Distance Preserving Embeddings for General *n*-Dimensional Manifolds

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Abstract

Low dimensional embeddings of manifold data have gained popularity in the last decade. However, a systematic finite sample analysis of manifold embedding algorithms largely eludes researchers. Here we present two algorithms that embed a general n-dimensional manifold into \mathbb{R}^d (where d only depends on some key manifold properties such as its intrinsic dimension, volume and curvature) that guarantee to approximately preserve all interpoint geodesic distances.

Keywords: Manifold Learning, Isometric Embeddings, Non-linear Dimensionality Reduction, Nash's Embedding Theorem

1. Introduction

Finding low dimensional representations of manifold data has gained popularity in the last decade. One typically assumes that points are sampled from an n-dimensional manifold residing in some high-dimensional ambient space \mathbb{R}^D and analyzes to what extent their low dimensional embedding maintains some important manifold property, say, interpoint geodesic distances.

Despite an abundance of manifold embedding algorithms, only a few provide any kind of distance preserving guarantee. Isomap (Tenebaum et al., 2000), for instance, provides an asymptotic guarantee that as one increases the amount of data sampled from an underlying manifold, one can approximate the geodesic distances between the sample points well (Bernstein et al., 2000). Then, under a very restricted class of *n*-dimensional manifolds, one can show that the *n*-dimensional embedding returned by Isomap is approximately distance preserving on the input samples.

Unfortunately any kind of systematic finite sample analysis of manifold embedding algorithms—especially for general classes of manifolds—still largely eludes the manifold learning community. Part of the difficulty is due to the restriction of finding an embedding in exactly n dimensions. It turns out that many simple manifolds (such as a closed loop, a cylinder, a section of a sphere) cannot be isometrically embedded in \mathbb{R}^n , where n is the manifold's intrinsic dimension. If these manifolds reside in some high dimensional ambient space, we would at least like to embed them in a lower dimensional space (possibly slightly larger than n) while still preserving interpoint geodesic distances.

Here we are interested in investigating low-dimensional distance-preserving manifold embeddings more formally. Given a sample X from an underlying n-dimensional manifold $M \subset \mathbb{R}^D$, and an embedding procedure $\mathcal{A}: M \to \mathbb{R}^d$ that (uses X in training and) maps points from M into some low dimensional space \mathbb{R}^d , we define the quality of the embedding \mathcal{A} as $(1 \pm \epsilon)$ -isometric if for all $p, q \in M$:

$$(1 - \epsilon)D_G(p, q) \le D_G(\mathcal{A}(p), \mathcal{A}(q)) \le (1 + \epsilon)D_G(p, q),$$

where D_G denotes the geodesic distance. We would like to know i) can one come up with an embedding algorithm \mathcal{A} that achieves $(1 \pm \epsilon)$ -isometry for *all* points in M? ii) how much can one reduce the target dimension d and still have $(1 \pm \epsilon)$ -isometry? and, iii) what kinds of restrictions (if any) does one need on M and X?

Since \mathcal{A} only gets to access a finite size sample X from the underlying non-linear manifold M, it is essential to assume certain amount of curvature regularity on M. Niyogi et al. (2008) provide a nice characterization of manifold curvature via a notion of manifold condition number that will be useful throughout the text (details later).

Perhaps the first algorithmic result for embedding a general n-dimensional manifold is due to Baraniuk and Wakin (2009). They show that an orthogonal linear projection of a well-conditioned n-dimensional manifold $M \subset \mathbb{R}^D$ into a sufficiently high dimensional random subspace is enough to approximately preserve all pairwise geodesic distances. To get $(1\pm\epsilon)$ -isometry, they show that a target dimension d of size about $O\left(\frac{n}{\epsilon^2}\log\frac{VD}{\tau}\right)$ is sufficient, where V is the n-dimensional volume of the manifold and τ is the manifold's curvature condition number. This result was sharpened by Clarkson (2008) and Verma (2011) by completely removing the dependence on ambient dimension D and partially substituting the curvature-condition τ with more average-case manifold properties. In either case, the $1/\epsilon^2$ dependence is troublesome: if we want an embedding with all distances within 99% of the original distances (i.e., $\epsilon=0.01$), the bounds require the dimension of the target space to be at least 10,000!

1.1 Our Contributions

In this work, we give two algorithms that achieve $(1 \pm \epsilon)$ -isometry where the dimension of the target space is *independent* of the isometry constant ϵ . As one expects, this dependency shows up in the sampling density (i.e. the size of X) required to compute the embedding. The first algorithm we propose is simple and easy to implement but embeds the given n-dimensional manifold in $\tilde{O}(2^{cn})$ dimensions¹ (where c is an absolute constant). The second algorithm, a variation on the first, focuses on minimizing the target dimension. It is computationally more involved and serves a more theoretical purpose: it shows that one can embed the manifold in just $\tilde{O}(n)$ dimensions.

We would like to highlight that both of our proposed algorithms work for a very general class of well-conditioned manifolds. There is no requirement that the underlying manifold is connected, or is globally isometric (or even globally diffeomorphic) to some subset of \mathbb{R}^n as is frequently assumed by several manifold embedding algorithms. In addition, unlike

^{1.} $\tilde{O}(\cdot)$ notation suppresses the logarithmic dependence on quantities that depend on the intrinsic geometry of the underlying manifold, such as its volume and curvature-condition terms.

spectrum-based embedding algorithms in the literature, our algorithms yield an explicit embedding that cleanly embeds out-of-sample data points, and provide isometry guarantees over the entire manifold (not just the input samples).

As we shall discuss in the next section, our algorithms are heavily inspired by Nash's embedding technique (Nash, 1954). It is worth noting that the techniques used in our proof are different from what Nash uses in his work; unlike traditional differential-geometric settings, we can only access the underlying manifold through a finite size sample. This makes it difficult to compute quantities (such as the curvature tensor and local functional form of the input manifold, etc.) that are important in Nash's approach for constructing an isometric embedding. Our work provides insight on how and under what conditions can one use just the samples to construct an approximate isometric embedding of the underlying manifold. In that sense, this work can be viewed as an algorithmic realization of Nash's Embedding Theorem.

2. Isometrically Embedding *n*-Dimensional Manifolds: Intuition

Given an underlying n-dimensional manifold $M \subset \mathbb{R}^D$, we shall use ideas from Nash's embedding (Nash, 1954) to develop our algorithms. To ease the burden of finding a $(1 \pm \epsilon)$ -isometric embedding directly, our proposed algorithm will be divided in two stages. The first stage will embed M in a lower dimensional space without having to worry about preserving any distances. Since interpoint distances will potentially be distorted by the first stage, the second stage will focus on adjusting these distances by applying a series of corrections. The combined effect of both stages is a distance preserving embedding of M in lower dimensions. We now describe the stages in detail.

2.1 Embedding Stage

We shall use the random projection result by Clarkson (2008) (with ϵ set to a constant) to embed M into $d = \tilde{O}(n)$ dimensions. This gives an easy one-to-one low-dimensional embedding that doesn't collapse interpoint distances. Note that a projection does contract interpoint distances; by appropriately scaling the random projection, we can make sure that the distances are contracted by at most a constant amount, with high probability.

2.2 Correction Stage

Since the random projection can contract different parts of the manifold by different amounts, we will apply several corrections—each corresponding to a different local region—to stretchout and restore the local distances.

To understand a single correction better, we can consider its effect on a small section of the contracted manifold. Since manifolds are locally linear, the section effectively looks like a contracted n-dimensional affine space. Our correction map needs to restore distances over this n-flat.

For simplicity, let's temporarily assume n=1 (this corresponds to a 1-dimensional manifold), and let $t \in [0,1]$ parameterize a unit-length segment of the contracted 1-flat. Suppose we want to stretch the segment by a factor of $L \geq 1$ to restore the contracted distances. How can we accomplish this?

Perhaps the simplest thing to do is apply a linear correction $\Psi: t \mapsto Lt$. While this mapping works well for individual local regions, it turns out that this mapping makes it difficult to control the interference between different corrections with overlapping localities.

We instead use extra coordinates and apply a non-linear map $\Psi: t \mapsto (t, \sin(Ct), \cos(Ct))$ where C controls the stretch-size. Note that such a spiral map stretches the length of the tangent vectors by a factor of $\sqrt{1+C^2}$, since $\|\Psi'\| = \|d\Psi/dt\| = \|(1,C\cos(Ct),-C\sin(Ct))\| = \sqrt{1+C^2}$. Now since the geodesic distance between any two points p and q on a manifold is given by the expression $\int \|\gamma'(s)\|ds$, where γ is a parameterization of the geodesic curve between points p and q (that is, length of a curve is infinitesimal sum of the length of tangent vectors along its path), Ψ stretches the interpoint geodesic distances by a factor of $\sqrt{1+C^2}$ on the resultant surface as well. Thus, to stretch the distances by a factor of L, we can set $C:=\sqrt{L^2-1}$.

Now generalizing this to a local region for an arbitrary n-dimensional manifold, let $U := [u^1, \ldots, u^n]$ be a $d \times n$ matrix whose columns form an orthonormal basis for the (local) contracted n-flat in the embedded space \mathbb{R}^d and let $\sigma^1, \ldots, \sigma^n$ be the corresponding shrinkages along the n orthogonal directions. Then one can consider applying an n-dimensional analog of the spiral mapping: $\Psi: t \mapsto (t, \Psi_{\sin}(t), \Psi_{\cos}(t))$, where $t \in \mathbb{R}^d$

$$\Psi_{\sin}(t) := (\sin((Ct)_1), \dots, \sin((Ct)_n)), \text{ and } \Psi_{\cos}(t) := (\cos((Ct)_1), \dots, \cos((Ct)_n)).$$

Here C is an $n \times d$ "correction" matrix that encodes how much of the surface needs to stretch in the various orthogonal directions. It turns out that if one sets C to be the matrix SU^{T} , where S is a diagonal matrix with entry $S_{ii} := \sqrt{(1/\sigma^i)^2 - 1}$ (recall that σ^i was the shrinkage along direction u^i), then the correction Ψ precisely restores the shrinkages along the n orthonormal directions on the resultant surface (see Section 5.2.1 for a detailed derivation).

This takes care of the local regions individually. Now, globally, since different parts of the contracted manifold need to be stretched by different amounts, we localize the effect of the individual Ψ 's to a small enough neighborhood by applying a specific kind of kernel function known as the "bump" function in the analysis literature, given by (see also Figure 5 middle)

$$\lambda_x(t) := \mathbf{1}_{\{\|t-x\|<\rho\}} \cdot e^{-1/(1-(\|t-x\|/\rho)^2)}.$$

Applying different Ψ 's at different parts of the manifold has an aggregate effect of creating an approximate isometric embedding.

We now have a basic outline of our algorithm. Let M be an n-dimensional manifold in \mathbb{R}^D . We first find a contraction of M in $d = \tilde{O}(n)$ dimensions via a random projection. This embeds the manifold in low dimensions but distorts the interpoint geodesic distances. We estimate the distortion at different regions of the projected manifold by comparing a sample from M (i.e. X) with its projection. We then perform a series of corrections—each applied locally—to adjust the lengths in the local neighborhoods. We will conclude that restoring the lengths in all neighborhoods yields a globally consistent approximately isometric embedding of M. See also Figure 1.



Figure 1: A simple example demonstrating our embedding technique on a 1-dimensional manifold. Left: The original 1-dimensional manifold in some high dimensional space. Middle: A low dimensional mapping of the original manifold via, say, a linear projection onto the vertical plane. Different parts of the manifold are contracted by different amounts – distances at the tail-ends are contracted more than the distances in the middle. Right: Final embedding after applying a series of spiraling corrections. Small size spirals are applied to regions with small distortion (middle), large spirals are applied to regions with large distortions (tail-ends). Resulting embedding is isometric (i.e., geodesic distance preserving) to the original manifold.

As briefly mentioned earlier, a key issue in preserving geodesic distances across points in different neighborhoods is reconciling the interference between different corrections with overlapping localities. Based on exactly how we apply these different local Ψ 's gives rise to our two algorithms. For the first algorithm, we shall allocate a fresh set of coordinates for each correction Ψ so that the different corrections don't interfere with each other. Since a local region of an n-dimensional manifold can potentially have up to $O(2^{cn})$ overlapping regions, we shall require $O(2^{cn})$ additional coordinates to apply the corrections, making the final embedding dimension of $\tilde{O}(2^{cn})$ (where c is an absolute constant). For the second algorithm, we will follow Nash's technique (Nash, 1954) more closely and apply Ψ maps iteratively in the same embedding space without the use of extra coordinates. At each iteration we need to compute a pair of vectors normal to the embedded manifold. Since locally the manifold spreads across its tangent space, these normals indicate the locally empty regions in the embedded space. Applying the local Ψ correction in the direction of these normals gives a way to mitigate the interference between different Ψ 's. Since we don't use extra coordinates, the final embedding dimension remains $\tilde{O}(n)$.

3. Preliminaries

Let M be a smooth, n-dimensional compact Riemannian submanifold of \mathbb{R}^D . Note that we do not have any further topological restrictions on M; it may or may not have a boundary, or may or may not be orientable. We will frequently refer to such a manifold as an n-manifold.

Since we will be working with samples from M, we need to ensure certain amount of curvature regularity. Here we borrow the notation from Niyogi et al. (2008) about the condition number of M.

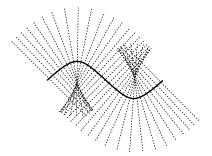


Figure 2: Tubular neighborhood of a manifold. Note that the normals (dotted lines) of a particular length incident at each point of the manifold (solid line) will intersect if the manifold is too curvy.

Definition 1 (condition number (Niyogi et al., 2008)) Let $M \subset \mathbb{R}^D$ be a compact Riemannian manifold. The condition number of M is $\frac{1}{\tau}$, if τ is the largest number such that the normals of length $r < \tau$ at any two distinct points $p, q \in M$ don't intersect.

The condition number is based on the notion of "reach" introduced by Federer (1959) and is closely related to the Second Fundamental Form of the manifold. Intuitively, it captures the complexity of a manifold in terms of the manifold's curvature. If M has condition number $1/\tau$, we can, for instance, bound the directional curvature at any $p \in M$ by τ . Figure 2 depicts the normals of a manifold. Notice that long non-intersecting normals are possible only if the manifold is relatively flat. Hence, the condition number of M gives us a handle on how curvy can M be. As a quick example, let's calculate the condition number of an n-dimensional sphere of radius r (embedded in \mathbb{R}^D). Note that in this case one can have non-intersecting normals of length less than r (since otherwise they will start intersecting at the center of the sphere). Thus, the condition number of such a sphere is 1/r. Henceforth we shall assume that M is well-conditioned, that is, M has condition number $1/\tau$. There are several useful properties of well-conditioned manifolds that would be helpful throughout the text; these are outlined in Appendix A.

Since we make minimal topological assumptions on M, even a well-conditioned M can have computational degeneracies: M, for instance, can have an unbounded number of well-conditioned connected components, yielding unusually large cover sizes. Since we make use of a random projection for the Embedding Stage, it is essential to have good manifold covers. Thus in order to avoid degenerate cases, we shall assume covering regularity on M.

Definition 2 (manifold regularity) Let $M \subset \mathbb{R}^D$ be an n-manifold with condition number $1/\tau$. We call M as C_M -regular, if for any $r \leq \tau/2$, the r-covering number of M is of size at most $(C_M/r)^n$, where C_M is a universal constant dependent only on intrinsic properties of M (such as its n-dimensional volume, etc.). That is, there exists a set $S \subset M$ of size at most $(C_M/r)^n$ such that for all $p \in M$, exists $x \in S$ such that $||p-x|| \leq r$.

