

A simple computation then gives

$$\rho_1(\delta) = \frac{\lambda}{mL_0}, \quad \rho_2(\delta) = \frac{\lambda}{m}, \quad \rho_3(\delta) = \delta,$$

and therefore we obtain the following from (5):

$$R_n(G) \lesssim \frac{1}{\sqrt{n}} \left( \frac{m^{3/2}}{\lambda} (C_{A,K} L_0 \sqrt{p} + C_{\mathcal{F},K} \sqrt{q}) + C_K \sqrt{d} \right).$$

Example 2. Consider all affine vector fields of the form $f(x) = Ax + u$, where the matrices $A \in \mathbb{R}^{d\times d}$ and the vectors $u \in \mathbb{R}^d$ are uniformly bounded: $\|A\| \leq 1$ ($\| \cdot \|$ denoting the spectral norm) and $|u| \leq 1$. Since

$$e^{t\bar{f}z} = e^{tA}z + \int_0^t e^{(t-s)A}u \, ds,$$

we can take $\bar{K} = B_2^0((R + 1)e^{mT})$, where $R = \max_{\xi \in \bar{K}} |\xi|$, $L := \max\{|T_0|, |T_1|\}$, and $B_2^0(r)$ is the $d$-dimensional Euclidean ball of radius $r$ centered at the origin. By Remark 1, we can construct a class $\mathcal{F}$ of vector fields that are affine on $\bar{K}$ and vanish outside a compact inflation of $\bar{K}$, and thus take $L_0 \lesssim R e^{mT}$, $L = 1$, $\beta(r, t) = r e^{|t|}$, and $\beta^j(r) = r e^{T_j}$.

The class $\mathcal{F}$ is parametrized by $\theta = (A, u)$, which takes values in a compact subset of $\mathbb{R}^{d \times d} \times \mathbb{R}^d$, so $q = d^2 + d$ and $C_{\mathcal{F},K} \lesssim R e^{mT}$. This shows that the Rademacher complexity $R_n(G)$ will have an exponential dependence on the number of layers $n$ and on $T$, although this can be removed under additional assumptions, e.g., $0 = T_0 < T_1 = T$ and all $A$ being uniformly Hurwitz, i.e., the real parts of all eigenvalues of $A$ are all smaller than $-\lambda$ for some $\lambda > 0$. The latter is a special case of the preceding example.

Example 3. Suppose that $\mathcal{F}$ consists of all vector fields of the form $f(x) = \sigma(Ax + u)$, where $\sigma : \mathbb{R}^{d} \to \mathbb{R}^d$ is a fixed bounded Lipschitz nonlinearity, i.e.,

$$|\sigma(x)| \leq 1 \quad \text{and} \quad |\sigma(x) - \sigma(y)| \leq |x - y|, \quad \forall x, y \in \mathbb{R}^d$$

and $A \in \mathbb{R}^{d \times d}$ and $u \in \mathbb{R}^d$ satisfy the same conditions as in Example 2. (The ODE $x = f(x)$ with $f$ of this form is a continuous-time recurrent neural net [17].) For any such $f$,

$$e^{t\bar{f}z} = e^{tA}z + \int_0^t e^{(t-s)A}u \, ds,$$

so Assumption 2 holds with $\bar{K} = B_2^0((R + mT)$ and $L_0 = L = 1$. The class $\mathcal{F}$ is parametrized by $\theta = (A, u) \in \mathbb{R}^{d \times d} \times \mathbb{R}^d$, so $q = d^2 + d$, but now $C_{\mathcal{F},K} \lesssim R + mT$.

In contrast to the preceding example, we now have $\beta(r, t) \leq \min\{e^{|t|}, r + 2|t|\}$, so in this setting it is possible for the Rademacher complexity to have polynomial dependence on $n$ and $T$ even without exponential stability.

IV. PROOF OF THEOREM 3

We first recall a standard technique for bounding expected suprema of random processes indexed by the elements of a metric space, the so-called Dudley entropy integral [18]:

Lemma 1. Let $(\mathcal{Z}_\theta)_{\theta \in \Theta}$ be a zero-mean subgaussian random process indexed by a metric space $(\Theta, d)$ — that is, for all $\theta, \theta' \in \Theta$, $E[\mathcal{Z}_\theta] = 0$ and

\[ \mathbb{P}(|\mathcal{Z}_\theta - \mathcal{Z}_{\theta'}| \geq t) \leq 2 \exp \left( - \frac{t^2}{2d^2(\|\theta - \theta'\|)} \right), \quad \forall t > 0. \]

