Manifold learning from a teacher’s demonstrations

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Abstract

We consider the problem of manifold learning. Extending existing approaches of learning from randomly sampled data points, we consider contexts where data may be chosen by a teacher. We analyze learning from teachers who can provide structured data such as points, comparisons (pairs of points), demonstrations (sequences). We prove results showing that the former two do not yield notable decreases in the amount of data required to infer a manifold. Teaching by demonstration can yield remarkable decreases in the amount of data required, if we allow the goal to be teaching up to topology. We further analyze teaching learners in the context of persistence homology. Teaching topology can greatly reduce the number of datapoints required to infer correct geometry, and allows learning from teachers who themselves do not have full knowledge of the true manifold. We conclude with implications for learning in humans and machines.

In machine learning, learners are assumed to operate in a relatively simplified problem space: data points sampled by a random process. Humans learn from a richer, stronger context. Two aspects that have received the most attention are the fact that data may be chosen by a more knowledgeable informant, such as a teacher [Shafto and Goodman, 2008, Shafto et al., 2014, Zhu, 2015], and that the data points may themselves be structured into pairs and sequences, as in comparison [Shafto and Goodman, 2008] and demonstration [Kuhl et al., 1997, Brand et al., 2002a]. In this paper, we consider how having teachers who select structured data may affect the complexity of learning.

We investigate the implications of teaching using structured data for the problem of manifold learning. Manifold learning is known to be a hard problem and is therefore a candidate domain where teaching with structured data might improve learning. Indeed, recent work has suggested it may be fruitful to view the problem as only learning up to topology, called Topological Data Analysis (TDA). Though TDA has demonstrated interesting results, including on perceptual problems [Carlsson et al., 2008], we know that even learning the topology of a manifold is hard. Nevertheless, many human learning problems—including perception [Tenenbaum, 1998, Jansen and Niyogi, 2006, Chen et al., 2018] and action learning [Slama et al., 2015]—are commonly viewed as manifold learning problems. Perhaps related to the fact that manifold learning is hard, many of these domains are viewed as benefiting from teaching.

Our goal is to understand theoretical bounds on learning manifolds and their topology from teaching via structured data, which we expect to inform debates in machine learning and human learning. We investigate manifolds because this is the learning problem, as most frequently posed. We particularly investigate the topology of manifolds for several reasons. First, the decomposition of learning into grounded and more abstract aspects parallels common wisdom across human and machine learning, which have converged on hierarchical (“deep”) models of learning. Second, teaching topology will prove to be data-efficient for manifold learning applications, such as clustering where only information about the global structure of manifold (e.g. number of connected components, number of holes, etc.) is needed. Third, teaching will be able to proceed without full knowledge of the geometry, and the requirement for the teacher can be relaxed by just knowing the homotopy type of the manifold.

We begin with preliminaries in Section 1. Section 2 provides results related to teaching the topology of manifolds via data points, comparisons, and demonstrations, showing that demonstrations can yield vastly more efficient teaching through the connection between groups and homology of manifolds. Section 3 considers teaching in a much more practical setting that allows the teacher to teach with partial knowledge and unconstrained data. Section 4 discusses related work and Section 5 provides concluding discussions.

1 Preliminaries

In this section, we will provide a brief overview of the necessary background, and refer the reader to [Hatcher, 2000, Munkres, 2000] for a complete introduction.

In machine learning, the manifold assumption states that high dimensional data in the real world are typically concentrated on a much lower dimensional manifold rather than every region of the possible domain [Zhu and Goldberg, 2009]. For instance, typically white noise does not appear in images of natural scenes, and natural
images do not occupy the entire space of possible pixel configurations. Therefore learning the manifold on which the data lie on or near is an important task. Because the difficulty of inferring the geometry of an arbitrary manifold is bounded by its worst local feature, quantified as the reach (defined below) of the manifold, we may only aim to reduce the sample complexity of learning a manifold by focusing on its global properties, which are encoded by the topology.

An $m$-dim manifold $\mathcal{M}$ is a topological object that locally resembles Euclidean space $\mathbb{R}^m$ near each point. They naturally arise as solution sets of a system of equations [Lee, 2010]. In this paper, $\mathcal{M}$ is an orientable compact sub-manifold in $\mathbb{R}^n$. We mainly focus on low dimensional manifolds such as curves (1-dim) and surfaces (2-dim). However, teaching methods developed in the following sections can be directly used to convey low dimensional topological features of any manifold.

The classical result on closed surfaces will be used, which states that any connected orientable closed surface is homeomorphic to either the sphere or the connected sum of $g$ tori, where $g \geq 1$ represents the genus.