We will use the notation $D_G(p,q)$ to indicate the geodesic distance between points p and q where the underlying manifold is understood from the context, and ||p-q|| to indicate

the Euclidean distance between points p and q where the ambient space is understood from the context.

To correctly estimate the distortion induced by the initial contraction mapping, our algorithm needs access to a high-resolution sample from our underlying manifold.

Definition 3 (bounded manifold cover) Let $M \subset \mathbb{R}^D$ be a Riemannian n-manifold. We call $X \subset M$ an α -bounded (ρ, δ) -cover of M if for all $p \in M$ and ρ -neighborhood $X_p := \{x \in X : ||x - p|| < \rho\}$ around p, we have

- there exist points $x_0, \ldots, x_n \in X_p$ such that $\left| \frac{x_i x_0}{\|x_i x_0\|} \cdot \frac{x_j x_0}{\|x_j x_0\|} \right| \le 1/2n$, for $i \ne j$. (local spread criterion)
- $|X_p| \le \alpha$. (local boundedness criterion)
- exists point $x \in X_p$ such that $||x p|| \le \rho/2$. (covering criterion)
- for any n+1 points in X_p satisfying the local spread criterion, let \hat{T}_p denote the n-dimensional affine space passing through them (note that \hat{T}_p does not necessarily pass through p). Then, for any unit vector \hat{v} in \hat{T}_p , we have $|\hat{v} \cdot \frac{v}{\|v\|}| \geq 1 \delta$, where v is the projection of \hat{v} onto the tangent space of M at p. (tangent space approximation criterion)

The above is an intuitive notion of manifold sampling that can estimate the local tangent spaces. Curiously, we haven't found such "tangent-space approximating" notions of manifold sampling in the literature. We do note in passing that our sampling criterion is similar in spirit to the (ϵ, δ) -sampling (also known as "tight" ϵ -sampling) criterion popular in the Computational Geometry literature (see e.g. Dev et al., 2002; Giesen and Wagner, 2003).

Remark 4 Given an n-manifold M with condition number $1/\tau$, and some $0 < \delta \le 1$. If $\rho \le \tau \delta/16n$, then there exists a 2^{13n} -bounded (ρ, δ) -cover of M (see Appendix B).

We can now state our two algorithms.

4. The Algorithms

Inputs. We assume the following quantities are given:

- (i) n the intrinsic dimension of M.
- (ii) $1/\tau$ the condition number of M.
- (iii) X an α -bounded (ρ, δ) -cover of M.
- (iv) ρ the ρ parameter of the cover.

Notation. Let ϕ be a random orthogonal projection map that maps points from \mathbb{R}^D into a random subspace of dimension d (n < d < D). We will have d to be about O(n). Set $\Phi := (2/3)(\sqrt{D/d})\phi$ as a scaled version of ϕ . Since Φ is linear, Φ can also be represented as a $d \times D$ matrix. In our discussion below we will use the function notation and the matrix notation interchangeably, that is, for any $p \in \mathbb{R}^D$, we will use the notation $\Phi(p)$ (applying function Φ to p) and the notation Φp (matrix-vector multiplication) interchangeably.

For any $x \in X$, let x_0, \ldots, x_n be n+1 points from the set $\{x' \in X : ||x-x'|| < \rho\}$ such that $\left|\frac{x_i-x_0}{\|x_i-x_0\|}\cdot\frac{x_j-x_0}{\|x_j-x_0\|}\right| \leq 1/2n$, for $i\neq j$ (cf. Definition 3). Let F_x be the $D\times n$ matrix whose column vectors form some orthonormal basis of the n-dimensional subspace spanned by the vectors $\{x_i - x_0\}_{i \in [n]}$. Note that F_x serves as a good approximation to the tangent spaces at different points in the neighborhood of $x \in M \subset \mathbb{R}^D$.

Estimating local contractions. We estimate the contraction caused by Φ at a small enough neighborhood of M containing the point $x \in X$, by computing the "thin" Singular Value Decomposition (SVD) $U_x \Sigma_x V_x^{\mathsf{T}}$ of the $d \times n$ matrix ΦF_x and representing the singular values in the conventional descending order. That is, $\Phi F_x = U_x \Sigma_x V_x^{\mathsf{T}}$, and since ΦF_x is a tall matrix $(n \leq d)$, we know that the bottom d-n singular values are zero. Thus, we only consider the top n (of d) left singular vectors in the SVD (so, U_x is $d \times n$, Σ_x is $n \times n$, and V_x is $n \times n$) and $\sigma_x^1 \geq \sigma_x^2 \geq \ldots \geq \sigma_x^n$ where σ_x^i is the *i*th largest singular value.

Observe that the singular values $\sigma_x^1, \ldots, \sigma_x^n$ are precisely the distortion amounts in the directions u_x^1, \ldots, u_x^n at $\Phi(x) \in \mathbb{R}^d$ $([u_x^1, \ldots, u_x^n] = U_x)$ when we apply Φ . To see this, consider the direction $w^i := F_x v_x^i$ in the column-span of F_x $([v_x^1, \dots, v_x^n] = V_x)$. Then $\Phi w^i = (\Phi F_x)v_x^i = \sigma_x^i u_x^i$, which can be interpreted as: Φ maps the vector w^i in the columnspace of F_x (in \mathbb{R}^D) to the vector u_x^i (in \mathbb{R}^d) with the scaling of σ_x^i .

Note that if $0 < \sigma_x^i \le 1$ (for all $x \in X$ and $1 \le i \le n$), we can define an $n \times d$ correction matrix (corresponding to each $x \in X$) $C^x := S_x U_x^{\mathsf{T}}$, where S_x is a diagonal matrix with $(S_x)_{ii} := \sqrt{(1/\sigma_x^i)^2 - 1}$. We can also write S_x as $(\Sigma_x^{-2} - I)^{1/2}$. The correction matrix C^x will have an effect of stretching the direction u_x^i by the amount $(S_x)_{ii}$ and killing any direction v that is orthogonal to (column-span of) U_x .

Algorithm 1 Compute Corrections C^x 's

- 1: for $x \in X$ (in any order) do
- Let $x_0, \ldots, x_n \in \{x' \in X : \|x' x\| < \rho\}$ be such that $\left|\frac{x_i x_0}{\|x_i x_0\|} \cdot \frac{x_j x_0}{\|x_j x_0\|}\right| \le 1/2n$ (for
- Let F_x be a $D \times n$ matrix whose columns form an orthonormal basis of the ndimensional span of the vectors $\{x_i - x_0\}_{i \in [n]}$.
- Let $U_x \Sigma_x V_x^{\mathsf{T}}$ be the "thin" SVD of ΦF_x . Set $C^x := (\Sigma_x^{-2} I)^{1/2} U_x^{\mathsf{T}}$.
- 6: end for

Algorithm 2 Embedding Technique I

Preprocessing Stage: Partition the given covering X into disjoint subsets such that no subset contains points that are too close to each other. Let $x_1, \ldots, x_{|X|}$ be the points in X in some arbitrary but fixed order. We can do the partition as follows:

- 1: Initialize $X^{(1)}, \ldots, X^{(K)}$ as empty sets.
- 2: for $x_i \in X$ (in any fixed order) do
- 3: Let j be the smallest positive integer such that x_i is not within distance 2ρ of any element in $X^{(j)}$. That is, the smallest j such that for all $x \in X^{(j)}$, $||x x_i|| \ge 2\rho$.
- 4: $X^{(j)} \leftarrow X^{(j)} \cup \{x_i\}.$
- 5: end for

The Embedding: For any $p \in M \subset \mathbb{R}^D$, embed it in \mathbb{R}^{d+2nK} as follows:

- 1: Let $t = \Phi(p)$.
- 2: Define $\Psi(t) := (t, \Psi_{1,\sin}(t), \Psi_{1,\cos}(t), \dots, \Psi_{K,\sin}(t), \Psi_{K,\cos}(t))$ where

$$\Psi_{j,\sin}(t) := (\psi_{j,\sin}^{1}(t), \dots, \psi_{j,\sin}^{n}(t)), \Psi_{j,\cos}(t) := (\psi_{j,\cos}^{1}(t), \dots, \psi_{j,\cos}^{n}(t)).$$

The individual terms are given by

$$\psi_{j,\sin}^{i}(t) := \sum_{x \in X^{(j)}} \left(\sqrt{\Lambda_{\Phi(x)}(t)} / \omega \right) \sin(\omega(C^{x}t)_{i}) \qquad i = 1, \dots, n;$$

$$\psi_{j,\cos}^{i}(t) := \sum_{x \in X^{(j)}} \left(\sqrt{\Lambda_{\Phi(x)}(t)} / \omega \right) \cos(\omega(C^{x}t)_{i}) \qquad j = 1, \dots, K$$

where
$$\Lambda_a(b) = \frac{\lambda_a(b)}{\sum_{q \in X} \lambda_{\Phi(q)}(b)}$$
.

3: **return** $\Psi(t)$ as the embedding of p in \mathbb{R}^{d+2nK} .

A few remarks are in order.

Remark 5 The goal of the Preprocessing Stage is to identify samples from X that can have overlapping $(\rho$ -size) local neighborhoods. The partitioning procedure described above ensures that corrections associated with nearby neighborhoods are applied in separate coordinates to minimize interference.

Remark 6 If $\rho \leq \tau/8$, the number of subsets (i.e. K) produced by Embedding I is at most $\alpha 2^{cn}$ for an α -bounded (ρ, δ) cover X of M (where $c \leq 4$). See Appendix C for details.

Remark 7 The function Λ acts as a (normalized) localizing kernel that helps in localizing the effects of the spiraling corrections (discussed in detail in Section 5.2).

Remark 8 $\omega > 0$ is a free parameter that controls the interference due to overlapping local corrections.

Algorithm 3 Embedding Technique II

The Embedding: Let $x_1, \ldots, x_{|X|}$ be the points in X in some arbitrary but fixed order. For any point $p \in M \subset \mathbb{R}^D$, we embed it in \mathbb{R}^{2d+3} by:

- 1: Let $t = \Phi(p)$.
- 2: Define $\Psi_{0,n}(t) := (t, \underbrace{0, \dots, 0}_{d+3})$. [Extension needed to efficiently find the normal vectors]
- 3: **for** i = 1, ..., |X| **do**
- 4: Define $\Psi_{i,0} := \Psi_{i-1,n}$.
- 5: **for** j = 1, ..., n **do**
- 6: Let $\eta_{i,j}(t)$ and $\nu_{i,j}(t)$ be two mutually orthogonal unit vectors normal to $\Psi_{i,j-1}(\Phi M)$ at $\Psi_{i,j-1}(t)$.
- 7: Define

$$\Psi_{i,j}(t) := \Psi_{i,j-1}(t) + \eta_{i,j}(t) \left(\frac{\sqrt{\Lambda_{\Phi(x_i)}(t)}}{\omega_{i,j}}\right) \sin(\omega_{i,j}(C^{x_i}t)_j) + \nu_{i,j}(t) \left(\frac{\sqrt{\Lambda_{\Phi(x_i)}(t)}}{\omega_{i,j}}\right) \cos(\omega_{i,j}(C^{x_i}t)_j),$$

where
$$\Lambda_a(b) = \frac{\lambda_a(b)}{\sum_{q \in X} \lambda_{\Phi(q)}(b)}$$
.

- 8: end for
- 9: end for
- 10: **return** $\Psi_{|X|,n}(t)$ as the embedding of p into \mathbb{R}^{2d+3} .

Remark 9 The function Λ , and the free parameters $\omega_{i,j}$ (one for each i, j iteration) have roles similar to those in Embedding I.

Remark 10 The success of Embedding II depends upon finding a pair of normal unit vectors η and ν in each iteration; we discuss how to approximate these in Appendix E.

For appropriate choice of d, ρ , δ and ω (or $\omega_{i,j}$), we have the following.

4.1 Main Result

Theorem 11 Let $M \subset \mathbb{R}^D$ be a C_M -regular n-manifold with condition number $1/\tau$. Let $d = \Omega\left(n\log(C_M/\tau)\right)$ be the target dimension of the initial random projection mapping such that $d \leq D$. For any $0 < \epsilon \leq 1$, let $\rho \leq (\tau d/D)(\epsilon/350)^2$, $\delta \leq (d/D)(\epsilon/250)^2$, and let $X \subset M$ be an α -bounded (ρ, δ) -cover of M. Now, given access to the sample X, let

- i. $N_{\rm I} \subset \mathbb{R}^{d+2\alpha n 2^{cn}}$ be the embedding of M returned by Algorithm I (where $c \leq 4$),
- ii. $N_{\rm II} \subset \mathbb{R}^{2d+3}$ be the embedding of M returned by Algorithm II.

Then, with probability at least 1-1/poly(n) over the choice of the initial random projection, for all $p, q \in M$ and their corresponding mappings $p_I, q_I \in N_I$ and $p_{II}, q_{II} \in N_{II}$, we have

i.
$$(1 - \epsilon)D_G(p, q) \le D_G(p_I, q_I) \le (1 + \epsilon)D_G(p, q)$$
,

ii.
$$(1 - \epsilon)D_G(p, q) \le D_G(p_{II}, q_{II}) \le (1 + \epsilon)D_G(p, q)$$
.

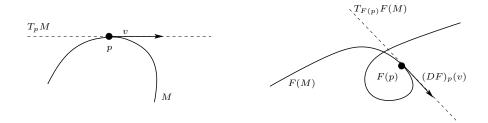


Figure 3: Effects of applying a smooth map F on various quantities of interest. Left: A manifold M containing point p. v is a vector tangent to M at p. Right: Mapping of M under F. Point p maps to F(p), tangent vector v maps to $(DF)_p(v)$.

5. Proof

Our goal is to show that the two proposed embeddings approximately preserve the lengths of all geodesic curves. Now, since the length of any given curve $\gamma:[a,b]\to M$ is given by $\int_a^b \|\gamma'(s)\|ds$, it is vital to study how our embeddings modify the length of the tangent vectors at any point $p\in M$.

In order to discuss tangent vectors, we need to introduce the notion of a tangent space T_pM at a particular point $p \in M$. Consider any smooth curve $c: (-\epsilon, \epsilon) \to M$ such that c(0) = p, then we know that c'(0) is the vector tangent to c at p. The collection of all such vectors formed by all such curves is a well defined vector space (with origin at p), called the tangent space T_pM . In what follows, we will fix an arbitrary point $p \in M$ and a tangent vector $v \in T_pM$ and analyze how the various steps of the algorithm modify the length of v.

Let Φ be the initial (scaled) random projection map (from \mathbb{R}^D to \mathbb{R}^d) that may contract distances on M by various amounts, and let Ψ be the subsequent correction map that attempts to restore these distances (as defined in Step 2 for Embedding I or as a sequence of maps in Step 7 for Embedding II). To get a firm footing for our analysis, we need to study how Φ and Ψ modify the tangent vector v. It is well known from differential geometry that for any smooth map $F: M \to N$ that maps a manifold $M \subset \mathbb{R}^k$ to a manifold $N \subset \mathbb{R}^{k'}$, there exists a linear map $(DF)_p: T_pM \to T_{F(p)}N$, known as the derivative map or the pushforward (at p), that maps tangent vectors incident at p in M to tangent vectors incident at F(p) in N. To see this, consider a vector u tangent to M at some point p. Then, there is some smooth curve $c:(-\epsilon,\epsilon)\to M$ such that c(0)=p and c'(0)=u. By mapping the curve c into N, i.e. F(c(t)), we see that F(c(t)) includes the point F(p) at t=0. Now, by calculus, we know that the derivative at this point, $\frac{dF(c(t))}{dt}\Big|_{t=0}$ is the directional derivative $(\nabla F)_p(u)$, where $(\nabla F)_p$ is a $k' \times k$ matrix called the gradient (at p). The quantity $(\nabla F)_p$ is precisely the matrix representation of this linear "pushforward" map that sends tangent vectors of M (at p) to the corresponding tangent vectors of N (at F(p)). Figure 3 depicts how these quantities are affected by applying F. Also note that if F is linear, then DF = F.