Then we have

$$E\left[ \sup_{\theta \in \Theta} \mathcal{Z}_\theta \right] \lesssim \int_0^D \sqrt{\log N(\Theta, d, \delta)} d\delta$$

where $N(\Theta, d, \delta)$ are the $\delta$-covering numbers and $D$ is the diameter of $(\Theta, d)$.
To apply the lemma, we consider the class $G$ of all reconstruction maps $G_{a,f,\xi} : \mathbb{R}^d \to \mathbb{R}^d$ indexed by $a \in \mathcal{A}^m$, $f \in \mathcal{F}^m$, and $\xi \in K$. Fix an $n$-tuple of points $(x_1, \ldots, x_n)$ in $K$ and consider the Rademacher process

$$Z_G := \frac{1}{\sqrt{n}} \sum_{i=1}^n \epsilon_i |x_i - G(x_i)|$$

indexed by $\mathcal{G}$, where $\epsilon_1, \ldots, \epsilon_n$ are i.i.d. Rademacher random variables. Then we have the following:

**Lemma 2.** The process (6) is subgaussian w.r.t. the metric

$$d(G, G') = \|G - G'\|_{C^0(K)} := \max_{x \in K} |G(x) - G'(x)|.$$ 

Since $G(K) \subseteq \tilde{K}$ for every $G \in \mathcal{G}$, the $C^0(K)$-diameter of $\mathcal{G}$ is bounded by $D$, the $\ell^2$ diameter of $\tilde{K}$. Therefore, the empirical Rademacher complexity of $\mathcal{G}$ is bounded by

$$\mathbb{R}_n(\mathcal{G}) \leq \frac{1}{\sqrt{n}} \int_0^D \sqrt{\log N(\mathcal{G}, \| \cdot \|_{C^0}, \delta)} \, d\delta.$$  

(7)

Our next order of business is to obtain upper bounds on the covering numbers $N(\mathcal{G}, \| \cdot \|_{C^0}, \delta)$.

### A. Covering number bounds

Let $\hat{\mathcal{A}}^m := \{ \hat{a} : \mathbb{R}^d \to [T_0, T_1]^m \}$ be a finite set of encoders that forms a minimal $\delta_1$-net of the metric space $(\mathcal{A}^m|K, \| \cdot \|_{\infty(C^0)})$. That is to say,

$$\sup_{a \in \mathcal{A}^m} \min_{\hat{a} \in \hat{\mathcal{A}}^m} \| a - \hat{a} \|_{\infty(C^0)} = \sup_{a \in \mathcal{A}^m} \min_{\hat{a} \in \hat{\mathcal{A}}^m} \max_{j=1}^m \max_{x \in K} |a_j(x) - \hat{a}_j(x)| \leq \delta_1.$$ 

Such a finite set exists because $\mathcal{A}^m|K$ consists of uniformly bounded and uniformly equicontinuous vector-valued maps supported on a compact set, hence is itself compact.

Similarly, let $\hat{\mathcal{F}}^m := \{ f : \mathbb{R}^d \to (\mathbb{R}^d)^m \}$ be a finite set of $m$-tuples of vector fields that forms a minimal $\delta_2$-net of $(\mathcal{F}^m|K, \| \cdot \|_{\infty(C^0)})$, and let $N(\mathcal{F}^m|K, \| \cdot \|_{\infty(C^0)}, \delta_2)$ denote the corresponding covering number. Finally, let $\hat{K} = \{ \hat{\xi} \in \hat{\mathcal{K}} \}$ be a finite set of points that forms a minimal $\delta_3$-net of $(K, \| \cdot \|)$ with covering number $N(\hat{K}, \| \cdot \|, \delta_3)$.

**Proposition 1.** Let $\hat{\mathcal{G}} := \{G_{\hat{a}, \hat{f}, \hat{\xi}} : \mathbb{R}^d \to \mathbb{R}^d : (\hat{a}, \hat{f}, \hat{\xi}) \in \hat{\mathcal{A}}^m \times \hat{\mathcal{F}}^m \times \hat{K} \} \subset \mathcal{G}$ where $\hat{\mathcal{A}}^m$, $\hat{\mathcal{F}}^m$, $\hat{K}$ are minimal $\delta_1$, $\delta_2$, $\delta_3$-nets of $\mathcal{A}^m|K$, $\mathcal{F}^m|K$, $K$, respectively. Then $\hat{\mathcal{G}}$ forms a $\delta$-net of $N(\mathcal{G}, \| \cdot \|_{C^0}, \delta)$ with

$$\delta \leq \sum_{j=0}^{m-1} \beta_j^l (L_0 B d_1) + \sum_{j=0}^{m-1} \beta_j^b (B d_2) + \tilde{\beta}^m (\delta_3),$$

where the functions $\tilde{\beta}^l$ are defined in (1) and the constant $B$ is defined in (2).