Algebraic topology provides powerful methods to study topological features of a space using algebraic tools. One main idea is that two topological spaces $X$ and $Y$ are considered to have ‘the same shape’ if one space can continuously deform into the other one. Formally, two continuous maps $h_0, h_1 : X \rightarrow Y$ are homotopic if there exists a continuous function $H : X \times [0,1] \rightarrow Y$ from the product of the space $X$ with the unit interval $[0,1]$ to $Y$ such that $H(x,0) = h_0(x)$ and $H(x,1) = h_1(x)$ hold for any $x \in X$. The spaces $X$ and $Y$ are said to be homotopy equivalent or to have the same homotopy type if there exists two maps $f : X \rightarrow Y$ and $g : Y \rightarrow X$ such that $f \circ g$ and $g \circ f$ are homotopic to the identity map between $X$ and $Y$ respectively. A space is said to be contractible if it is homotopy equivalent to a point.

Among all the topological invariants shared by spaces with the same homotopy type, homology is of the greatest interest to manifold learning. Because homology captures abstract topological properties of the underlying data space $\mathcal{M}$ in simple algebraic notions such as numbers and groups. There are several models of the homology theory. Throughout this paper, we will use simplicial homology with coefficient $\mathbb{Z}_2$. For each dimension $k$, the $k$-th homology group of $\mathcal{M}$, denoted by $H_k(\mathcal{M})$ is a commutative group in form of $\mathbb{Z}_2 \times \cdots \times \mathbb{Z}_2$. Roughly speaking, each copy of $\mathbb{Z}_2$ represents a $k$-dim ‘hole’ of $\mathcal{M}$ and the amount of copies represents the total number of independent $k$-dim ‘holes’ of $\mathcal{M}$. For example, $H_0(\mathcal{M}) = \mathbb{Z}_2 \times \mathbb{Z}_2$ indicates that $\mathcal{M}$ has two connected components, and non-trivial 1-st homology group $H_1(\mathcal{M})$ suggests that $\mathcal{M}$ contains 1-dim hole(s) and thus not contractible.

Another important characteristic of a manifold $\mathcal{M}$ that has been extensively used in manifold learning is the reach, which reflects the geometric aspect of $\mathcal{M}$ [Peifferman et al., 2016, Aamari et al., 2017]. The reach $\tau > 0$ of a manifold $\mathcal{M}$ is the largest number such that any point at distance less than $\tau$ from $\mathcal{M}$ has a unique nearest point on $\mathcal{M}$. Intuitively, around $\mathcal{M}$ one can freely roll a ball of radius less than its reach $\tau$. The reach measures the narrowest bottleneck-like width of $\mathcal{M}$, which also quantifies the curvature of $\mathcal{M}$.

For the formalism of teaching-learning algorithms, we consider $\mathcal{A}$ as a class of learning algorithms that construct approximations of $\mathcal{M}$ and/or identify the homotopy type of $\mathcal{M}$ from a set of data points sampled from $\mathcal{M}$. Examples of such algorithms are available in [Cheng et al., 2005, Niyogi et al., 2008, Boissonnat and Ghosh, 2014].

Given a manifold $\mathcal{M}$, a collection of data points $\mathcal{D} \subset \mathcal{M}$ is called a teaching set with respect to $\mathcal{A}$ if there exists a learning algorithm $\mathcal{A} \in \mathcal{A}$ that recovers the homotopy type of $\mathcal{M}$ using $\mathcal{D}$. $|\mathcal{D}|$ denotes the size of $\mathcal{D}$. A teaching set $\mathcal{D}$ is said to be minimal w.r.t. $\mathcal{M}$ if $|\mathcal{D}| \leq |\mathcal{D}^*|$ for any teaching set $\mathcal{D}^*$ of $\mathcal{M}$. Further, $\mathcal{D}$ is a minimal teaching set w.r.t. the homotopy type of $\mathcal{M}$ if $\mathcal{D}$ is a teaching set for some $\mathcal{M}'$ of the same homotopy type as $\mathcal{M}$ and $|\mathcal{D}| \leq |\mathcal{D}^*|$ for any teaching set $\mathcal{D}^*$ of a manifold homotopy equivalent to $\mathcal{M}$. The size of a minimal teaching set is called the minimal teaching number.

## 2 Structured data and manifold teaching

Our approach is inspired by human teaching together with their corresponding class of learners: examples [Shepard et al., 1961], comparisons [Gentner and Markman, 1994], or demonstrations [Brand et al., 2002b]. In this section, we propose three corresponding styles of methods to teach the topology of a manifold using structured data: isolated data points (individual examples), pairs of points (comparisons), and sequential data points (demonstrations). In particular, we provide lower bounds for teaching complexity of each method.