Observe that since pushforward maps are linear, without loss of generality we can assume that v has unit length. Also, since for n=0 there is nothing to prove, we shall assume that $n \ge 1$.

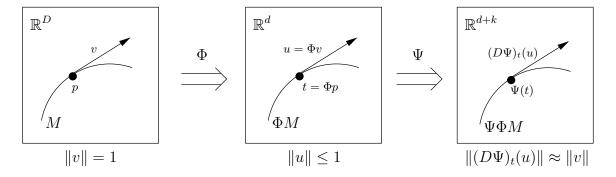


Figure 4: Two stage mapping of our embedding technique. Left: Underlying manifold $M \subset \mathbb{R}^D$ with the quantities of interest – a fixed point p and a fixed unit-vector v tangent to M at p. Center: A (scaled) linear projection of M into a random subspace of d dimensions. The point p maps to Φp and the tangent vector v maps to $u := (D\Phi)_p(v) = \Phi v$. The length of v contracts to ||u||. Right: Correction of ΦM via a non-linear mapping Ψ into \mathbb{R}^{d+k} . We have $k = O(\alpha 2^{cn})$ for correction technique I, and k = d+3 for correction technique II (see also Section 4). Our goal is to show that Ψ stretches length of contracted v (i.e. u) back to approximately its original length.

A quick roadmap for the proof. In the next three sections, we take a brief detour to study the effects of applying Φ , applying Ψ for Algorithm I, and applying Ψ for Algorithm II separately. This will give us the necessary tools to analyze the combined effect of applying $\Psi \circ \Phi$ on v (Section 5.4). We will conclude by relating tangent vectors to lengths of curves, showing approximate isometry (Section 5.5). Figure 4 provides a quick sketch of our two stage mapping with the quantities of interest. We defer the proofs of all the supporting lemmas to Appendix D.

5.1 Effects of Applying Φ

It is well known as an application of Sard's theorem from differential topology (see e.g. Milnor, 1972) that almost every smooth mapping of an n-dimensional manifold into \mathbb{R}^{2n+1} is a differential structure preserving embedding of M. In particular, a projection onto a random subspace (of dimension 2n + 1) constitutes such an embedding with probability 1.

This translates to stating that a random projection into \mathbb{R}^{2n+1} is enough to guarantee that Φ doesn't collapse the lengths of non-zero tangent vectors almost surely. However, due to computational issues, we additionally require that the lengths are bounded away from zero (that is, a statement of the form $||(D\Phi)_p(v)|| \geq \Omega(1)||v||$ for all v tangent to M at all points p).

We can thus appeal to the random projections result by Clarkson (2008) (with the isometry parameter set to a constant, say 1/4) to ensure this condition. In particular, the following holds.

Lemma 12 Let $M \subset \mathbb{R}^D$ be a C_M -regular n-manifold with condition number $1/\tau$. Let R be a random projection matrix that maps points from \mathbb{R}^D into a random subspace of

dimension d ($d \leq D$). Define $\Phi := (2/3)(\sqrt{D/d})R$ as a scaled projection mapping. If $d = \Omega(n \log(C_M/\tau))$, then with probability at least 1 - 1/poly(n) over the choice of the random projection matrix, we have

- (a) For all $p \in M$ and all tangent vectors $v \in T_pM$, $(1/2)\|v\| \le \|(D\Phi)_p(v)\| \le (5/6)\|v\|$.
- (b) For all $p, q \in M$, $(1/2)||p-q|| \le ||\Phi p \Phi q|| \le (5/6)||p-q||$.
- (c) For all $x \in \mathbb{R}^D$, $\|\Phi x\| \le (2/3)(\sqrt{D/d})\|x\|$.

In what follows, we assume that Φ is such a scaled random projection map. Then, a bound on the length of tangent vectors also gives us a bound on the spectrum of ΦF_x (recall the definition of F_x from Section 4).

Corollary 13 Let Φ , F_x and n be as described above (recall that $x \in X$ that forms a bounded (ρ, δ) -cover of M). Let σ_x^i represent the i^{th} largest singular value of the matrix ΦF_x . Then, for $\delta \leq d/32D$, we have $1/4 \leq \sigma_x^n \leq \sigma_x^1 \leq 1$ (for all $x \in X$).

We will be using these facts in our discussion below in Section 5.4.

5.2 Effects of Applying Ψ (Algorithm I)

As discussed in Section 2, the goal of Ψ is to restore the contraction induced by Φ on M. To understand the action of Ψ on a tangent vector better, we will first consider a simple case of flat manifolds (Section 5.2.1), and then develop the general case (Section 5.2.2).

5.2.1 Warm-up: flat M

Let's first consider applying a simple one-dimensional spiral map $\bar{\Psi}: \mathbb{R} \to \mathbb{R}^3$ given by $t \mapsto (t, \sin(Ct), \cos(Ct))$, where $t \in I = (-\epsilon, \epsilon)$. Let \bar{v} be a unit vector tangent to I (at, say, 0). Then note that

$$(D\bar{\Psi})_{t=0}(\bar{v}) = \frac{d\bar{\Psi}}{dt}\Big|_{t=0} = (1, C\cos(Ct), -C\sin(Ct))\Big|_{t=0}.$$

Thus, applying $\bar{\Psi}$ stretches the length of \bar{v} from 1 to $\|(1, C\cos(Ct), -C\sin(Ct))|_{t=0}\| = \sqrt{1+C^2}$. Notice the advantage of applying the spiral map in computing the lengths: the sine and cosine terms combine together to yield a simple expression for the size of the stretch. In particular, if we want to stretch the length of \bar{v} from 1 to, say, $L \geq 1$, then we simply need $C = \sqrt{L^2 - 1}$ (notice the similarity between this expression and our expression for the diagonal component S_x of the correction matrix C^x in Section 4).

We can generalize this to the case of n-dimensional flat manifold (a section of an n-flat) by considering a map similar to $\bar{\Psi}$. For concreteness, let F be a $D \times n$ matrix whose column vectors form some orthonormal basis of the n-flat manifold (in the original space \mathbb{R}^D). Let $U\Sigma V^{\mathsf{T}}$ be the "thin" SVD of ΦF . Then FV forms an orthonormal basis of the n-flat manifold (in \mathbb{R}^D) that maps to an orthogonal basis $U\Sigma$ of the projected n-flat manifold (in \mathbb{R}^d) via the contraction mapping Φ . Define the spiral map $\bar{\Psi}: \mathbb{R}^d \to \mathbb{R}^{d+2n}$

in this case as follows. $\bar{\Psi}(t) := (t, \bar{\Psi}_{\sin}(t), \bar{\Psi}_{\cos}(t))$, with $\bar{\Psi}_{\sin}(t) := (\bar{\psi}_{\sin}^1(t), \dots, \bar{\psi}_{\sin}^n(t))$ and $\bar{\Psi}_{\cos}(t) := (\bar{\psi}_{\cos}^1(t), \dots, \bar{\psi}_{\cos}^n(t))$. The individual terms are given as

$$\bar{\psi}_{\sin}^{i}(t) := \sin((Ct)_{i})
\bar{\psi}_{\cos}^{i}(t) := \cos((Ct)_{i}) \qquad i = 1, \dots, n,$$

where C is now an $n \times d$ correction matrix. It turns out that setting $C = (\Sigma^{-2} - I)^{1/2} U^{\mathsf{T}}$ precisely restores the contraction caused by Φ to the tangent vectors (notice the similarity between this expression with the correction matrix in the general case C^x in Section 4 and our motivating intuition in Section 2). To see this, let v be a vector tangent to the n-flat at some point p (in \mathbb{R}^D). We will represent v in the FV basis (that is, $v = \sum_i \alpha_i (Fv^i)$ where $[Fv^1, \dots, Fv^n] = FV$). Note that $\|\Phi v\|^2 = \|\sum_i \alpha_i \Phi F v^i\|^2 = \|\sum_i \alpha_i \sigma^i u^i\|^2 = \sum_i (\alpha_i \sigma^i)^2$ (where σ^i are the individual singular values of Σ and u^i are the left singular vectors forming the columns of U). Now, let w be the pushforward of v (that is, $w = (D\Phi)_p(v) = \Phi v = \sum_i w_i e^i$, where $\{e^i\}_i$ forms the standard basis of \mathbb{R}^d). Now, since $D\bar{\Psi}$ is linear, we have $\|(D\bar{\Psi})_{\Phi(p)}(w)\|^2 = \|\sum_i w_i(D\bar{\Psi})_{\Phi(p)}(e^i)\|^2$, where $(D\bar{\Psi})_{\Phi(p)}(e^i) = \frac{d\bar{\Psi}}{dt^i}|_{t=\Phi(p)} = \left(\frac{dt}{dt^i}, \frac{d\bar{\Psi}_{\text{sin}}(t)}{dt^i}, \frac{d\bar{\Psi}_{\text{cos}}(t)}{dt^i}\right)|_{t=\Phi(p)}$. The individual components are given by

$$d\bar{\psi}_{\sin}^{k}(t)/dt^{i} = +\cos((Ct)_{k})C_{k,i} d\bar{\psi}_{\cos}^{k}(t)/dt^{i} = -\sin((Ct)_{k})C_{k,i}$$
 $k = 1, ..., n; i = 1, ..., d.$

By algebra, we see that

$$\begin{split} \|(D(\bar{\Psi} \circ \Phi))_{p}(v)\|^{2} &= \|(D\bar{\Psi})_{\Phi(p)}((D\Phi)_{p}(v))\|^{2} = \|(D\bar{\Psi})_{\Phi(p)}(w)\|^{2} \\ &= \sum_{i=1}^{d} w_{i}^{2} \left(\frac{dt}{dt^{i}}\right)^{2} + \sum_{i=1}^{d} \sum_{k=1}^{n} w_{i}^{2} \left(\frac{d\psi_{\sin}^{k}(t)}{dt^{i}}\right)^{2} + \sum_{i=1}^{d} \sum_{k=1}^{n} w_{i}^{2} \left(\frac{d\psi_{\cos}^{k}(t)}{dt^{i}}\right)^{2} \Big|_{t=\Phi(p)} \\ &= \sum_{k=1}^{d} w_{k}^{2} + \sum_{k=1}^{n} \cos^{2}((C\Phi(p))_{k})((C\Phi v)_{k})^{2} + \sum_{k=1}^{n} \sin^{2}((C\Phi(p))_{k})((C\Phi v)_{k})^{2} \\ &= \sum_{k=1}^{d} w_{k}^{2} + \sum_{k=1}^{n} ((C\Phi v)_{k})^{2} = \|\Phi v\|^{2} + \|C\Phi v\|^{2} = \|\Phi v\|^{2} + (\Phi v)^{\mathsf{T}} C^{\mathsf{T}} C(\Phi v) \\ &= \|\Phi v\|^{2} + (\sum_{i} \alpha_{i} \sigma^{i} u^{i})^{\mathsf{T}} U(\Sigma^{-2} - I) U^{\mathsf{T}} (\sum_{i} \alpha_{i} \sigma^{i} u^{i}) \\ &= \|\Phi v\|^{2} + [\alpha_{1} \sigma^{1}, \dots, \alpha_{n} \sigma^{n}] (\Sigma^{-2} - I) [\alpha_{1} \sigma^{1}, \dots, \alpha_{n} \sigma^{n}]^{\mathsf{T}} \\ &= \|\Phi v\|^{2} + (\sum_{i} \alpha_{i}^{2} - \sum_{i} (\alpha_{i} \sigma^{i})^{2}) = \|\Phi v\|^{2} + \|v\|^{2} - \|\Phi v\|^{2} = \|v\|^{2}. \end{split}$$

In other words, our non-linear correction map $\bar{\Psi}$ can exactly restore the contraction caused by Φ for any vector tangent to an n-flat manifold.

In the fully general case, the situation gets slightly more complicated since we need to apply different spiral maps, each corresponding to a different size correction at different locations on the contracted manifold. Recall that we localize the effect of a correction by applying the so-called "bump" function (details below). These bump functions, although

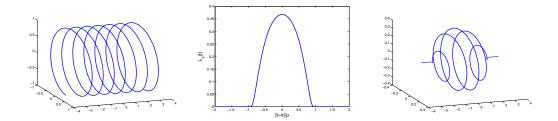


Figure 5: Effects of applying a bump function on a spiral mapping. Left: Spiral mapping $t \mapsto (t, \sin(t), \cos(t))$. Middle: Bump function λ_x : a smooth function with compact support. The parameter x controls the location while ρ controls the width. Right: The combined effect: $t \mapsto (t, \lambda_x(t) \sin(t), \lambda_x(t) \cos(t))$. Note that the effect of the spiral is localized while keeping the mapping smooth.

important for localization, have an undesirable effect on the stretched length of the tangent vector. Thus, to ameliorate their effect on the length of the resulting tangent vector, we control their contribution via a free parameter ω .

5.2.2 The General Case

More specifically, Embedding Technique I restores the contraction induced by Φ by applying a non-linear map $\Psi(t) := (t, \Psi_{1,\sin}(t), \Psi_{1,\cos}(t), \dots, \Psi_{K,\sin}(t), \Psi_{K,\cos}(t))$ (recall that K is the number of subsets we decompose X into – cf. description in Embedding I in Section 4), with $\Psi_{j,\sin}(t) := (\psi_{j,\sin}^1(t), \dots, \psi_{j,\sin}^n(t))$ and $\Psi_{j,\cos}(t) := (\psi_{j,\cos}^1(t), \dots, \psi_{j,\cos}^n(t))$. The individual terms are given as

$$\psi_{j,\sin}^{i}(t) := \sum_{x \in X^{(j)}} \left(\sqrt{\Lambda_{\Phi(x)}(t)} / \omega \right) \sin(\omega(C^{x}t)_{i})$$

$$\psi_{j,\cos}^{i}(t) := \sum_{x \in X^{(j)}} \left(\sqrt{\Lambda_{\Phi(x)}(t)} / \omega \right) \cos(\omega(C^{x}t)_{i})$$

$$i = 1, \dots, n; j = 1, \dots, K,$$

where C^x 's are the correction amounts for different locations x on the manifold, $\omega > 0$ controls the frequency (cf. Section 4), and $\Lambda_{\Phi(x)}(t)$ is defined to be $\lambda_{\Phi(x)}(t)/\sum_{q\in X}\lambda_{\Phi(q)}(t)$, with

$$\lambda_{\Phi(x)}(t) := \left\{ \begin{array}{ll} \exp(-1/(1 - \|t - \Phi(x)\|^2/\rho^2)) & \text{if } \|t - \Phi(x)\| < \rho. \\ 0 & \text{otherwise.} \end{array} \right.$$

 λ is a classic example of a bump function (see Figure 5 middle). It is a smooth function with compact support. Its applicability arises from the fact that it can be made "to specifications". That is, it can be made to vanish outside any interval of our choice. Here we exploit this property to localize the effect of our corrections. The normalization of λ (the function Λ) creates the so-called smooth partition of unity that helps to vary smoothly between the spirals applied at different regions of M.