**Proof.** Fix any $a, f, \xi$ and consider the reconstruction map

$$G_{a,f,\xi} : \mathbb{R}^d \to \mathbb{R}^d, \quad x \mapsto e^{a(x)} f_m \circ \cdots \circ e^{a(x)} f_1 \xi.$$ 

Let $\hat{a}, \hat{f}, \hat{\xi}$ be the closest elements in their respective coverings. Then by the triangle inequality

$$\|G_{\hat{a}, \hat{f}, \hat{\xi}} - G_{a,f,\xi}\|_{C^0} \leq \|G_{\hat{a}, \hat{f}, \hat{\xi}} - G_{\hat{a}, \hat{f}, \hat{\xi}}\|_{C^0} + \|G_{\hat{a}, \hat{f}, \hat{\xi}}(x) - G_{a,f,\xi}(x)\|_{C^0} + \|G_{a,f,\xi} - G_{a,f,\xi}\|_{C^0} =: D_1 + D_2 + D_3.$$ 

We now estimate the three error terms $D_1$, $D_2$, and $D_3$ individually using Lemmas 3–5 in the next section.

To estimate $D_1$, given a fixed initial condition $\xi$, fixed vector fields $(f_1, \ldots, f_m)$, and two tuples of times $(t_1, \ldots, t_m)$ and $(t_1', \ldots, t'_m)$ such that $|t_j - t_j'| \leq \delta_1$ for every $j = 1, \ldots, m$, we want to bound the difference between decoder outputs $e^{t_m} f_m \circ \cdots \circ e^{t_1} f_1 \xi$ and $e^{t'_m} f_m \circ \cdots \circ e^{t'_1} f_1 \xi$. We can equivalently consider a single tuple of times $(1, \ldots, 1)$ and two tuples of scaled vector fields $(t_1 f_1, \ldots, t_m f_m)$ and $(t'_1 f_1, \ldots, t'_m f_m)$, which yields the same decoder outputs. In this case, the difference between the vector fields is bounded by $\|t_j f_j - t'_j f_j\|_{C^0(K)} = |t_j - t'_j| \|f_j\|_{C^0(K)} \leq \delta_0 d_1$. Now, if a vector field $f$ admits the comparison function $\beta(r, t)$, then, for any $r \in [T_0, T_1]$, the rescaled vector field $r f$ admits the comparison function $(r, t) \mapsto \beta(r, \tau t)$. We can therefore apply Lemma 5 with $(1, \ldots, 1) \leftrightarrow (t_1, \ldots, t_m)$, $t_j f_j \leftrightarrow t'_j f_j$, and comparison function $(r, t) \mapsto \max_{r \in [T_0, T_1]} \beta(r, \tau t)$ to get

$$D_1 = \max_{x \in K} |G_{\hat{a}, \hat{f}, \hat{\xi}}(x) - G_{a,f,\xi}(x)| \leq \sum_{j=0}^{m-1} \tilde{\beta}^l (L_0 B d_1).$$

For $D_2$, we apply Lemma 5 and use the fact that $\|f_j - f_j\|_{C^0(K)} \leq \delta_2$ for all $j$, as well as the monotonicity of $r \mapsto \tilde{\beta}^l(r)$, to get

$$D_2 = \max_{x \in K} |G_{\hat{a}, \hat{f}, \hat{\xi}}(x) - G_{a,f,\xi}(x)| \leq \sum_{j=0}^{m-1} \tilde{\beta}^l (B d_2).$$

Finally, for $D_3$, we apply Lemma 4 with $k = m$ and use the fact that $|\xi - \hat{\xi}| \leq \delta_3$ to get

$$D_3 = \max_{x \in K} |G_{\hat{a}, \hat{f}, \hat{\xi}}(x) - G_{a,f,\xi}(x)| \leq \tilde{\beta}^m (\delta_3).$$

The proof is completed by taking the supremum over all $(a, f, \xi) \in \mathcal{A}^m \times \mathcal{F}^m \times K$. 