### 2.1 Manifold teaching from sample points

The pioneering work in [Niyogi et al., 2008] introduced a framework to reconstruct manifolds from random sampling. Their work can be rephrased as a manifold teaching problem. Suppose two agents, which we call a teacher and a learner, wish to communicate a manifold $\mathcal{M} \subset \mathbb{R}^n$. In their setting, the teacher passes a collection of randomly sampled data points $\mathcal{D} = \{x_1, \ldots, x_k\}$ to the learner, who then builds a manifold by a learning algorithm in the class $\mathcal{A}(\epsilon)$: the learner first picks a parameter $\epsilon \in \mathbb{R}^+$, then for each $x_i \in \mathcal{D}$, makes an
n-dimensional ball $B_r(x_i)$ centered at $x_i$ of radius $\epsilon$. Here $n$ is the dimension of the ambient space which can be inferred from data points’ coordinate size. The union of all these balls $U_i(\mathcal{D}) = \cup_{x \in \mathcal{D}} B_r(x)$ constitutes the learned space.

The main result in [Niyogi et al., 2008] provides an estimation $N_\epsilon$ on the number of data that are needed to guarantee that the learned space $U_\epsilon$ and the target manifold $\mathcal{M}$ are homotopy equivalent with high confidence. $N_\epsilon$ depends on the confidence level, the volume and the reach of $\mathcal{M}$, and also the learner’s choice of $\epsilon$.

Considering $N_\epsilon$ as a sufficient bound on the minimal teaching number of $\mathcal{M}$, we seek a necessary condition. The calculation of $N_\epsilon$ proposed in [Niyogi et al., 2008] requires knowledge about the critical features of $\mathcal{M}$ (volume and reach), which translated to our context implies that either the teacher knows the true manifold. In Section 3, we will show that this assumption can be relaxed in many practical cases.

Suppose that the teacher uses the class of algorithms $\mathcal{A}(\epsilon)$, what is a minimal teaching set to convey the homotopy type of a manifold $\mathcal{M}$? The case when $\mathcal{M}$ is a non-contractible 1-dim manifold is extremely neat. Since every such $\mathcal{M}$ is homotopy equivalent to a circle, at least three points are needed as explained below.

**Example 2.1.** Let $S^1$ be a unit circle embedded in $\mathbb{R}^2$, and $\mathcal{A}(\epsilon)$ be the class of learning algorithms described above. It is clear that any data set with only one or two points will result contractible $U_\epsilon$ for any choice of $\epsilon$. However, as illustrated in Figure 1(a), with three equidistant points sampled on $S^1$, any learner $\mathcal{A}(\epsilon)$ with $\frac{\sqrt{3}}{2} \leq \epsilon < 1$ will recover the correct topology of $S^1$ from the union of three connected disks with a hole in the middle. Thus the minimal teaching number for a circle is three.

Now suppose that $\mathcal{M}$ is a closed orientable surface. Two basic examples are given below.

**Example 2.2.** Let $S^2$ be a unit sphere. Only four points are needed: four vertices of an inscribed regular tetrahedron. Any learner $\mathcal{A}(\epsilon)$ with $\frac{2\sqrt{2}}{3} \leq \epsilon < 1$, recovers the correct topology of $S^2$.

![Figure 1: Teaching sets for 1-dim manifolds](image)

**Example 2.3.** Let $T^2$ be a torus embedded in $\mathbb{R}^3$ as shown in Figure 2. $T^2$ can be obtained by rotating the red circle $l_1$ around the green circle $l_2$. Denote the radii of $l_1$ and $l_2$ by $r_1$ and $r_2$ respectively. Two 1-dim holes of $T^2$ are represented by $l_1$ and $l_2$. As in Example 2.1, each $l_i$ needs at least three teaching points. Since the learner $\mathcal{A}(\epsilon)$ picks one $\epsilon$ for all data points, more data points are needed for $l_i$ when $\frac{\sqrt{4}}{2} r_i \geq r_j$, where $i, j \in \{1, 2\}$ and $i \neq j$. Hence to find the minimal teaching set for the homotopy type of $T^2$, we may assume that $r_1 = r_2 = r$. Suppose that any three data points sharing a circle in Figure 2 are equidistant points. Then $D_1 = \{a_1, a_2, a_3, b_1, c_1\}$ can be used to teach $l_1$ and $l_2$. To recover the only 2-dim hole of $T^2$, it is natural to add $\{b_2, b_3, c_2, c_3\}$ into $D_1$ to complete the red dotted circles going through $b_1$ and $c_1$. Ideally, $\epsilon$-balls centered at these 9 points should form a torus. However, there are large undesirable gaps left open between the red circles because the learner is restricted to pick $\frac{\sqrt{2}}{2} r < \epsilon < r$.