Since any tangent vector in \mathbb{R}^d can be expressed in terms of the basis vectors, it suffices to study how $D\Psi$ acts on the standard basis $\{e^i\}$. Note that

$$(D\Psi)_t(e^i) = \left(\frac{dt}{dt^i}, \frac{d\Psi_{1,\sin}(t)}{dt^i}, \frac{d\Psi_{1,\cos}(t)}{dt^i}, \dots, \frac{d\Psi_{K,\sin}(t)}{dt^i}, \frac{d\Psi_{K,\cos}(t)}{dt^i}\right)\Big|_t,$$

where

$$\frac{d\psi_{j,\sin}^{k}(t)}{dt^{i}} = \sum_{x \in X^{(j)}} \frac{1}{\omega} \left(\sin(\omega(C^{x}t)_{k}) \frac{d\Lambda_{\Phi(x)}^{1/2}(t)}{dt^{i}} \right) + \sqrt{\Lambda_{\Phi(x)}(t)} \cos(\omega(C^{x}t)_{k}) C_{k,i}^{x} \qquad k \in [n]; \ i \in [d]$$

$$\frac{d\psi_{j,\cos}^{k}(t)}{dt^{i}} = \sum_{x \in X^{(j)}} \frac{1}{\omega} \left(\cos(\omega(C^{x}t)_{k}) \frac{d\Lambda_{\Phi(x)}^{1/2}(t)}{dt^{i}} \right) - \sqrt{\Lambda_{\Phi(x)}(t)} \sin(\omega(C^{x}t)_{k}) C_{k,i}^{x} \qquad j \in [K]$$

One can now observe the advantage of having the term ω . By picking ω sufficiently large, we can make the first part of the expression sufficiently small. Now, for any tangent vector $u = \sum_i u_i e^i$ such that $||u|| \leq 1$, we have (by algebra)

$$\begin{split} \|(D\Psi)_{t}(u)\|^{2} &= \|\sum_{i} u_{i}(D\Psi)_{t}(e^{i})\|^{2} \\ &= \sum_{i=1}^{d} u_{i}^{2} \left(\frac{dt}{dt^{i}}\right)^{2} + \sum_{i=1}^{d} \sum_{j=1}^{K} \sum_{k=1}^{n} u_{i}^{2} \left(\frac{d\psi_{j,\sin}^{k}(t)}{dt^{i}}\right)^{2} + \sum_{i=1}^{d} \sum_{j=1}^{K} \sum_{k=1}^{n} u_{i}^{2} \left(\frac{d\psi_{j,\cos}^{k}(t)}{dt^{i}}\right)^{2} \\ &= \sum_{k=1}^{d} u_{k}^{2} + \sum_{k=1}^{n} \sum_{j=1}^{K} \left[\sum_{x \in X^{(j)}} \left(\frac{A_{\sin}^{k,x}(t)}{\omega}\right) + \sqrt{\Lambda_{\Phi(x)}(t)} \cos(\omega(C^{x}t)_{k})(C^{x}u)_{k}\right]^{2} \\ &+ \left[\sum_{x \in X^{(j)}} \left(\frac{A_{\cos}^{k,x}(t)}{\omega}\right) - \sqrt{\Lambda_{\Phi(x)}(t)} \sin(\omega(C^{x}t)_{k})(C^{x}u)_{k}\right]^{2}, \end{split}$$
(1)

where $A_{\sin}^{k,x}(t) := \sum_i u_i \sin(\omega(C^x t)_k) (d\Lambda_{\Phi(x)}^{1/2}(t)/dt^i)$ and $A_{\cos}^{k,x}(t) := \sum_i u_i \cos(\omega(C^x t)_k) (d\Lambda_{\Phi(x)}^{1/2}(t)/dt^i)$. We can further simplify Eq. (1) and get

Lemma 14 Let t be any point in $\Phi(M)$ and u be any vector tangent to $\Phi(M)$ at t such that $||u|| \leq 1$. Let d, ϵ , ρ and α be as per the statement of Theorem 11. Pick $\omega \geq \Omega(n\alpha^2 16^n \sqrt{d}/\rho\epsilon)$, then

$$\|(D\Psi)_t(u)\|^2 = \|u\|^2 + \sum_{x \in X} \Lambda_{\Phi(x)}(t) \sum_{k=1}^n (C^x u)_k^2 + \zeta, \tag{2}$$

where $|\zeta| \leq \epsilon/2$.

We will use this derivation of $||(D\Psi)_t(u)||^2$ to study the combined effect of $\Psi \circ \Phi$ on M in Section 5.4.

5.3 Effects of Applying Ψ (Algorithm II)

The goal of the second algorithm is to apply the spiraling corrections while using the coordinates more economically. We achieve this goal by applying them sequentially in the same embedding space (rather than simultaneously by making use of extra 2nK coordinates as done in the first algorithm), see also Nash (1954). Since all the corrections will be sharing the same coordinate space, one needs to keep track of a pair of normal vectors in order to prevent interference among the different local corrections.

More specifically, $\Psi: \mathbb{R}^d \to \mathbb{R}^{2d+3}$ (in Algorithm II) is defined recursively as $\Psi := \Psi_{|X|,n}$ such that (see also Embedding II in Section 4)

$$\Psi_{i,j}(t) := \Psi_{i,j-1}(t) + \eta_{i,j}(t) \frac{\sqrt{\Lambda_{\Phi(x_i)}(t)}}{\omega_{i,j}} \sin(\omega_{i,j}(C^{x_i}t)_j) + \nu_{i,j}(t) \frac{\sqrt{\Lambda_{\Phi(x_i)}(t)}}{\omega_{i,j}} \cos(\omega_{i,j}(C^{x_i}t)_j),$$

where $\Psi_{i,0}(t) := \Psi_{i-1,n}(t)$, and the base function $\Psi_{0,n}(t)$ is given as $t \mapsto (t, 0, \dots, 0)$. $\eta_{i,j}(t)$ and $\nu_{i,j}(t)$ are mutually orthogonal unit vectors that are approximately normal to $\Psi_{i,j-1}(\Phi M)$ at $\Psi_{i,j-1}(t)$. In this section we assume that the normals η and ν have the following properties:

- $|\eta_{i,j}(t)\cdot v| \leq \epsilon_0$ and $|\nu_{i,j}(t)\cdot v| \leq \epsilon_0$ for all unit-length v tangent to $\Psi_{i,j-1}(\Phi M)$ at $\Psi_{i,j-1}(t)$. (quality of normal approximation)
- For all $1 \leq l \leq d$, we have $||d\eta_{i,j}(t)/dt^l|| \leq K_{i,j}$ and $||d\nu_{i,j}(t)/dt^l|| \leq K_{i,j}$. (bounded directional derivatives)

We refer the reader to Appendix E for details on how to estimate such normals.

Now, as before, representing a tangent vector $u = \sum_{l} u_{l} e^{l}$ (such that $||u||^{2} \leq 1$) in terms of its basis vectors, it suffices to study how $D\Psi$ acts on basis vectors. Observe that $(D\Psi_{i,j})_{t}(e^{l}) = \left(\frac{d\Psi_{i,j}(t)}{dt^{l}}\right)_{k=1}^{2d+3} \Big|_{t}$, with the k^{th} component given as

$$\begin{split} \left(\frac{d\Psi_{i,j-1}(t)}{dt^{l}}\right)_{k} + (\eta_{i,j}(t))_{k}\sqrt{\Lambda_{\Phi(x_{i})}(t)}C_{j,l}^{x_{i}}B_{\cos}^{i,j}(t) - (\nu_{i,j}(t))_{k}\sqrt{\Lambda_{\Phi(x_{i})}(t)}C_{j,l}^{x_{i}}B_{\sin}^{i,j}(t) \\ + \frac{1}{\omega_{i,j}}\Big[\Big(\frac{d\eta_{i,j}(t)}{dt^{l}}\Big)_{k}\sqrt{\Lambda_{\Phi(x_{i})}(t)}B_{\sin}^{i,j}(t) + \Big(\frac{d\nu_{i,j}(t)}{dt^{l}}\Big)_{k}\sqrt{\Lambda_{\Phi(x_{i})}(t)}B_{\cos}^{i,j}(t) \\ + (\eta_{i,j}(t))_{k}\frac{d\Lambda_{\Phi(x_{i})}^{1/2}(t)}{dt^{l}}B_{\sin}^{i,j}(t) + (\nu_{i,j}(t))_{k}\frac{d\Lambda_{\Phi(x_{i})}^{1/2}(t)}{dt^{l}}B_{\cos}^{i,j}(t)\Big], \end{split}$$

where $B_{\cos}^{i,j}(t) := \cos(\omega_{i,j}(C^{x_i}t)_j)$ and $B_{\sin}^{i,j}(t) := \sin(\omega_{i,j}(C^{x_i}t)_j)$. For ease of notation, let $R_{i,j}^{k,l}$ be the terms in the bracket (being multiplied to $1/\omega_{i,j}$) in the above expression. Then, we have (for any i, j)

$$\|(D\Psi_{i,j})_{t}(u)\|^{2} = \|\sum_{l} u_{l}(D\Psi_{i,j})_{t}(e^{l})\|^{2}$$

$$= \sum_{k=1}^{2d+3} \left[\underbrace{\sum_{l} u_{l} \left(\frac{d\Psi_{i,j-1}(t)}{dt^{l}} \right)_{k}}_{\zeta_{i,j}^{k,1}} + \underbrace{(\eta_{i,j}(t))_{k} \sqrt{\Lambda_{\Phi(x_{i})}(t)} \cos(\omega_{i,j}(C^{x_{i}}t)_{j}) \sum_{l} C_{j,l}^{x_{i}} u_{l}}_{\zeta_{i,j}^{k,2}} \right]^{2}$$

$$\underbrace{-(\nu_{i,j}(t))_{k} \sqrt{\Lambda_{\Phi(x_{i})}(t)} \sin(\omega_{i,j}(C^{x_{i}}t)_{j}) \sum_{l} C_{j,l}^{x_{i}} u_{l}}_{\zeta_{i,j}^{k,3}} + (1/\omega_{i,j}) \underbrace{\sum_{l} u_{l} R_{i,j}^{k,l}}_{\zeta_{i,j}^{k,4}} \right]^{2}}_{\zeta_{i,j}^{k,3}}$$

$$= \underbrace{\|(D\Psi_{i,j-1})_{t}(u)\|^{2}}_{=\sum_{k} \left(\zeta_{i,j}^{k,1}\right)^{2}} + \underbrace{\Lambda_{\Phi(x_{i})}(t)(C^{x_{i}}u)_{j}^{2}}_{=\sum_{k} \left(\zeta_{i,j}^{k,2}\right)^{2} + \left(\zeta_{i,j}^{k,3}\right)^{2}} + \underbrace{\sum_{k} \left[\left(\zeta_{i,j}^{k,4}/\omega_{i,j}\right)^{2} + \left(2\zeta_{i,j}^{k,4}/\omega_{i,j}\right)\left(\zeta_{i,j}^{k,1} + \zeta_{i,j}^{k,2} + \zeta_{i,j}^{k,3}\right) + 2\left(\zeta_{i,j}^{k,1}\zeta_{i,j}^{k,2} + \zeta_{i,j}^{k,1}\zeta_{i,j}^{k,3}\right)\right]}_{Z_{i,j}}, (3)$$

where the last equality is by expanding the square and by noting that $\sum_k \zeta_{i,j}^{k,2} \zeta_{i,j}^{k,3} = 0$ since η and ν are orthogonal to each other. The base case $\|(D\Psi_{0,n})_t(u)\|^2$ equals $\|u\|^2$.

Again, by picking $\omega_{i,j}$ sufficiently large, and by noting that the cross terms $\sum_{k} (\zeta_{i,j}^{k,1} \zeta_{i,j}^{k,2})$ and $\sum_{k} (\zeta_{i,j}^{k,1} \zeta_{i,j}^{k,3})$ are very close to zero since η and ν are approximately normal to the tangent vector, we have

Lemma 15 Let t be any point in $\Phi(M)$ and u be any vector tangent to $\Phi(M)$ at t such that $||u|| \leq 1$. Let ϵ be the isometry parameter chosen in Theorem 11. Pick $\omega_{i,j} \geq \Omega((K_{i,j} + (\alpha 16^n/\rho))(nd|X|)^2/\epsilon)$ (recall that $K_{i,j}$ is the bound on the directional derivative of η and ν). If $\epsilon_0 \leq O(\epsilon/\sqrt{d}(n|X|)^2)$ (recall that ϵ_0 is the quality of approximation of the normals η and ν), then we have

$$\|(D\Psi)_t(u)\|^2 = \|(D\Psi_{|X|,n})_t(u)\|^2 = \|u\|^2 + \sum_{i=1}^{|X|} \Lambda_{\Phi(x_i)}(t) \sum_{j=1}^n (C^{x_i}u)_j^2 + \zeta, \tag{4}$$

where $|\zeta| \leq \epsilon/2$.

5.4 Combined Effect of $\Psi(\Phi(M))$

We can now analyze the aggregate effect of both our embeddings on the length of an arbitrary unit vector v tangent to M at p. Let $u := (D\Phi)_p(v) = \Phi v$ be the pushforward of v. Then $||u|| \le 1$ (cf. Lemma 12). See also Figure 4.

Now, recalling that $D(\Psi \circ \Phi) = D\Psi \cdot D\Phi$, and noting that pushforward maps are linear, we have $\|(D(\Psi \circ \Phi))_p(v)\|^2 = \|(D\Psi)_{\Phi(p)}(u)\|^2$. Thus, representing u as $\sum_i u_i e^i$ in ambient coordinates of \mathbb{R}^d , and using Eq. (2) (for Algorithm I) or Eq. (4) (for Algorithm II), we get

$$\|(D(\Psi \circ \Phi))_p(v)\|^2 = \|(D\Psi)_{\Phi(p)}(u)\|^2 = \|u\|^2 + \sum_{x \in X} \Lambda_{\Phi(x)}(\Phi(p)) \|C^x u\|^2 + \zeta,$$

where $|\zeta| \leq \epsilon/2$. We can give simple lower and upper bounds for the above expression by noting that $\Lambda_{\Phi(x)}$ is a localization function. Define $N_p := \{x \in X : \|\Phi(x) - \Phi(p)\| < \rho\}$ as the neighborhood around p (ρ as per the theorem statement). Then only the points in N_p contribute to above equation, since $\Lambda_{\Phi(x)}(\Phi(p)) = d\Lambda_{\Phi(x)}(\Phi(p))/dt^i = 0$ for $\|\Phi(x) - \Phi(p)\| \geq \rho$. Also note that for all $x \in N_p$, $\|x - p\| < 2\rho$ (cf. Lemma 12).

Let $x_M := \arg \max_{x \in N_p} \|C^x u\|^2$ and $x_m := \arg \min_{x \in N_p} \|C^x u\|^2$ be the quantities that attain the maximum and the minimum respectively. Then:

$$||u||^{2} + ||C^{x_{m}}u||^{2} - \epsilon/2 \le ||(D(\Psi \circ \Phi))_{p}(v)||^{2} \le ||u||^{2} + ||C^{x_{M}}u||^{2} + \epsilon/2.$$
 (5)

Notice that ideally we would like to have the correction factor " C^pu " in Eq. (5) since that would give the perfect stretch around the point p. But what about correction C^xu for nearby x's? The following lemma helps us continue in this situation.