Using this proposition, we can now estimate the covering numbers of $\mathcal{G}$ as follows: Fix any $\delta \geq 0$ and any $\gamma_1, \gamma_2, \gamma_3 > 0$ such that $\gamma_1 + 2 \gamma_2 + 2 \gamma_3 = 1$. Then, with $\rho_1(\cdot)$, $\rho_2(\cdot)$, $\rho_3(\cdot)$ defined in (3), we have

$$\sum_{j=0}^{m-1} \tilde{\beta}^l (L_0 B \rho_1(\gamma_1 \delta)) + \sum_{j=0}^{m-1} \tilde{\beta}^b (B \rho_2(\gamma_2 \delta)) + \tilde{\beta}^m (\rho_3(\gamma_3 \delta)) \leq \delta.$$ 

Therefore, letting $\hat{\mathcal{A}}^m$, $\hat{\mathcal{F}}^m$, and $\hat{K}$ be the minimal $\rho_1(\gamma_1 \delta)$-, $\rho_2(\gamma_2 \delta)$-, and $\rho_3(\gamma_3 \delta)$-nets of $\mathcal{A}^m|K$, $\mathcal{F}^m|K$, and $K$ respec-
tively, we see that
\[
\log \mathcal{N}(\mathcal{G}, \| \cdot \|_{C^0(K)}, \delta) \leq \log \mathcal{N}(\mathcal{A}^m|K, \| \cdot \|_{\ell^\infty(C^0)}, \rho_1(\gamma_1 \delta)) \\
+ \log \mathcal{N}(\mathcal{F}^m|\tilde{K}, \| \cdot \|_{\ell^\infty(C^0)}, \rho_2(\gamma_2 \delta)) \\
+ \log \mathcal{N}(K, \| \cdot \|, \rho_3(\gamma_3 \delta))
\]

We can further upper-bound the quantities on the right-hand side using the fact that
\[
\log \mathcal{N}(\mathcal{A}^m|K, \| \cdot \|_{\ell^\infty(C^0)}, \delta) \leq m \log \mathcal{N}(A|K, \| \cdot \|_{C^0}, \delta), \\
\log \mathcal{N}(\mathcal{F}^m|\tilde{K}, \| \cdot \|_{\ell^\infty(C^0)}, \delta) \leq m \log \mathcal{N}(F|\tilde{K}, \| \cdot \|_{C^0}, \delta).
\]

The bound (4) follows by substituting the above covering number estimates into the Dudley entropy integral in (7) and then optimizing over all choices of \(\gamma_1, \gamma_2, \gamma_3\).

\section{B. Lemmas on iterated flows}

The proofs for the following lemmas are omitted due to space limitations; see the full version [19].

\begin{lemma}
For any \(f, f' \in \mathcal{F}\), any \(t \in [T_0, T_1]\), and any \(\xi \in \mathbb{R}^d\) such that \(e^{tf}\xi \in \tilde{K}\) for all \(s \in [T_0, T_1]\), we have
\[
|e^{tf}\xi - e^{tf'}\xi| \leq \tilde{B}\|f - f'\|_{\ell^\infty(C^0)},
\]
where \(\tilde{B}\) is defined in Eq. (2).
\end{lemma}

\begin{lemma}
For all \(k\)-tuples \(t \in [T_0, T_1]^k\) and \(f \in \mathcal{F}^k\) and for all points \(\xi, \xi'\),
\[
|e^{tf}\xi - e^{tf'}\xi'| \leq \tilde{B}^k(|\xi - \xi'|).
\]
\end{lemma}

\begin{lemma}
For all \(m\)-tuples \(t \in [T_0, T_1]^m\) and \(f, f' \in \mathcal{F}^m\) and all points \(\xi \in K\),
\[
|e^{tf}\xi - e^{tf'}\xi| \leq \sum_{j=1}^{m} \tilde{B}^{m-j}\|f - f'\|_{C^0(\tilde{K})}.
\]
\end{lemma}

\section{V. Conclusions}

In this work we have developed an encoder-decoder architecture for learning immersed submanifolds based on the construction in Sussmann’s orbit theorem, and provided high-probability bounds on its generalization error. Capitalizing on the natural recursive structure present in differential equations allows for complex generative models to be built from comparatively simple vector field parameterizations. This architecture generalizes some well-known learning algorithms to the nonlinear setting. For example, principal component analysis (PCA) is recovered by choosing orthogonal projection encoders and taking \(\mathcal{F}\) to consist of constant vector fields. Various nonlinear generalizations of PCA can also be recovered by choosing an appropriate family of vector fields that enables the application of a nonlinear kernel to the input. Thus, applications to parametric manifold learning and nonlinear dimensionality reduction are practicable. We can also find utility in this architecture for high-dimensional sampling problems and generative modeling, since the latent space (of times) can be much simpler and of lower dimension than the complexity of features produced by the decoder.

This formulation naturally lends itself to a neural net implementation based on recent work on neural ODEs [20], since the compositional structure of deep neural nets — i.e., composition of nonlinear layers — is clearly manifested in the recursive structure of ODE flows, \(e^{tf} = e^{(t-s)f} \circ e^{sf}\), an even richer class of models can be obtained by allowing controlled ODEs [14].

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