We now compute how many extra points are needed to fill in all these gaps. Direct calculation shows that the radius of the dashed blue circle $l_3$ is 2.5$r$ and nine equidistant data points on $l_3$ are needed to teach it with $\frac{\sqrt{4}}{2} r < \epsilon < r$. If we rotate $l_1$ around $l_2$ nine times with each step $2\pi/9,$ then the trace of $\{a_1, a_2, a_3\}$ produces 27 data points (including all 9 points in $D_1$). With these 27 points, we almost form a torus but still have many
small gaps. One may count that in total there are 27 such gaps. So 54 points are enough. Moreover, notice that the inner green circle $l_2$ is over taught, one may check that 3 teaching points can be removed from $l_2$. Hence we may teach $T^2$ with 51 points.

The approach we used in Example 2.3 can be generalized to all orientable surfaces.

**Proposition 2.4.** Let $M_g \subset \mathbb{R}^3$ be a closed orientable surface with genus $g$. Then the minimal teaching number for the homotopy type of $M_g$ with respect to $A(\epsilon)$ is bounded by $49g + 2$.

**Proof.** We will proceed by induction. When $g = 1$, $M_1$ is homotopy equivalent to $T^2$. So the homotopy type of $M_1$ can be taught by 51 points. Suppose that the claim holds for any $M_g$ with $g < n$. Then when $g < n$, $M_{g,1}$, surface with genus $g$ and 1 boundary component, can be taught by $49g + 1$ points. Notice that there exists a $M_n$ which can be obtained by gluing a $M_{1,1}$ with a $M_{n-1,1}$. Hence we may teach $M_n$ with $[49 + 1] + [49(n - 1) + 1] = 49n + 2$ data points. □

**Remark 2.5.** The teaching set prescribed in Proposition 2.4 for $M_g$ is robust to parameter $\epsilon$. For different choices of $\epsilon$, if the learned space $U_\epsilon$ is not homotopy equivalent to the target manifold $M_g$, then $U_\epsilon$ is either contractible or disconnected. Therefore, if the learner and the teacher agree the target manifold is connected and not contractible, then the learner is able to learn the correct manifold (homology) using any proper choice of $\epsilon$.

**Remark 2.6.** Let $M_{g,b} \subset \mathbb{R}^3$ be a genus $g$ orientable surface with $b$ boundary components. Note that $M_{g,b}$ can be obtained from $M_g$ by removing $b$ disconnect disks. Therefore, the minimal teaching number of $M_{g,b}$ with respect to $A(\epsilon)$ is bounded by $49g + 2 - b$.

The above analysis suggests that teaching manifolds by isolated data is not always efficient: the examples show that even a simple manifold as a regular torus requires a large set of teaching points. Based on manifold’s topological features, below we propose two new classes of teaching algorithms.

### 2.2 Manifold teaching from comparison

Manifolds are locally Euclidean. It is natural to teach a manifold by showing its local pieces first, then patching them together to obtain a global structure. In Section 2.1 each local piece is an $\epsilon$-ball of the ambient dimension and each such ball is taught by a data point at its center. In this section we will describe a class of algorithms where each local piece is a square of the intrinsic dimension. [Shafto and Goodman, 2008] showed that a square in $\mathbb{R}^2$ can be efficiently taught by a pair of vertices, which forms one of its diagonals. In the same spirit, a pair of points in $\mathbb{R}^n$ determines a collection of squares. For example, let $\overline{a_1a_2}$ be the segment connecting two points $a_1$ and $a_2$ in $\mathbb{R}^3$. There are infinitely many squares in $\mathbb{R}^3$ having $\overline{a_1a_2}$ as its diagonal. These squares can be parameterized, for example, by their normal vectors.

As a direct extension, 2-dim manifolds embedded in $\mathbb{R}^3$ can be taught by passing pairs of data points. In this setting, the teacher passes $D = \{(p_1, q_1), \ldots, (p_m, q_m)\}$ a collection of pairs of data points to the learner. The learner builds a manifold by a learning algorithm in the class $A(n_1)$: for each pair $(p_i, q_i)$, the learner first picks a direction $n_i$, then construct a square with diagonal $\overline{p_iq_i}$ and normal vector $n_i$. The union of these squares $U = \cup_{(p_i, q_i) \in D} S_{n_i}(p_i, q_i)$ is the learned space. To make the $A(n_1)$ robust to the choice of $n_i$, we may further assume that the teacher and the learner agree that $(*)$: if two pairs share a common point, then their corresponding squares sharing an edge.