Lemma 16 Let p, v, u be as above. For any $x \in N_p \subset X$, let C^x and F_x also be as discussed above (recall that $||p-x|| < 2\rho$, and $X \subset M$ forms a bounded (ρ, δ) -cover of the fixed underlying manifold M with condition number $1/\tau$). Define $\xi := (4\rho/\tau) + \delta + 4\sqrt{\rho\delta/\tau}$. If $\rho \leq \tau/4$ and $\delta \leq d/32D$, then

$$1 - \|u\|^2 - 40 \cdot \max\left\{\sqrt{\xi D/d}, \xi D/d\right\} \le \|C^x u\|^2 \le 1 - \|u\|^2 + 51 \cdot \max\left\{\sqrt{\xi D/d}, \xi D/d\right\}.$$

Note that we chose $\rho \leq (\tau d/D)(\epsilon/350)^2$ and $\delta \leq (d/D)(\epsilon/250)^2$ (cf. theorem statement). Thus, combining Eq. (5) and Lemma 16, we get (recall ||v|| = 1)

$$(1 - \epsilon) \|v\|^2 \le \|(D(\Psi \circ \Phi))_p(v)\|^2 \le (1 + \epsilon) \|v\|^2.$$

So far we have shown that our embedding approximately preserves the length of a fixed tangent vector at a fixed point. Since the choice of the vector and the point was arbitrary, it follows that our embedding approximately preserves the tangent vector lengths throughout the embedded manifold uniformly. We will now show that preserving the tangent vector lengths implies preserving the geodesic curve lengths.

5.5 Preservation of the Geodesic Lengths

Pick any two (path-connected) points p and q in M, and let α be the geodesic² path between p and q. Further let \bar{p} , \bar{q} and $\bar{\alpha}$ be the images of p, q and α under our embedding. Note that $\bar{\alpha}$ is not necessarily the geodesic path between \bar{p} and \bar{q} , thus we need an extra piece of notation: let $\bar{\beta}$ be the geodesic path between \bar{p} and \bar{q} (under the embedded manifold) and β be its inverse image in M. We need to show $(1 - \epsilon)L(\alpha) \leq L(\bar{\beta}) \leq (1 + \epsilon)L(\alpha)$, where $L(\cdot)$ denotes the length of the path \cdot (end points are understood).

First recall that for any differentiable map F and curve γ , $\bar{\gamma} = F(\gamma) \Rightarrow \bar{\gamma}' = (DF)(\gamma')$. By $(1 \pm \epsilon)$ -isometry of tangent vectors, this immediately gives us $(1 - \epsilon)L(\gamma) \leq L(\bar{\gamma}) \leq (1 + \epsilon)L(\gamma)$ for any path γ in M and its image $\bar{\gamma}$ in embedding of M. So,

$$(1 - \epsilon)D_G(p, q) = (1 - \epsilon)L(\alpha) \le (1 - \epsilon)L(\beta) \le L(\bar{\beta}) = D_G(\bar{p}, \bar{q}).$$

Similarly,

$$D_G(\bar{p}, \bar{q}) = L(\bar{\beta}) \le L(\bar{\alpha}) \le (1 + \epsilon)L(\alpha) = (1 + \epsilon)D_G(p, q).$$

6. Conclusion

This work provides two algorithms for $(1 \pm \epsilon)$ -isometric embedding of generic *n*-dimensional manifolds. Our algorithms are similar in spirit to Nash's construction (Nash, 1954), and manage to remove the dependence on the isometry constant ϵ from the final embedding

^{2.} Globally, geodesic paths between points are not necessarily unique; we are interested in a path that yields the shortest distance between the points.

dimension. Note that this dependency does necessarily show up in the sampling density required to make the corrections.

The correction procedure discussed here can also be readily adapted to create isometric embeddings from any manifold embedding procedure (under some mild conditions). Take any off-the-shelf manifold embedding algorithm \mathcal{A} (such as LLE, Laplacian Eigenmaps, etc.) that maps an n-dimensional manifold in, say, d dimensions, but does not necessarily guarantee an approximate isometric embedding. Then as long as one can ensure that \mathcal{A} is a one-to-one mapping that doesn't collapse interpoint distances, we can scale the output returned by \mathcal{A} to create a contraction. The scaled version of \mathcal{A} acts as the Embedding Stage of our algorithm. We can thus apply the Corrections Stage (either the one discussed in Algorithm I or Algorithm II) to produce an approximate isometric embedding of the given manifold in slightly higher dimensions. In this sense, the correction procedure presented here serves as a universal procedure for approximate isometric manifold embeddings.

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Appendix A. Properties of a Well-conditioned Manifold

Throughout this section we will assume that M is a compact submanifold of \mathbb{R}^D of dimension n, and condition number $1/\tau$. The following are some properties of such a manifold that would be useful throughout the text.

Lemma 17 (relating nearby tangent vectors – implicit in the proof of Proposition 6.2 Niyogi et al. (2008)) Pick any two (path-connected) points $p, q \in M$. Let $u \in T_pM$ be a unit length tangent vector and $v \in T_qM$ be its parallel transport along the (shortest) geodesic path to q. Then³, i) $u \cdot v \ge 1 - D_G(p, q)/\tau$, ii) $||u - v|| \le \sqrt{2D_G(p, q)/\tau}$.

Lemma 18 (relating geodesic distances to ambient distances – Proposition 6.3 of Niyogi et al. (2008)) If $p, q \in M$ such that $||p - q|| \le \tau/2$, then $D_G(p, q) \le \tau(1 - \sqrt{1 - 2||p - q||/\tau}) \le 2||p - q||$.

Lemma 19 (projection of a section of a manifold onto the tangent space) Pick any $p \in M$ and define $M_{p,r} := \{q \in M : ||q-p|| \le r\}$. Let f denote the orthogonal linear projection of $M_{p,r}$ onto the tangent space T_pM . Then, for any $r \le \tau/4$

(i) the map $f:M_{p,r}\to T_pM$ is one-to-one. (follows from Lemma 5.4, 6.1-6.3 of Niyogi et al. (2008))

^{3.} Technically, it is not possible to directly compare two vectors that reside in different tangent spaces. However, since we only deal with manifolds that are immersed in some ambient space, we can treat the tangent spaces as n-dimensional affine subspaces. We can thus parallel translate the vectors to the origin of the ambient space, and do the necessary comparison (such as take the dot product, etc.). We will make a similar abuse of notation for any calculation that uses vectors from different affine subspaces to mean to first translate the vectors and then perform the necessary calculation.

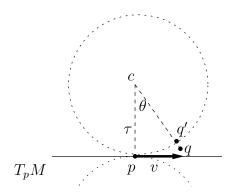


Figure 6: Plane spanned by vectors q - p and $v \in T_pM$ (where v is the projection of q - p onto T_pM), with τ -balls tangent to p. Note that q' is the point on the ball such that $\angle pcq = \angle pcq' = \theta$.

(ii) for any
$$x, y \in M_{p,r}$$
, $||f(x) - f(y)||^2 \ge \left(1 - \left(\frac{r}{\tau} + \sqrt{\frac{2r}{\tau}}\right)^2\right) \cdot ||x - y||^2$. (follows from Lemma 5.3, 6.2, 6.3 of Niyogi et al. (2008))

Lemma 20 (coverings of a section of a manifold) Pick any $p \in M$ and define $M_{p,r} := \{q \in M : ||q-p|| \le r\}$. If $r \le \tau/4$, then there exists $C \subset M_{p,r}$ of size at most 16^n with the property: for any $p' \in M_{p,r}$, exists $c \in C$ such that $||p'-c|| \le r/2$.

Proof The proof closely follows the arguments presented in the proof of Theorem 22 of Dasgupta and Freund (2008).

For $r \leq \tau/4$, note that $M_{p,r} \subset \mathbb{R}^D$ is (path-)connected. Let f denote the projection of $M_{p,r}$ onto $T_pM \cong \mathbb{R}^n$. Quickly note that f is one-to-one (see Lemma 19(i)). Then, $f(M_{p,r}) \subset \mathbb{R}^n$ is contained in an n-dimensional ball of radius r. By standard volume arguments, $f(M_{p,r})$ can be covered by at most 16^n balls of radius r/7 (see e.g. Lemma 5.2 of Vershynin (2010)). WLOG we can assume that the centers of these covering balls are in $f(M_{p,r})$. Note that the inverse image of each of these covering balls (in \mathbb{R}^n) is contained in a D-dimensional ball of radius r/2 that is centered at some point in $M_{p,r}$ (by noting $r \leq \tau/4$ and using Lemma 19(ii)). Thus, the centers of these D-dimensional balls (containing the inverse images) forms the desired covering.

Lemma 21 (relating nearby manifold points to tangent vectors) Pick any point $p \in M$ and let $q \in M$ (distinct from p) be such that $D_G(p,q) \leq \tau$. Let $v \in T_pM$ be the projection of the vector q - p onto T_pM . Then, i) $\left| \frac{v}{\|v\|} \cdot \frac{q-p}{\|q-p\|} \right| \geq 1 - (D_G(p,q)/2\tau)^2$, ii) $\left\| \frac{v}{\|v\|} - \frac{q-p}{\|q-p\|} \right\| \leq D_G(p,q)/\tau\sqrt{2}$.

Proof If vectors v and q-p are in the same direction, we are done. Otherwise, consider the plane spanned by vectors v and q-p. Then since M has condition number $1/\tau$, we know that the point q cannot lie within any τ -ball tangent to M at p (see Figure 6). Consider

such a τ -ball (with center c) whose center is closest to q and let q' be the point on the surface of the ball which subtends the same angle ($\angle pcq'$) as the angle formed by q ($\angle pcq$). Let this angle be called θ . Then using cosine rule, we have $\cos \theta = 1 - ||q' - p||^2/2\tau^2$.

Define α as the angle subtended by vectors v and q-p, and α' the angle subtended by vectors v and q'-p. WLOG we can assume that the angles α and α' are less than $\pi/2$. Then, $\cos \alpha \ge \cos \alpha' = \cos \theta/2$. Using the trigonometric identity $\cos \theta = 2\cos^2\left(\frac{\theta}{2}\right) - 1$, and noting $||q-p||^2 \ge ||q'-p||^2$, we have

$$\left| \frac{v}{\|v\|} \cdot \frac{q-p}{\|q-p\|} \right| = \cos \alpha \ge \cos \frac{\theta}{2} \ge \sqrt{1 - \|q-p\|^2 / 4\tau^2} \ge 1 - (D_G(p,q)/2\tau)^2.$$

Now, by applying the cosine rule, we have $\left\| \frac{v}{\|v\|} - \frac{q-p}{\|q-p\|} \right\|^2 = 2(1-\cos\alpha)$. The lemma follows.

Lemma 22 (approximating tangent space by nearby samples) Let $0 < \delta \le 1$. Pick any point $p_0 \in M$ and let $p_1, \ldots, p_n \in M$ be n points distinct from p_0 such that (for all $1 \le i \le n$)

(i)
$$D_G(p_0, p_i) \le \tau \delta / \sqrt{n}$$
,

(ii)
$$\left| \frac{p_i - p_0}{\|p_i - p_0\|} \cdot \frac{p_j - p_0}{\|p_i - p_0\|} \right| \le 1/2n \ (\text{for } i \ne j).$$

Let \hat{T} be the n dimensional subspace spanned by vectors $\{p_i - p_0\}_{i \in [n]}$. For any unit vector $\hat{u} \in \hat{T}$, let u be the projection of \hat{u} onto $T_{p_0}M$. Then, $|\hat{u} \cdot \frac{u}{|u|}| \geq 1 - \delta$.

Proof Define the vectors $\hat{v}_i := \frac{p_i - p_0}{\|p_i - p_0\|}$ (for $1 \le i \le n$). Observe that $\{\hat{v}_i\}_{i \in [n]}$ forms a basis of \hat{T} . For $1 \le i \le n$, define v_i as the projection of vector \hat{v}_i onto $T_{p_0}M$. Also note that by applying Lemma 21, we have that for all $1 \le i \le n$, $\|\hat{v}_i - v_i\|^2 \le \delta^2/2n$.

Now consider any unit $\hat{u} \in \hat{T}$, and its projection u in $T_{p_0}M$. Let $V = [\hat{v}_1, \dots, \hat{v}_n]$ be the $D \times n$ matrix with columns v_1, \dots, v_n . We represent the unit vector \hat{u} as $V\alpha = \sum_i \alpha_i \hat{v}_i$. Also, since u is the projection of \hat{u} , we have $u = \sum_i \alpha_i v_i$. Then, $\|\alpha\|^2 \leq 2$. To see this, we first identify \hat{T} with \mathbb{R}^n via an isometry S (a linear map that preserves the lengths and angles of all vectors in \hat{T}). Note that S can be represented as an $n \times D$ matrix, and since the columns of V form a basis for \hat{T} , SV is an $n \times n$ invertible matrix. Then, since $S\hat{u} = SV\alpha$, we have $\alpha = (SV)^{-1}S\hat{u}$. Thus, (recall $\|S\hat{u}\| = 1$)

$$\|\alpha\|^{2} \leq \max_{x \in S^{n-1}} \|(SV)^{-1}x\|^{2} = \lambda_{\max}((SV)^{-\mathsf{T}}(SV)^{-1})$$

$$= \lambda_{\max}((SV)^{-1}(SV)^{-\mathsf{T}}) = \lambda_{\max}((V^{\mathsf{T}}V)^{-1}) = 1/\lambda_{\min}(V^{\mathsf{T}}V)$$

$$\leq 1/(1 - ((n-1)/2n)) \leq 2,$$

where i) $\lambda_{\max}(A)$ and $\lambda_{\min}(A)$ denote the largest and smallest eigenvalues of a square symmetric matrix A respectively, and ii) the second inequality is by noting that $V^{\mathsf{T}}V$ is an $n \times n$ matrix with 1's on the diagonal and at most 1/2n on the off-diagonal elements, and applying the Gershgorin circle theorem.

Now we can bound the quantity of interest. Note that

$$\left| \hat{u} \cdot \frac{u}{\|u\|} \right| \geq \left| \hat{u}^{\mathsf{T}} (\hat{u} - (\hat{u} - u)) \right| \geq 1 - \|\hat{u} - u\| = 1 - \|\sum_{i} \alpha_{i} (\hat{v}_{i} - v_{i}) \|$$

$$\geq 1 - \sum_{i} |\alpha_{i}| \|\hat{v}_{i} - v_{i}\| \geq 1 - (\delta/\sqrt{2n}) \sum_{i} |\alpha_{i}| \geq 1 - \delta,$$

where the last inequality is by noting $\|\alpha\|_1 \leq \sqrt{2n}$.

Appendix B. On Constructing a Bounded Manifold Cover

Given a compact *n*-manifold $M \subset \mathbb{R}^D$ with condition number $1/\tau$, and some $0 < \delta \le 1$. We can construct an α -bounded (ρ, δ) cover X of M (with $\alpha \le 2^{13n}$ and $\rho \le \tau \delta/16n$) as follows.

Set $\rho \leq \tau \delta/16n$ and pick a $(\rho/2)$ -net C of M (that is $C \subset M$ such that, i. for $c, c' \in C$ such that $c \neq c'$, $||c - c'|| \geq \rho/2$, ii. for all $p \in M$, exists $c \in C$ such that $||c - p|| < \rho/2$). WLOG we shall assume that all points of C are in the interior of M. Then, for each $c \in C$, define $M_{c,\rho/2} := \{p \in M : ||p - c|| \leq \rho/2\}$, and the orthogonal projection map $f_c : M_{c,\rho/2} \to T_c M$ that projects $M_{c,\rho/2}$ onto $T_c M$ (note that, cf. Lemma 19(i), f_c is one-to-one). Note that $T_c M$ can be identified with \mathbb{R}^n with the c as the origin. We will denote the origin as $x_0^{(c)}$, that is, $x_0^{(c)} = f_c(c)$.

Now, let B_c be any n-dimensional closed ball centered at the origin $x_0^{(c)} \in T_cM$ of radius r > 0 that is completely contained in $f_c(M_{c,\rho/2})$ (that is, $B_c \subset f_c(M_{c,\rho/2})$). Pick a set of n points $x_1^{(c)}, \ldots, x_n^{(c)}$ on the surface of the ball B_c such that $(x_i^{(c)} - x_0^{(c)}) \cdot (x_j^{(c)} - x_0^{(c)}) = 0$ for $i \neq j$.