The assumption $(*)$ implicitly indicates how squares are chosen and glued together. For example, let $o = (0, 0, 0), p_1 = (1, 1, 0), p_2 = (1, 0, 1)$ be three points in $\mathbb{R}^3$ and the teaching set be $D = \{(o, p_1), (o, p_2)\}$. A priori, the learner has infinitely many choices over normal vectors for both pairs. However, as two output squares shall share an edge, it is only possible if the normal vectors chosen for $(o, p_1)$ and $(o, p_2)$ are $(0, 0, 1)$ and $(0, 1, 0)$ respectively.

More generally, higher dimensional manifolds can also be taught by pairs. To teach an $m$-dim manifold, the only modification should be made to the learning algorithm $A(n_1)$ is that for each teaching pair, instead of making a square, the learner should make an $m$-dim cube. Correspondingly, in assumption $(*)$, two cubes should share a face (instead of an edge) if their teaching pairs have a common point.

![Figure 3: 1-toroid and 2-toroid](image)
Example 2.7. A torus can be viewed as the boundary of an 1-toroid made by 8 cubes as shown in Figure 3(a). The boundary is made by 32 squares. Hence a torus can be taught by 32 pairs of points consisting at most 32 distinct data points (each point may be reused in at least two different pairs).

Proposition 2.8. Let $M_g \subset \mathbb{R}^3$ be a closed orientable surface with genus $g$. Then the minimal teaching number for the homotopy type of $M_g$ with respect to $A(n)$ is bounded by $20g + 12$ pairs.

Proof. There exists a $M_g$ can be viewed as the boundary of a $g$-toroid. A $g$-toroid can be obtained from a $(g-1)$-toroid by adding a handle. For example, Figure 3(b) is a 2-toroid obtained from (a) by adding a handle consisting 5-cubes. Inductively, we can show that $5g + 3$ cubes may build a $g$-toroid. Each cube has 4-faces on the boundary. Hence the boundary of such cubic $g$-toroid is made by $20g + 12$ squares. □

2.3 Manifold teaching from demonstrations

A main task in manifold teaching is passing the correct topology. This task forces large amount of data for any local to global teaching procedure due to the locally Euclidean nature of manifolds. In this section we will describe a method that teaches the topology directly from demonstrations where each demonstration is a sequence of data points describing a loop.

Teaching with sequences of data points is efficient because topologies of manifolds are intuitively captured by loops in various dimensions. As in Example 2.7, a unit circle can be taught by three points. In fact, any sequence of data points describing a loop.

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red curves for the first time, assumption (\$2\$) ensures the learner always picks the red curves during the entire learning process.

**Example 2.10.** The torus in Example 2.3 can be taught by a sequence of four sequences:

$$D_{\text{torus}} = \langle [a_1, a_2, a_3, a_1], [b_1, b_2, b_3, b_1], [c_1, c_2, c_3, c_1], [a_1, a_2, a_3, a_1] \rangle$$

as shown in Figure 3. This teaching set only contains the 9 basic points which fits our initial intuition.

**Proposition 2.11.** Let $$M_g \subset \mathbb{R}^3$$ be a closed orientable surface with genus $$g \geq 2$$. Then the minimal teaching number of $$M_g$$ with respect to $$A(I)$$ is bounded by $$3g - 3$$ sequences, where each sequence consists of at most 4 data points.

**Proof.** A classical result of surfaces states that for any $$M_g$$ there is a system of $$3g - 3$$ disjoint simple closed curves which cut $$M_g$$ into pairs of pants (see for example, \[Farb and Margalit, 2011\]). Note that each simple closed curve can be taught by a sequence of 4 points; each pair of pants can be taught by a sequence that consists of three sequences representing its boundary curves. Moreover, two legs of a pair of pants can be glued along their boundary curves through a sequential data. For instance, two blue boundary curves in Figure 3(b) can be glued by $$[[b_1, b_2, b_3, b_1], [b_4, b_5, b_1]]$$. Hence the claim holds. □

There are two levels—topology and geometry—in learning a manifold $$M$$. In the topological level, the goal is to convey the homotopy type of $$M$$, whereas in the geometric level, one aims to minimize the Hausdorff distance between the learned space and the target manifold. Teaching by points as in Sec 2.1 combines these two objectives together. According to the main result in \[Niyogi et al., 2008\], the learned space $$U_\epsilon$$ is topologically the same as the true manifold $$M$$ with high confidence only if $$\epsilon$$ is chosen close to the reach of $$M$$. This also indicates that every point in $$U_\epsilon$$ is $$\epsilon$$ close to $$M$$. In contrast, teaching by comparison and demonstration prioritize topology which leads to a large reduction on the minimal teaching number. However, the distance between the learned space and $$M$$ could be large. To close this gap, we show in the following section that even learners interested in the geometry of $$M$$ would benefit from learning the topological information.