Define the bounded manifold cover as

$$X := \bigcup_{c \in C, i=0,\dots,n} f_c^{-1}(x_i^{(c)}). \tag{6}$$

Lemma 23 Let $0 < \delta \le 1$ and $\rho \le \tau \delta/16n$. Let C be a $(\rho/2)$ -net of M as described above, and X be as in Eq. (6). Then X forms a 2^{13n} -bounded (ρ, δ) cover of M.

Proof Pick any point $p \in M$ and define $X_p := \{x \in X : ||x - p|| < \rho\}$. Let $c \in C$ be such that $||p - c|| < \rho/2$. Then X_p has the following properties.

Local spread criterion: For $0 \le i \le n$, since $||f_c^{-1}(x_i^{(c)}) - c|| \le \rho/2$ (by construction), we have $||f_c^{-1}(x_i^{(c)}) - p|| < \rho$. Thus, $f_c^{-1}(x_i^{(c)}) \in X_p$ (for $0 \le i \le n$). Now, for $1 \le i \le n$, noting that $D_G(f_c^{-1}(x_i^{(c)}), f_c^{-1}(x_0^{(c)})) \le 2||f_c^{-1}(x_i^{(c)}) - f_c^{-1}(x_0^{(c)})|| \le \rho$ (cf. Lemma 18), we have that for the vector $\hat{v}_i^{(c)} := \frac{f_c^{-1}(x_i^{(c)}) - f_c^{-1}(x_0^{(c)})}{||f_c^{-1}(x_i^{(c)}) - f_c^{-1}(x_0^{(c)})||}$ and its (normalized) projection $v_i^{(c)} := \frac{x_i^{(c)} - x_0^{(c)}}{||x_i^{(c)} - x_0^{(c)}||}$ onto $T_c M$, $||\hat{v}_i^{(c)} - v_i^{(c)}|| \le \rho/\sqrt{2}\tau$ (cf. Lemma 21). Thus, for $i \ne j$, we have (recall, by construction, we have $v_i^{(c)} \cdot v_j^{(c)} = 0$)

$$|\hat{v}_i^{(c)} \cdot \hat{v}_j^{(c)}| = |(\hat{v}_i^{(c)} - v_i^{(c)} + v_i^{(c)}) \cdot (\hat{v}_j^{(c)} - v_j^{(c)} + v_j^{(c)})|$$

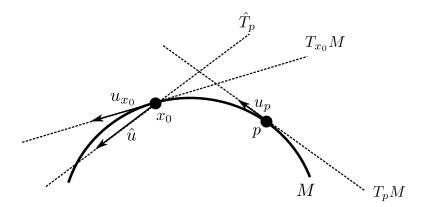


Figure 7: An example manifold M with various quantities of interest. \hat{T}_p is a sample-based approximation to T_pM (using the nearby samples x_0, \ldots, x_n). The angle between \hat{u} and its projection u_p (into T_pM) is bounded by bounding \hat{u} and its projection u_{x_0} (into $T_{x_0}M$) and relating u_{x_0} with its transport to T_pM .

$$= |(\hat{v}_{i}^{(c)} - v_{i}^{(c)}) \cdot (\hat{v}_{j}^{(c)} - v_{j}^{(c)}) + v_{i}^{(c)} \cdot (\hat{v}_{j}^{(c)} - v_{j}^{(c)}) + (\hat{v}_{i}^{(c)} - v_{i}^{(c)}) \cdot v_{j}^{(c)}|$$

$$\leq ||(\hat{v}_{i}^{(c)} - v_{i}^{(c)})||||(\hat{v}_{j}^{(c)} - v_{j}^{(c)})|| + ||\hat{v}_{i}^{(c)} - v_{i}^{(c)}|| + ||\hat{v}_{j}^{(c)} - v_{j}^{(c)}||$$

$$\leq 3\rho/\sqrt{2}\tau \leq 1/2n.$$

Covering criterion: There exists $x \in X_p$, namely $f_c^{-1}(x_0^{(c)})$ (= c), such that $||p-x|| \le \rho/2$.

Local boundedness criterion: Define $M_{p,3\rho/2}:=\{q\in M:\|q-p\|<3\rho/2\}$. Note that $X_p\subset\{f_c^{-1}(x_i^{(c)}):c\in C\cap M_{p,3\rho/2},0\leq i\leq n\}$. Now, using Lemma 20 we have that there exists a cover $N\subset M_{p,3\rho/2}$ of size at most 16^{3n} such that for any point $q\in M_{p,3\rho/2}$, there exists $n'\in N$ such that $\|q-n'\|<\rho/4$. Note that, by construction of C, there cannot be an $n'\in N$ such that it is within distance $\rho/4$ of two (or more) distinct $c,c'\in C$ (since otherwise the distance $\|c-c'\|$ will be less than $\rho/2$, contradicting the packing of C). Thus, $|C\cap M_{p,3\rho/2}|\leq 16^{3n}$. It follows that $|X_p|\leq (n+1)16^{3n}\leq 2^{13n}$.

Tangent space approximation criterion: Pick any n+1 (distinct) points in X_p (viz. x_0, \ldots, x_n) that satisfy the local spread criterion, that is, $\left|\frac{x_i-x_0}{\|x_i-x_0\|}\cdot\frac{x_j-x_0}{\|x_j-x_0\|}\right| \leq 1/2n$ $(i\neq j)$. Let \hat{T}_p be the n-dimensional affine space passing through x_0, \ldots, x_n (note that \hat{T}_p does not necessarily pass through p). Then, for any unit vector $\hat{u}\in\hat{T}_p$, we need to show that its projection u_p onto T_pM has the property $|\hat{u}\cdot\frac{u_p}{\|u_p\|}|\geq 1-\delta$. Let θ be the angle between vectors \hat{u} and u_p . Let u_{x_0} be the projection of \hat{u} onto $T_{x_0}M$, and θ_1 be the angle between vectors \hat{u} and u_{x_0} , and let θ_2 be the angle between vectors u_{x_0} (at x_0) and its parallel transport along the geodesic path to p (see Figure 7). WLOG we can assume that θ_1 and θ_2 are at most $\pi/2$. Then, $\theta \leq \theta_1 + \theta_2 \leq \pi$. We get the bound on the individual angles as follows. By applying Lemma 22, $\cos(\theta_1) \geq 1 - \delta/4$, and by applying Lemma 17, $\cos(\theta_2) \geq 1 - \delta/4$. Finally, by using Lemma 24, we have $|\hat{u}\cdot\frac{u_p}{\|u_p\|}| = \cos(\theta) \geq \cos(\theta_1 + \theta_2) \geq 1 - \delta$.

Lemma 24 Let $0 \le \epsilon_1, \epsilon_2 \le 1$. If $\cos \alpha \ge 1 - \epsilon_1$ and $\cos \beta \ge 1 - \epsilon_2$, then $\cos(\alpha + \beta) \ge 1 - \epsilon_1 - \epsilon_2 - 2\sqrt{\epsilon_1 \epsilon_2}$.

Proof Applying the identity $\sin \theta = \sqrt{1 - \cos^2 \theta}$ immediately yields $\sin \alpha \le \sqrt{2\epsilon_1}$ and $\sin \beta \le \sqrt{2\epsilon_2}$. Now, $\cos(\alpha + \beta) = \cos \alpha \cos \beta - \sin \alpha \sin \beta \ge (1 - \epsilon_1)(1 - \epsilon_2) - 2\sqrt{\epsilon_1 \epsilon_2} \ge 1 - \epsilon_1 - \epsilon_2 - 2\sqrt{\epsilon_1 \epsilon_2}$.

Remark 25 A dense enough sample from M constitutes as a tangent space approximating cover. One can selectively prune the dense sampling to control the total number of points in each neighborhood, while still maintaining the cover properties, forming a bounded cover as per Definition 3.

Appendix C. Bounding the Number of Subsets K in Embedding I

By construction (see the preprocessing stage of Embedding I), $K = \max_{x \in X} |X \cap B(x, 2\rho)|$ (where B(x, r) denotes a Euclidean ball centered at x of radius r). That is, K is the largest number of x's ($\in X$) that are within a 2ρ ball of some $x \in X$.

Now, pick any $x \in X$ and consider the set $M_x := M \cap B(x, 2\rho)$. Then, if $\rho \leq \tau/8$, M_x can be covered by 2^{cn} balls of radius ρ (see Lemma 20). By recalling that X forms an α -bounded (ρ, δ) -cover, we have $|X \cap B(x, 2\rho)| = |X \cap M_x| \leq \alpha 2^{cn}$ (where $c \leq 4$).

Appendix D. Various Proofs

D.1 Proof of Lemma 12

Since R is a random orthoprojector from \mathbb{R}^D to \mathbb{R}^d , it follows that

Lemma 26 (random projection of n-manifolds – adapted from Theorem 1.5 of Clarkson (2008)) Let M be a C_M -regular n-manifold with condition number $1/\tau$. Let $\bar{R} := \sqrt{D/d}R$ be a scaling of R. Pick any $0 < \epsilon \le 1$ and $0 < \delta \le 1$. If $d = \Omega(\epsilon^{-2}n\log(C_M/\tau) + \epsilon^{-2}n\log(1/\epsilon) + \log(1/\delta))$, then with probability at least $1 - \delta$, for all $p, q \in M$

$$(1 - \epsilon) \|p - q\| \le \|\bar{R}p - \bar{R}q\| \le (1 + \epsilon) \|p - q\|.$$

We apply this result with $\epsilon = 1/4$. Then, for $d = \Omega(n \log(C_M/\tau))$, with probability at least 1 - 1/poly(n), $(3/4)\|p - q\| \le \|\bar{R}p - \bar{R}q\| \le (5/4)\|p - q\|$. Now let $\Phi : \mathbb{R}^D \to \mathbb{R}^d$ be defined as $\Phi x := (2/3)\bar{R}x = (2/3)(\sqrt{D/d})x$ (as per the lemma statement). Then we immediately get $(1/2)\|p - q\| \le \|\Phi p - \Phi q\| \le (5/6)\|p - q\|$.

Also note that for any $x \in \mathbb{R}^D$, we have $\|\Phi x\| = (2/3)(\sqrt{D/d})\|Rx\| \le (2/3)(\sqrt{D/d})\|x\|$ (since R is an orthoprojector).

Finally, for any point $p \in M$, a unit vector u tangent to M at p can be approximated arbitrarily well by considering a sequence $\{p_i\}_i$ of points (in M) converging to p (in M) such that $(p_i - p)/\|p_i - p\|$ converges to u. Since for all points p_i , $(1/2) \leq \|\Phi p_i - \Phi p\|/\|p_i - p\| \leq (5/6)$ (with high probability), it follows that $(1/2) \leq \|(D\Phi)_p(u)\| \leq (5/6)$.

D.2 Proof of Corollary 13

Let v_x^1 and v_x^n ($\in \mathbb{R}^n$) be the right singular vectors corresponding to singular values σ_x^1 and σ_x^n respectively of the matrix ΦF_x . Then, quickly note that $\sigma_x^1 = \|\Phi F_x v^1\|$, and $\sigma_x^n = \|\Phi F_x v^n\|$. Note that since F_x is orthonormal, we have that $\|F_x v^1\| = \|F_x v^n\| = 1$. Now, since $F_x v^n$ is in the span of column vectors of F_x , by the sampling condition (cf. Definition 3), there exists a unit length vector \bar{v}_x^n tangent to M (at x) such that $|F_x v_x^n \cdot \bar{v}_x^n| \ge 1 - \delta$. Thus, decomposing $F_x v_x^n$ into two vectors a_x^n and b_x^n such that $a_x^n \perp b_x^n$ and $a_x^n := (F_x v_x^n \cdot \bar{v}_x^n) \bar{v}_x^n$, we have (by Lemma 12)

$$\sigma_x^n = \|\Phi(F_x v^n)\| = \|\Phi((F_x v_x^n \cdot \bar{v}_x^n) \bar{v}_x^n) + \Phi b_x^n\|$$

$$\geq (1 - \delta) \|\Phi \bar{v}_x^n\| - \|\Phi b_x^n\|$$

$$\geq (1 - \delta)(1/2) - (2/3)\sqrt{2\delta D/d},$$

since $||b_x^n||^2 = ||F_x v_x^n||^2 - ||a_x^n||^2 \le 1 - (1 - \delta)^2 \le 2\delta$ and $||\Phi b_x^n|| \le (2/3)(\sqrt{D/d})||b_x^n|| \le (2/3)\sqrt{2\delta D/d}$. Similarly decomposing $F_x v_x^1$ into two vectors a_x^1 and b_x^1 such that $a_x^1 \perp b_x^1$ and $a_x^1 := (F_x v_x^1 \cdot \bar{v}_x^1)\bar{v}_x^1$ (where \bar{v}_x^1 is a unit vector tangent to M at x such that $|F_x v_x^1 \cdot \bar{v}_x^1| \le 1 - \delta$), we have (by Lemma 12)

$$\sigma_x^1 = \|\Phi(F_x v_x^1)\| = \|\Phi((F_x v_x^1 \cdot \bar{v}_x^1) \bar{v}_x^1) + \Phi b_x^1\|
\leq \|\Phi \bar{v}_x^1\| + \|\Phi b_x^1\|
\leq (5/6) + (2/3)\sqrt{2\delta D/d},$$

where the last inequality is by noting $\|\Phi b_x^1\| \leq (2/3)\sqrt{2\delta D/d}$. Now, by our choice of δ ($\leq d/32D$), and by noting that $d \leq D$, the corollary follows.

D.3 Proof of Lemma 14

We can simplify Eq. (1) by recalling how the subsets $X^{(j)}$ were constructed (see preprocessing stage of Embedding I). Note that for any fixed t, at most one term in the set $\{\Lambda_{\Phi(x)}(t)\}_{x\in X^{(j)}}$ is non-zero. Thus,

$$\begin{split} \|(D\Psi)_{t}(u)\|^{2} &= \sum_{k=1}^{d} u_{k}^{2} + \sum_{k=1}^{n} \sum_{x \in X} \Lambda_{\Phi(x)}(t) \cos^{2}(\omega(C^{x}t)_{k}) (C^{x}u)_{k}^{2} + \Lambda_{\Phi(x)}(t) \sin^{2}(\omega(C^{x}t)_{k}) (C^{x}u)_{k}^{2} \\ &+ \frac{1}{\omega} \left[\underbrace{\left(\left(A_{\sin}^{k,x}(t) \right)^{2} + \left(A_{\cos}^{k,x}(t) \right)^{2} \right) / \omega}_{\zeta_{1}} + \underbrace{2 A_{\sin}^{k,x}(t) \sqrt{\Lambda_{\Phi(x)}(t)} \cos(\omega(C^{x}t)_{k}) (C^{x}u)_{k}}_{\zeta_{2}} \right] \\ &= \|u\|^{2} + \sum_{x \in X} \Lambda_{\Phi(x)}(t) \sum_{k=1}^{n} (C^{x}u)_{k}^{2} + \zeta, \end{split}$$

where $\zeta := (\zeta_1 + \zeta_2 + \zeta_3)/\omega$. Noting that i) the terms $|A_{\sin}^{k,x}(t)|$ and $|A_{\cos}^{k,x}(t)|$ are at most $O(\alpha 16^n \sqrt{d}/\rho)$ (see Lemma 27), ii) $|(C^x u)_k| \le 4$, and iii) $\sqrt{\Lambda_{\Phi(x)}(t)} \le 1$, we can pick ω

sufficiently large (say, $\omega \geq \Omega(n\alpha^2 16^n \sqrt{d}/\rho\epsilon)$ such that $|\zeta| \leq \epsilon/2$ (where ϵ is the isometry constant from our main theorem).