### 3 Learning from teacher with partial knowledge

All teaching methods discussed in previous sections assume teacher has full access to the true manifold. However, in reality, the teacher often does not know the underlying manifold and often does not have full control over which data can be used to teach. In this section, we consider teaching in a much more practical scenario that allows a teacher, who may have limited knowledge, to teach with unconstrained data. We illustrate how this would assist the learner to improve their estimation of the relevant topological and geometrical information from the data.

Following the standard setting of topological data analysis \[Carlsson, 2009\] \[Chazal and Michel, 2017\], we assume that the data $$D$$ is a finite set of points sampled from the true manifold $$M$$. Using an algorithm in class $$A(\epsilon)$$ (Sec 2.1) with different $$\epsilon$$’s, the learner obtains a summary of estimations of $$M$$ in form of persistent homology (Sketched below, see details in \Edelsbrunner and Harer, 2010\ \[Chazal et al., 2016\]). Rather than picking a teaching set directly from $$M$$, the teacher first selects a subset $$D_T$$ from $$D$$, then passes $$D_T$$ to the learner in a proper sequential format according to algorithm $$A(I)$$ (Sec 2.3) to demonstrate desired topological features of $$M$$.

Roughly speaking, persistent homology tracks topological changes as the learner’s approximation of $$M$$ varies with $$\epsilon$$. Based on algorithm $$A(\epsilon)$$, for each $$\epsilon \in \mathbb{R}^+$$, the learner builds a union of balls $$U_\epsilon = \bigcup_{x \in D} B_\epsilon(x)$$, centered at $$D$$ with radii equal to $$\epsilon$$. Consider the nested family of $$\{U_\epsilon\}_{x \in \mathbb{R}^+}$$. Given a non-negative integer $$k$$, the inclusion $$U_{r_1} \subset U_{r_2}$$ for $$r_1 < r_2$$, naturally induces a linear map between their $$k$$-th homology groups $$H_k(U_{r_1})$$ and $$H_k(U_{r_2})$$. The set of all $$k$$-th homology groups $$\{H_k(U_{r})\}_{r \in \mathbb{R}^+}$$ together with all the linear maps induced by inclusions form a persistence module, which can be intuitively viewed as \[H_k(U_0) \rightarrow \cdots \rightarrow H_k(U_{r_1}) \rightarrow \cdots \rightarrow H_k(U_{r_2}) \rightarrow \cdots\]

It is shown in \[Chazal et al., 2016\] that when $$D$$ is finite, the persistence module obtained for a fixed $$k$$ can be decomposed into direct sum of interval modules of the form:

$$H_k(U_b) \cup H_k(U_d) \to 0 \to \cdots \to Z_2 \to 0 \to \cdots$$

where $$Z_2 \to Z_2$$ is the identity map. Recall that each $$k$$-th homology group is a direct sum of $$\mathbb{Z}_2$$, with each copy of $$\mathbb{Z}_2$$ represents a $$k$$-dim loop. Hence, essentially each interval module records the lifespan of a loop, which can be depicted by a interval $$[b, d]$$ from the birth radius $$b$$ to the death radius $$d$$ of the loop. Therefore, each
persistence module forms a collection of intervals called the persistence barcode. Conventionally, the longer an interval in the barcode, the more persistent, and thus relevant, is the corresponding topological feature.

As discussed before, the difficulty of learning a manifold $M$ increases dramatically as the reach of $M$ drops. Now we illustrate how teaching helps in these situations by the following example. Our example is based on a two dimensional manifold embedded in $\mathbb{R}^2$, but method works for all manifolds.

**Example 3.1.** Let the true manifold $M$ be the blue barbell shaped annulus shown in Figure 5 with reach $\tau = 0.26$. Assume that the learner analyzes randomly sampled data by TDA and the teacher knows that $M$ contains a 1-dim hole. Based on $\mathcal{A}(I)$, three distinct points are required to form a teaching sequence for this hole. When fewer than three data points are observed by the learner, the teacher would simply wait until more data were collected. Suppose that the learner gets three data $D_3 = \{a, b, c\}$ as shown. The corresponding persistence barcode of $D_3$ is empty for $H_1$ (no 1-dim loop is ever formed for any choice of $\epsilon$). With $D_1$, the teacher may teach by marking these points sequentially as for example $[a, b, c, a]$. Comparing the teacher’s demonstration with the barcode, the learner would realize that $M$ is homotopy equivalent to a circle and currently points gathered are not sufficient to extract any accurate geometrical information.

Further suppose that the learner intends to estimate the geometry of $M$ and so more points are sampled. A given data set $D$ is called feasible, if the learner is able to derive the true geometry of $M$ from $D$ with some $\epsilon$, i.e. if there exists $\epsilon^* < \tau = 0.26$ such that $U_{\epsilon^*}(D)$ is homotopy equivalent to $M$. To estimate the lower bound on size of a feasible data set, we randomly sample data sets from $M$ with increasing sizes and 20 simulations for each size. Empirically it shows that feasible data sets appear only after $|D| > 150$ and and appears in every simulation for $|D| \geq 500$.

Figure 5(a) shows the persistence barcode for a data set of size 500. The red bars are the longest four intervals for $H_0$, which reflects the number of connected components. After $\epsilon > 0.156$, only one red bar remains which indicates $U_{\epsilon}$ contains a single component for any $\epsilon > 0.156$. The green bars are the intervals for $H_1$ (ignoring intervals of length less than 0.05), which represents the number of 1-dim holes. The top green bar spans over (0.158, 1.751) and indicates that there is a 1-dim loop forms at $\epsilon = 0.158$ and persists until $\epsilon = 1.751$. The bottom green bar spans over (0.357, 1.747) and indicates that another 1-dim loop forms at $\epsilon = 0.357$ and persists until $\epsilon = 1.747$. All randomly sampled data sets of size 500 exhibit similar persistence barcode with two long intervals for $H_1$ as shown. Focusing on the range of $\epsilon$ where 1-dim holes exist, on average 78% choice of $\epsilon$ (with variance 0.0002) indicates two 1-dim loops over all simulations. Thus, without teaching, the learner would likely to conclude a wrong topological information, $H_1(M) = \mathbb{Z}_2 \times \mathbb{Z}_2$, with high confidence. In contrast, with a teaching set of three points, the learner is able to not only infer the correct topology immediately after teaching but also accurately estimate the geometry of $M$ by focusing on $U_{\epsilon}$ with $0.158 < \epsilon < 0.357$.

Figure 5(b) plots the average learning accuracy of $M$’s geometry for different types of learners. The blue curve shows the learners with a topological teacher who are assumed to follow a Bernoulli distribution since they are able to infer the correct geometry with every feasible data set. The orange curve is corresponding to learners who choose $\epsilon$ uniformly from the interval where barcode for $H_1(M)$ is not empty (Variances are omitted as their magnitudes are bounded above by 0.01). The green curve shows learners, who approximate $M$ by $U_{\epsilon}$ with the most persistent homology, stay incorrect on geometry even with increasing data size. Clearly learner’s acquisition of geometry are accelerated by teaching topology.

Persistent homology has started to attract attention in machine learning [Carlsson et al., 2008, Chazal et al., 2013, Li et al., 2014, Reininghaus et al., 2015]. However, leveraging these topological features for learning poses considerable challenges because the relevant topological information is not carried by the whole persistence barcode but is concentrated in a small region of $\epsilon$ that may not be obvious [Holer et al., 2017]. Teaching by demonstration resolves these challenges by allowing the the learner to extract the most suitable topological information after the correct homology appears in the persistence barcode, and zooming the analysis of $M$’s geometry into the most appropriate range of $\epsilon$ with high data efficiency.

More importantly, teaching by demonstration allows accumulation of information across learners, whereas other forms of teaching can only transmit information from an already knowledgeable teacher. As pointed out in Sec 2.1, the method of teaching by sampling points essentially assumes that the teacher knows the true manifold.

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$^5$It is possible that $U_{\epsilon}(D)$ is homotopy equivalent to $M$ for $\epsilon > \tau$. However the top and the bottom of the narrow middle part of $M$ will be connected up in such $U_{\epsilon}(D)$, which leads to wrong geometry.

$^6$The barcode was constructed using the GHDHI library [Maria et al., 2014].
However, given the intractability of manifold learning in general, there is no plausible way for the teacher to have access to $\mathcal{M}$. On such accounts, teaching does not resolve the true challenge of learning and instead passes off the problem to a teacher for whom the learning problem does not exist. The key advantage of teaching from demonstrations is that it allows the teacher to convey critical information of $\mathcal{M}$ without knowing the entire manifold. For example, let $\mathcal{M}$ be a torus as in Figure 2, with $r_1 << r_2$. The teacher may only have enough observations to conclude that there is a loop homotopy equivalent to the green circle $l_2$. With sequential data, the teacher could easily pass the only loop $l_2$ he observed, which allows the learner to focus on the region of $\epsilon$ where $l_2$ exists.