Lemma 27 For all k, x and t, the terms $|A_{\sin}^{k,x}(t)|$ and $|A_{\cos}^{k,x}(t)|$ are at most $O(\alpha 16^n \sqrt{d}/\rho)$.

Proof We shall focus on bounding $|A_{\sin}^{k,x}(t)|$ (the steps for bounding $|A_{\cos}^{k,x}(t)|$ are similar). Note that

$$|A_{\sin}^{k,x}(t)| = \left| \sum_{i=1}^{d} u_i \sin(\omega(C^x t)_k) \frac{d\Lambda_{\Phi(x)}^{1/2}(t)}{dt^i} \right| \le \sum_{i=1}^{d} |u_i| \cdot \left| \frac{d\Lambda_{\Phi(x)}^{1/2}(t)}{dt^i} \right| \le \sqrt{\sum_{i=1}^{d} \left| \frac{d\Lambda_{\Phi(x)}^{1/2}(t)}{dt^i} \right|^2},$$

since $||u|| \le 1$. Thus, we can bound $|A_{\sin}^{k,x}(t)|$ by $O(\alpha 16^n \sqrt{d}/\rho)$ by noting the following lemma.

Lemma 28 For all i, x and t, $|d\Lambda_{\Phi(x)}^{1/2}(t)/dt^i| \leq O(\alpha 16^n/\rho)$.

Proof Pick any $t \in \Phi(M)$, and let $p_0 \in M$ be (the unique element) such that $\Phi(p_0) = t$. Define $N_{p_0} := \{x \in X : \|\Phi(x) - \Phi(p_0)\| < \rho\}$ as the neighborhood around p_0 . Fix an arbitrary $x_0 \in N_{p_0} \subset X$ (since if $x_0 \notin N_{p_0}$ then $d\Lambda_{\Phi(x_0)}^{1/2}(t)/dt^i = 0$), and consider the function

$$\Lambda_{\Phi(x_0)}^{1/2}(t) = \left(\frac{\lambda_{\Phi(x_0)}(t)}{\sum_{x \in N_{p_0}} \lambda_{\Phi(x)}(t)}\right)^{1/2} = \left(\frac{e^{-1/(1 - (\|t - \Phi(x_0)\|^2/\rho^2))}}{\sum_{x \in N_{p_0}} e^{-1/(1 - (\|t - \Phi(x)\|^2/\rho^2))}}\right)^{1/2}.$$

Define $A_t(x) := 1/(1-(||t-\Phi(x)||^2/\rho^2))$. Now, pick an arbitrary coordinate $i_0 \in \{1,\ldots,d\}$ and consider the (directional) derivative of this function

$$\frac{d\Lambda_{\Phi(x_0)}^{1/2}(t)}{dt^{i_0}} \ = \ \frac{1}{2} \left(\Lambda_{\Phi(x_0)}^{-1/2}(t)\right) \left(\frac{d\Lambda_{\Phi(x_0)}(t)}{dt^{i_0}}\right) \\ = \ \frac{\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right)^{1/2}}{2\left(e^{-A_t(x_0)}\right)^{1/2}} \left[\frac{\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right) \left(\frac{-2(t_{i_0} - \Phi(x_0)_{i_0})}{\rho^2}(A_t(x_0))^2\right) \left(e^{-A_t(x_0)}\right)}{\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right)^2} - \frac{\left(e^{-A_t(x_0)}\right) \left(\sum_{x \in N_{p_0}} \frac{-2(t_{i_0} - \Phi(x)_{i_0})}{\rho^2}(A_t(x))^2e^{-A_t(x)}\right)}{\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right)^2} \right] \\ = \ \frac{\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right) \left(\frac{-2(t_{i_0} - \Phi(x_0)_{i_0})}{\rho^2}(A_t(x_0))^2\right) \left(e^{-A_t(x_0)}\right)^{1/2}}{2\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right)^{1.5}}$$

$$-\frac{\left(e^{-A_t(x_0)}\right)^{1/2} \left(\sum_{x \in N_{p_0}} \frac{-2(t_{i_0} - \Phi(x)_{i_0})}{\rho^2} (A_t(x))^2 e^{-A_t(x)}\right)}{2\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right)^{1.5}}$$

Observe that the domain of the function A_t is $\{x \in X : ||t - \Phi(x)|| < \rho\}$ and the range is $[1, \infty)$. Recalling that for any $\beta \ge 1$, $|\beta^2 e^{-\beta}| \le 1$ and $|\beta^2 e^{-\beta/2}| \le 3$, we have that $|A_t(\cdot)^2 e^{-A_t(\cdot)}| \le 1$ and $|A_t(\cdot)^2 e^{-A_t(\cdot)/2}| \le 3$. Thus,

$$\left| \frac{d\Lambda_{\Phi(x_0)}^{1/2}(t)}{dt^{i_0}} \right| \leq \frac{3 \cdot \left| \sum_{x \in N_{p_0}} e^{-A_t(x)} \right| \cdot \left| \frac{2(t_{i_0} - \Phi(x_0)_{i_0})}{\rho^2} \right| + \left| e^{-A_t(x_0)/2} \right| \cdot \left| \sum_{x \in N_{p_0}} \frac{2(t_{i_0} - \Phi(x)_{i_0})}{\rho^2} \right|}{2\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right)^{1.5}}$$

$$\leq \frac{(3)(2/\rho) \left| \sum_{x \in N_{p_0}} e^{-A_t(x)} \right| + \left| e^{-A_t(x_0)/2} \right| \sum_{x \in N_{p_0}} (2/\rho)}{2\left(\sum_{x \in N_{p_0}} e^{-A_t(x)}\right)^{1.5}}$$

$$\leq O(\alpha 16^n/\rho),$$

where the last inequality is by noting: i) $|N_{p_0}| \le \alpha 16^n$ (since for all $x \in N_{p_0}$, $||x - p_0|| \le 2\rho$ – cf. Lemma 12, X is an α -bounded cover, and by noting that for $\rho \le \tau/8$, a ball of radius 2ρ can be covered by 16^n balls of radius ρ on the given n-manifold – cf. Lemma 20), ii) $|e^{-A_t(x)}| \le |e^{-A_t(x)/2}| \le 1$ (for all x), and iii) $\sum_{x \in N_{p_0}} e^{-A_t(x)} \ge \Omega(1)$ (since our cover X ensures that for any p_0 , there exists $x \in N_{p_0} \subset X$ such that $||p_0 - x|| \le \rho/2$ – see also Remark 4, and hence $e^{-A_t(x)}$ is non-negligible for some $x \in N_{p_0}$).

D.4 Proof of Lemma 15

Note that by definition, $\|(D\Psi)_t(u)\|^2 = \|(D\Psi_{|X|,n})_t(u)\|^2$. Thus, using Eq. (3) and expanding the recursion, we have

$$\begin{split} \|(D\Psi)_{t}(u)\|^{2} &= \|(D\Psi_{|X|,n})_{t}(u)\|^{2} \\ &= \|(D\Psi_{|X|,n-1})_{t}(u)\|^{2} + \Lambda_{\Phi(x_{|X|})}(t)(C^{x_{|X|}}u)_{n}^{2} + Z_{|X|,n} \\ &\vdots \\ &= \|(D\Psi_{0,n})_{t}(u)\|^{2} + \left[\sum_{i=1}^{|X|} \Lambda_{\Phi(x_{i})}(t)\sum_{j=1}^{n} (C^{x_{i}}u)_{j}^{2}\right] + \sum_{i,j} Z_{i,j}. \end{split}$$

Note that $(D\Psi_{i,0})_t(u) := (D\Psi_{i-1,n})_t(u)$. Now recalling that $||(D\Psi_{0,n})_t(u)||^2 = ||u||^2$ (the base case of the recursion), all we need to show is that $|\sum_{i,j} Z_{i,j}| \le \epsilon/2$. This follows directly from the lemma below.

Lemma 29 Let $\epsilon_0 \leq O(\epsilon/\sqrt{d}(n|X|)^2)$, and for any i, j, let $\omega_{i,j} \geq \Omega((K_{i,j} + (\alpha 16^n/\rho))(nd|X|)^2/\epsilon)$ (as per the statement of Lemma 15). Then, for any $i, j, |Z_{i,j}| \leq \epsilon/2n|X|$.

Proof Recall that (cf. Eq. (3))

$$Z_{i,j} = \underbrace{\frac{1}{\omega_{i,j}^2} \sum_{k} \left(\zeta_{i,j}^{k,4}\right)^2}_{(a)} + 2 \underbrace{\sum_{k} \frac{\zeta_{i,j}^{k,4}}{\omega_{i,j}} \left(\zeta_{i,j}^{k,1} + \zeta_{i,j}^{k,2} + \zeta_{i,j}^{k,3}\right)}_{(b)} + 2 \underbrace{\sum_{k} \zeta_{i,j}^{k,1} \zeta_{i,j}^{k,2} + 2 \underbrace{\sum_{k} \zeta_{i,j}^{k,1} \zeta_{i,j}^{k,3}}_{(d)}}_{(d)}.$$

Term (a): Note that $|\sum_k (\zeta_{i,j}^{k,4})^2| \leq O(d^3(K_{i,j} + (\alpha 16^n/\rho))^2)$ (cf. Lemma 30 (iv)). By our choice of $\omega_{i,j}$, we have term (a) at most $O(\epsilon/n|X|)$.

Term (b): Note that $\left|\zeta_{i,j}^{k,1}+\zeta_{i,j}^{k,2}+\zeta_{i,j}^{k,3}\right| \leq O(n|X|+(\epsilon/dn|X|))$ (by noting Lemma 30 (i)-(iii), recalling the choice of $\omega_{i,j}$, and summing over all i',j'). Thus, $\left|\sum_k \zeta_{i,j}^{k,4}(\zeta_{i,j}^{k,1}+\zeta_{i,j}^{k,2}+\zeta_{i,j}^{k,3})\right| \leq O\left(\left(d^2(K_{i,j}+(\alpha 16^n/\rho))\right)\left(n|X|+(\epsilon/dn|X|)\right)\right)$. Again, by our choice of $\omega_{i,j}$, term (b) is at most $O(\epsilon/n|X|)$.

Terms (c) and (d): We focus on bounding term (c) (the steps for bounding term (d) are same). Note that $|\sum_k \zeta_{i,j}^{k,1} \zeta_{i,j}^{k,2}| \le 4|\sum_k \zeta_{i,j}^{k,1} (\eta_{i,j}(t))_k|$ (by combining the definition of $\zeta_{i,j}^1$ and $\zeta_{i,j}^2$ from Eq. (3) with Lemma 32(b) and Corollary 13). Now, observe that $(\zeta_{i,j}^{k,1})_{k=1,\dots,2d+3}$ is a tangent vector with length at most $O(\sqrt{dn}|X|)$ (cf. Lemma 30 (i)). Thus, by noting that $\eta_{i,j}$ is almost normal (with quality of approximation ϵ_0), we have term (c) at most $O(\epsilon/n|X|)$.

By choosing the constants in the order terms appropriately, we can get the lemma.

Lemma 30 Let $\zeta_{i,j}^{k,1}$, $\zeta_{i,j}^{k,2}$, $\zeta_{i,j}^{k,3}$, and $\zeta_{i,j}^{k,4}$ be as defined in Eq. (3). Then for all $1 \le i \le |X|$ and $1 \le j \le n$, we have

(i)
$$|\zeta_{i,j}^{k,1}| \le 1 + 8n|X| + \sum_{i'=1}^{i} \sum_{j'=1}^{j-1} O(d(K_{i',j'} + (\alpha 16^n/\rho))/\omega_{i',j'}),$$

- (ii) $|\zeta_{i,j}^{k,2}| \le 4$,
- $(iii) \ |\zeta_{i,j}^{k,3}| \leq 4,$
- (iv) $|\zeta_{i,j}^{k,4}| \le O(d(K_{i,j} + (\alpha 16^n/\rho))).$

Proof First note for any $||u|| \le 1$ and for any $x_i \in X$, $1 \le j \le n$ and $1 \le l \le d$, we have $|\sum_l C_{j,l}^{x_i} u_l| = |(C^{x_i} u)_j| \le 4$ (cf. Lemma 32 (b) and Corollary 13).

Noting that for all *i* and *j*, $\|\eta_{i,j}\| = \|\nu_{i,j}\| = 1$, we have $|\zeta_{i,j}^{k,2}| \leq 4$ and $|\zeta_{i,j}^{k,3}| \leq 4$.

Observe that $\zeta_{i,j}^{k,4} = \sum_l u_l R_{i,j}^{k,l}$. For all i, j, k and l, note that i) $||d\eta_{i,j}(t)/dt^l|| \leq K_{i,j}$ and $||d\nu_{i,j}(t)/dt^l|| \leq K_{i,j}$ and ii) $|d\lambda_{\Phi(x)}^{1/2}(t)/dt^l| \leq O(\alpha 16^n/\rho)$ (cf. Lemma 28). Thus we have

$$|\zeta_{i,j}^{k,4}| \le O(d(K_{i,j} + (\alpha 16^n/\rho))).$$

Now for any i, j, note that $\zeta_{i,j}^{k,1} = \sum_l u_l d\Psi_{i,j-1}(t)/dt^l$. Thus by recursively expanding, $|\zeta_{i,j}^{k,1}| \leq 1 + 8n|X| + \sum_{i'=1}^i \sum_{j'=1}^{j-1} O(d(K_{i',j'} + (\alpha 16^n/\rho))/\omega_{i',j'})$.

D.5 Proof of Lemma 16

We start by stating the following useful observations:

Lemma 31 Let A be a linear operator such that $\max_{\|x\|=1} \|Ax\| \le \delta_{\max}$. Let u be a unit-length vector. If $\|Au\| \ge \delta_{\min} > 0$, then for any unit-length vector v such that $|u \cdot v| \ge 1 - \epsilon$, we have

$$1 - \frac{\delta_{\max} \sqrt{2\epsilon}}{\delta_{\min}} \le \frac{\|Av\|}{\|Au\|} \le 1 + \frac{\delta_{\max} \sqrt{2\epsilon}}{\delta_{\min}}.$$

Proof Let v' = v if $u \cdot v > 0$, otherwise let v' = -v. Quickly note that $||u - v'||^2 = ||u||^2 + ||v'||^2 - 2u \cdot v' = 2(1 - u \cdot v') \le 2\epsilon$. Thus, we have,

i.
$$||Av|| = ||Av'|| \le ||Au|| + ||A(u - v')|| \le ||Au|| + \delta_{\max} \sqrt{2\epsilon}$$
,

ii.
$$||Av|| = ||Av'|| \ge ||Au|| - ||A(u - v')|| \ge ||Au|| - \delta_{\max} \sqrt{2\epsilon}$$
.

Noting that $||Au|| \ge \delta_{\min}$ yields the result.

Lemma 32 Let $x_1, \ldots, x_n \in \mathbb{R}^D$ be a set of orthonormal vectors, $F := [x_1, \ldots, x_n]$ be a $D \times n$ matrix and let Φ be a linear map from \mathbb{R}^D to \mathbb{R}^d ($n \leq d \leq D$) such that for all non-zero $a \in span(F)$ we have $0 < \|\Phi a\| \leq \|a\|$. Let $U\Sigma V^{\mathsf{T}}$ be the thin SVD of ΦF . Define $C = (\Sigma^{-2} - I)^{1/2} U^{\mathsf{T}}$. Then,

- (a) $||C(\Phi a)||^2 = ||a||^2 ||\Phi a||^2$, for any $a \in span(F)$,
- (b) $||C||^2 \le (1/\sigma^n)^2$, where $||\cdot||$ denotes the spectral norm of a matrix and σ^n is the n^{th} largest singular value of ΦF .

Proof Note that the columns of FV form an orthonormal basis for the subspace spanned by columns of F, such that $\Phi(FV) = U\Sigma$. Thus, since $a \in \text{span}(F)$, let y be such that a = FVy. Note that i) $||a||^2 = ||y||^2$, ii) $||\Phi a||^2 = ||U\Sigma y||^2 = y^{\mathsf{T}}\Sigma^2 y$. Now,

$$\begin{split} \|C\Phi a\|^2 &= \|((\Sigma^{-2} - I)^{1/2} U^{\mathsf{T}}) \Phi F V y\|^2 \\ &= \|(\Sigma^{-2} - I)^{1/2} U^{\mathsf{T}} U \Sigma V^{\mathsf{T}} V y\|^2 \\ &= \|(\Sigma^{-2} - I)^{1/2} \Sigma y\|^2 \\ &= y^{\mathsf{T}} y - y^{\mathsf{T}} \Sigma^2 y \\ &= \|a\|^2 - \|\Phi a\|^2. \end{split}$$

Now, consider $||C||^2$.

$$||C||^{2} \leq ||(\Sigma^{-2} - I)^{1/2}||^{2}||U^{\mathsf{T}}||^{2}$$

$$\leq \max_{||x||=1} ||(\Sigma^{-2} - I)^{1/2}x||^{2}$$

$$\leq \max_{||x||=1} x^{\mathsf{T}} \Sigma^{-2} x$$

$$= \max_{||x||=1} \sum_{i} x_{i}^{2} / (\sigma^{i})^{2}$$

$$\leq (1/\sigma^{n})^{2},$$

where σ^i are the (top n) singular values forming the diagonal matrix Σ .

Lemma 33 Let $M \subset \mathbb{R}^D$ be a compact Riemannian n-manifold with condition number $1/\tau$. Pick any $x \in M$ and let F_x be any n-dimensional affine space with the property: for any unit vector v_x tangent to M at x, and its projection v_{xF} onto F_x , $\left|v_x \cdot \frac{v_{xF}}{\|v_{xF}\|}\right| \geq 1 - \delta$. Then for any $p \in M$ such that $\|x - p\| \leq \rho \leq \tau/2$, and any unit vector v tangent to M at p, $(\xi := (2\rho/\tau) + \delta + 2\sqrt{2\rho\delta/\tau})$

$$i. \left| v \cdot \frac{v_F}{\|v_F\|} \right| \ge 1 - \xi,$$

ii.
$$||v_F||^2 \ge 1 - 2\xi$$
,

$$iii. \|v_r\|^2 \le 2\xi,$$

where v_F is the projection of v onto F_x and v_r is the residual (i.e. $v = v_F + v_r$ and $v_F \perp v_r$).

Proof Let γ be the angle between v_F and v. We will bound this angle.

Let v_x (at x) be the parallel transport of v (at p) via the (shortest) geodesic path via the manifold connection. Let the angle between vectors v and v_x be α . Let v_{xF} be the projection of v_x onto the subspace F_x , and let the angle between v_x and v_{xF} be β . WLOG, we can assume that the angles α and β are acute. Then, since $\gamma \leq \alpha + \beta \leq \pi$, we have that $\left|v \cdot \frac{v_F}{\|v_F\|}\right| = \cos \gamma \geq \cos(\alpha + \beta)$. We bound the individual terms $\cos \alpha$ and $\cos \beta$ as follows.

Now, since $||p-x|| \le \rho$, using Lemmas 17 and 18, we have $\cos(\alpha) = |v \cdot v_x| \ge 1 - 2\rho/\tau$. We also have $\cos(\beta) = \left|v_x \cdot \frac{v_{xF}}{\|v_{xF}\|}\right| \ge 1 - \delta$. Then, using Lemma 24, we finally get $\left|v \cdot \frac{v_F}{\|v_F\|}\right| = |\cos(\gamma)| \ge 1 - 2\rho/\tau - \delta - 2\sqrt{2\rho\delta/\tau} = 1 - \xi$.

Also note since
$$1 = \|v\|^2 = (v \cdot \frac{v_F}{\|v_F\|})^2 \left\| \frac{v_F}{\|v_F\|} \right\|^2 + \|v_r\|^2$$
, we have $\|v_r\|^2 = 1 - \left(v \cdot \frac{v_F}{\|v_F\|}\right)^2 \le 2\xi$, and $\|v_F\|^2 = 1 - \|v_r\|^2 \ge 1 - 2\xi$.

Now we are in a position to prove Lemma 16. Let v_F be the projection of the unit vector v (at p) onto the subspace spanned by (the columns of) F_x and v_r be the residual

(i.e. $v = v_F + v_r$ and $v_F \perp v_r$). Then, noting that p, x, v and F_x satisfy the conditions of Lemma 33 (with ρ in the Lemma 33 replaced with 2ρ from the statement of Lemma 16), we have $(\xi := (4\rho/\tau) + \delta + 4\sqrt{\rho\delta/\tau})$

- a) $|v \cdot \frac{v_F}{||v_F||}| \ge 1 \xi$,
- b) $||v_F||^2 \ge 1 2\xi$,
- c) $||v_r||^2 \le 2\xi$.

We can now bound the required quantity $||C^x u||^2$. Note that

$$||C^{x}u||^{2} = ||C^{x}\Phi v||^{2} = ||C^{x}\Phi(v_{F} + v_{r})||^{2}$$

$$= ||C^{x}\Phi v_{F}||^{2} + ||C^{x}\Phi v_{r}||^{2} + 2C^{x}\Phi v_{F} \cdot C^{x}\Phi v_{r}$$

$$= \underbrace{||v_{F}||^{2} - ||\Phi v_{F}||^{2}}_{(a)} + \underbrace{||C^{x}\Phi v_{r}||^{2}}_{(b)} + \underbrace{2C^{x}\Phi v_{F} \cdot C^{x}\Phi v_{r}}_{(c)}$$

where the last equality is by observing v_F is in the span of F_x and applying Lemma 32 (a). We now bound the terms (a),(b), and (c) individually.

Term (a): Note that $1 - 2\xi \le ||v_F||^2 \le 1$ and observing that Φ satisfies the conditions of Lemma 31 with $\delta_{\max} = (2/3)\sqrt{D/d}$, $\delta_{\min} = (1/2) \le ||\Phi v||$ (cf. Lemma 12) and $|v \cdot \frac{v_F}{||v_F||}| \ge 1 - \xi$, we have (recall $||\Phi v|| = ||u|| \le 1$)

$$||v_{F}||^{2} - ||\Phi v_{F}||^{2} \leq 1 - ||v_{F}||^{2} \left\| \Phi \frac{v_{F}}{||v_{F}||} \right\|^{2}$$

$$\leq 1 - (1 - 2\xi) \left\| \Phi \frac{v_{F}}{||v_{F}||} \right\|^{2}$$

$$\leq 1 + 2\xi - \left\| \Phi \frac{v_{F}}{||v_{F}||} \right\|^{2}$$

$$\leq 1 + 2\xi - (1 - (4/3)\sqrt{2\xi D/d})^{2} ||\Phi v||^{2}$$

$$\leq 1 - ||u||^{2} + (2\xi + (8/3)\sqrt{2\xi D/d}), \tag{7}$$

where the fourth inequality is by using Lemma 31. Similarly, in the other direction

$$||v_F||^2 - ||\Phi v_F||^2 \ge 1 - 2\xi - ||v_F||^2 \left\| \Phi \frac{v_F}{||v_F||} \right\|^2$$

$$\ge 1 - 2\xi - \left\| \Phi \frac{v_F}{||v_F||} \right\|^2$$

$$\ge 1 - 2\xi - \left(1 + (4/3)\sqrt{2\xi D/d} \right)^2 ||\Phi v||^2$$

$$\ge 1 - ||u||^2 - \left(2\xi + (32/9)\xi(D/d) + (8/3)\sqrt{2\xi D/d} \right). \tag{8}$$

Term (b): Note that for any x, $\|\Phi x\| \leq (2/3)(\sqrt{D/d})\|x\|$. We can apply Lemma 32 (b) with $\sigma_x^n \geq 1/4$ (cf. Corollary 13) and noting that $\|v_r\|^2 \leq 2\xi$, we immediately get

$$0 \le \|C^x \Phi v_r\|^2 \le 4^2 \cdot (4/9)(D/d)\|v_r\|^2 \le (128/9)(D/d)\xi. \tag{9}$$

Term (c): Recall that for any x, $\|\Phi x\| \leq (2/3)(\sqrt{D/d})\|x\|$, and using Lemma 32 (b) we have that $\|C^x\|^2 \leq 16$ (since $\sigma_x^n \geq 1/4$ – cf. Corollary 13).

Now let $a := C^x \Phi v_F$ and $b := C^x \Phi v_r$. Then $||a|| = ||C^x \Phi v_F|| \le ||C^x|| ||\Phi v_F|| \le 4$ (since $||C^x|| \le 4$, and noting that v_F is vector in the column-span of F_x such that $||v_F|| \le 1$ and the largest singular value of ΦF_x is at most 1 by Corollary 13), and $||b|| = ||C^x \Phi v_F|| \le (8/3)\sqrt{2\xi D/d}$ (see Eq. (9)).

Thus, $|2a \cdot b| \le 2||a|| ||b|| \le 2 \cdot 4 \cdot (8/3) \sqrt{2\xi D/d} = (64/3) \sqrt{2\xi D/d}$. Equivalently,

$$-(64/3)\sqrt{2\xi D/d} \le 2C^x \Phi v_F \cdot C^x \Phi v_r \le (64/3)\sqrt{2\xi D/d}.$$
 (10)

Combining (7)-(10), and noting $d \leq D$, yields the lemma.

Appendix E. Computing the Normal Vectors

The success of the second embedding technique crucially depends upon finding (at each iteration step) a pair of mutually orthogonal unit vectors that are normal to the embedding of manifold M (from the previous iteration step) at a given point p. At a first glance finding such normal vectors seems infeasible since we only have access to a finite size sample Xfrom M. The saving grace comes from noting that the corrections are applied to the ndimensional manifold $\Phi(M)$ that is actually a submanifold of d-dimensional space \mathbb{R}^d . Let's denote this space \mathbb{R}^d as a flat d-manifold N (containing our manifold of interest $\Phi(M)$). Note that even though we only have partial information about $\Phi(M)$ (since we only have samples from it), we have full information about N (since it is the entire space \mathbb{R}^d). What it means is that given some point of interest $\Phi p \in \Phi(M) \subset N$, finding a vector normal to N (at Φp) automatically is a vector normal to $\Phi(M)$ (at Φp). Of course, to find two mutually orthogonal normals to a d-manifold N, N itself needs to be embedded in a larger dimensional Euclidean space (although embedding into d+2 should suffice, for computational reasons we will embed N into Euclidean space of dimension 2d+3). This is precisely the first thing we do before applying any corrections (cf. Step 2 of Embedding II in Section 4). See Figure 8 for an illustration of the setup before finding any normals.

Now for every iteration of the algorithm, note that we have complete knowledge of N and exactly what function (namely $\Psi_{i,j}$ for iteration i, j) is being applied to N. Thus with additional computation effort, one can compute the necessary normal vectors.

More specifically, We can estimate a pair of mutually orthogonal unit vectors that are normal to $\Psi_{i,j}(N)$ at Φp (for any step i, j) as follows.

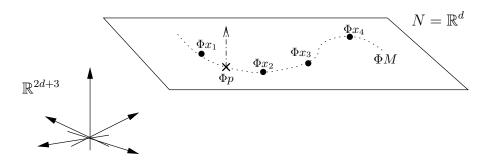


Figure 8: Basic setup for computing the normals to the underlying n-manifold ΦM at the point of interest Φp . Observe that even though it is difficult to find vectors normal to ΦM at Φp within the containing space \mathbb{R}^d (because we only have a finite-size sample from ΦM , viz. Φx_1 , Φx_2 , etc.), we can treat the point Φp as part of the bigger ambient manifold N (= \mathbb{R}^d , that contains ΦM) and compute the desired normals in a space that contains N itself. Now, for each i, j iteration of Algorithm II, $\Psi_{i,j}$ acts on the entire N, and since we have complete knowledge about N, we can compute the desired normals.

Algorithm 4 Compute Normal Vectors

Preprocessing Stage:

1: Let $\eta_{i,j}^{\mathrm{rand}}$ and $\nu_{i,j}^{\mathrm{rand}}$ be vectors in \mathbb{R}^{2d+3} drawn independently at random from the surface of the unit-sphere (for $1 \leq i \leq |X|, \ 1 \leq j \leq n$).

Compute Normals: For any point of interest $p \in M$, let $t := \Phi p$ denote its projection into \mathbb{R}^d . Now, for any iteration i,j (where $1 \leq i \leq |X|$, and $1 \leq j \leq n$), we shall assume that $\Psi_{i,j-1}$ (cf. Step 3) from the previous iteration i,j-1 is already given. Then we can compute the (approximated) normals $\eta_{i,j}(t)$ and $\nu_{i,j}(t)$ for the iteration i,j as follows.

- 1: Let $\Delta > 0$ be the quality of approximation.
- 2: **for** k = 1, ..., d **do**
- 3: Approximate the k^{th} tangent vector as

$$T^k := \frac{\Psi_{i,j-1}(t + \Delta e^k) - \Psi_{i,j-1}(t)}{\Delta},$$

where $\Psi_{i,j-1}$ is as defined in Section 5.3, and e^k is the k^{th} standard vector.

- 4: end for
- 5: Let $\eta = \eta_{i,j}^{\text{rand}}$, and $\nu = \nu_{i,j}^{\text{rand}}$.
- 6: Use Gram-Schmidt orthogonalization process to extract $\hat{\eta}$ (from η) that is orthogonal to vectors $\{T^1, \dots, T^d\}$.
- 7: Use Gram-Schmidt orthogonalization process to extract $\hat{\nu}$ (from ν) that is orthogonal to vectors $\{T^1, \dots, T^d, \hat{\eta}\}$.
- 8: **return** $\hat{\eta}/\|\hat{\eta}\|$ and $\hat{\nu}/\|\hat{\nu}\|$ as mutually orthogonal unit vectors that are approximately normal to $\Psi_{i,j-1}(\Phi M)$ at $\Psi_{i,j-1}(t)$.

A few remarks are in order.

Remark 34 The choice of target dimension of size 2d+3 (instead of d+2) ensures that a pair of random unit-vectors η and ν are not parallel to any vector in the tangent bundle of $\Psi_{i,j-1}(N)$ with probability 1. This follows from Sard's theorem (see e.g. Milnor, 1972), and is the key observation in reducing the embedding size in Whitney's embedding (Whitney, 1936). This also ensures that our orthogonalization process (Steps 6 and 7) will not result in a null vector.

Remark 35 By picking Δ sufficiently small, we can approximate the normals η and ν arbitrarily well by approximating the tangents T^1, \ldots, T^d well.

Remark 36 For each iteration i, j, the vectors $\hat{\eta}/\|\hat{\eta}\|$ and $\hat{\nu}/\|\hat{\nu}\|$ that are returned (in Step 8) are a smooth modification to the starting vectors $\eta_{i,j}^{\mathrm{rand}}$ and $\nu_{i,j}^{\mathrm{rand}}$ respectively. Now, since we use the same starting vectors $\eta_{i,j}^{\mathrm{rand}}$ and $\nu_{i,j}^{\mathrm{rand}}$ regardless of the point of application $(t = \Phi p)$, it follows that the respective directional derivatives of the returned vectors are bounded as well.

By noting Remarks 35 and 36, the approximate normals we return satisfy the conditions needed for Embedding II (see our discussion in Section 5.3).

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