In addition, from a teacher’s perspective, much less data is needed to learn the topology of an irregular manifold $\mathcal{M}$ than its geometry. For instance, let $\mathcal{M}$ be the 1-dim manifold shown in Figure 1(b). Denote the reach of $\mathcal{M}$ by $\tau$ and the radius of the left arc in $\mathcal{M}$ by $r$. Note that the teacher only needs $\tau$-dense data to learn the topology of $\mathcal{M}$, whereas $\tau$-dense data to learn the geometry. In fact, for any manifold $\mathcal{M}$, we may define its topological reach $\eta$ to be the largest number such that $U_\epsilon(\mathcal{M})$ is homotopy equivalent to $\mathcal{M}$ for any $\epsilon \leq \eta$, where $U_\epsilon(\mathcal{M}) = \bigcup_{p \in \mathcal{M}} B_\epsilon(p)$. According to Proposition 3.2 in [Niyogi et al., 2008], for the same confidence level, points needed to achieve $\epsilon$-dense is polynomial increasing with $1/\epsilon$. Therefore when $\mathcal{M}$ is irregular, i.e. $\tau$ is significantly less than $\eta$, the amount of data needed to achieve $\eta$-dense is much fewer than $\tau$-dense. Since the topology of $U_\epsilon(\mathcal{M})$ remains the same for data beyond $\eta$-dense, it requires much less data to learning the topology of an irregular manifold than its geometry.

### 4 Related work

There are three main areas of related work: formal approaches to manifold learning, machine teaching, and human learning from teaching.

[Niyogi et al., 2008] describe a PAC learning framework for learning the homology of a manifold, which we directly build upon in Section 2.1. Extensions have, for example, directly tested the manifold hypothesis [Fefferman et al., 2016], and estimated the reach of a manifold [Aamari et al., 2017]. This line of work assumes data are isolated sample points and are not formulated by a teacher.

The literatures on machine teaching, algorithmic teaching, and Bayesian teaching investigate the implications of having a teacher for machine learning algorithms. Machine teaching has focused on the problem of teaching standard machine learning algorithms, most commonly formalizing the single best set of teaching points (maximize the probability of the true hypothesis) [Zhu, 2015, Liu and Zhu, 2016]. Algorithmic teaching similarly investigates the problem of teaching but within the deterministic algorithmic learning framework [Doliwa et al., 2014]. Bayesian teaching has been investigated with standard probabilistic machine learning algorithms [Eaves Jr and Shafto, 2016, Yang and Shafto, 2017]. All of these assume that the relevant data are points, rather than more structured data and all require that the teacher knows the correct answer.

The literature on human learning emphasizes the structured nature of the data presented by teachers in the forms of pairing data to form comparisons [Shafto and Goodman, 2008, Shafto et al., 2014] and series data to form demonstrations [Brand et al., 2002a, Ho et al., 2016]. Both the machine teaching and Bayesian teaching approaches listed above have also been applied to teaching human learners in simple cognitive science-style experiments. Bayesian teaching has been used model more realistic phenomena such as infant-directed speech [Eaves Jr et al., 2016].
5 Conclusions

We considered the problem of teaching low-dimensional manifolds using structured data, which extends mathematical approaches to manifold learning and research in machine learning toward learning contexts more consistent with the richness of human learning. Building on prior work in manifold learning, we formalize teaching manifolds from data and comparisons, observe that contrary to intuition, teaching does not facilitate learning as much as one would expect due to constraints imposed by the reach of the manifold. Considering learning from teaching demonstrations—sequences of data points—we show that learning can be greatly facilitated by teaching. This approach relies on separating teaching the geometry of the manifold itself from teaching the topology of the manifold. Focusing on teaching only the topology, we show that sequences of points can be used to represent the homology groups of the manifold, which compactly capture important abstract structure that can be used to facilitate future learning. Moreover, this relaxes the overly stringent and implausible requirement that the teacher must know the manifold exactly. Instead, the teacher can proceed with only an accurate reconstruction of the topologically-relevant reach, which is almost always less stringent than the true reach. Due to the polynomial increase in data required to achieve reductions in the reach, this is a substantial improvement. Future work may extend this approach toward more naturalistic learning problems faced by humans or solved by machine learning. The approaches are not restricted to manifold teaching and it would be interesting to explore teaching more general mathematical objects with low dimensional topological structures, such as graphs, CW-complexes and even groups.

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