

Spectral convergence of the connection Laplacian from random samples

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Spectral methods that are based on eigenvectors and eigenvalues of discrete graph Laplacians, such as Diffusion Maps and Laplacian Eigenmaps, are often used for manifold learning and nonlinear dimensionality reduction. It was previously shown by Belkin & Niyogi (2007, Convergence of Laplacian eigenmaps, vol. 19. *Proceedings of the 2006 Conference on Advances in Neural Information Processing Systems*. The MIT Press, p. 129.) that the eigenvectors and eigenvalues of the graph Laplacian converge to the eigenfunctions and eigenvalues of the Laplace–Beltrami operator of the manifold in the limit of infinitely many data points sampled independently from the uniform distribution over the manifold. Recently, we introduced Vector Diffusion Maps and showed that the connection Laplacian of the tangent bundle of the manifold can be approximated from random samples. In this article, we present a unified framework for approximating other connection Laplacians over the manifold by considering its principle bundle structure. We prove that the eigenvectors and eigenvalues of these Laplacians converge in the limit of infinitely many independent random samples. We generalize the spectral convergence results to the case where the data points are sampled from a non-uniform distribution, and for manifolds with and without boundary.

Keywords: graph connection Laplacian; vector diffusion maps; vector diffusion distance; orientable diffusion maps; diffusion maps; principal bundle; connection Laplacian.

1 Introduction

A recurring problem in fields such as neuroscience, computer graphics and image processing is that of organizing a set of 3-dimension/dimensional objects by pairwise comparisons. For example, the objects can be 3-dimension/dimensional brain functional magnetic resonance imaging (fMRI) images [21] that correspond to similar functional activity. In order to separate the actual sources of variability among the images from the nuisance parameters that correspond to different conditions of the acquisition process, the images are initially registered and aligned. Similarly, the shape space analysis problem in computer graphics [29] involves the organization of a collection of shapes. Also in this problem it is desired to factor out nuisance shape deformations, such as rigid transformations.

Once the nuisance parameters have been factored out, methods such as Diffusion Maps (DM) [11] or Laplacian Eigenmaps (LE) [3] can be used for nonlinear dimensionality reduction, classification

and clustering. In [33], we introduced Vector Diffusion Maps (VDM) as an algorithmic framework for organization of such data sets that simultaneously takes into account the nuisance parameters and the data affinities by a single computation of the eigenvectors and eigenvalues of the graph connection Laplacian (GCL) that encodes both types of information. In [33], we also proved pointwise convergence of the GCL to the connection Laplacian of the tangent bundle of the data manifold in the limit of infinitely many sample points. The main contribution of the current article is a proof for the spectral convergence of the CGL to the connection Laplacian operator over the vector bundle of the data manifold. In passing, we also provide a spectral convergence result for the graph Laplacian (normalized properly) to the Laplace–Beltrami operator in the case of non-uniform sampling and for manifolds with non-empty boundary, thus broadening the scope of a previous result of Belkin & Niyogi [5].

At the center of LE, DM and VDM is a weighted undirected graph, whose vertices correspond to the data objects, and the weights quantify the affinities between them. A commonly used metric is the Euclidean distance, and the affinity can then be described using a kernel function of the distance. For example, if the data set $\{x_1, x_2, \dots, x_n\}$ consists of n functions in $L_2(\mathbb{R}^3)$, then the distances are given by

$$d_E(x_i, x_j) := \|x_i - x_j\|_{L^2(\mathbb{R}^3)}, \quad (1.1)$$

and the weights can be defined using the Gaussian kernel with width \sqrt{h} as

$$w_{ij} = e^{-\frac{d_E^2(x_i, x_j)}{2h}}. \quad (1.2)$$

However, the Euclidean distance is sensitive to the nuisance parameters. In order to factor out the nuisance parameters, it is required to use a metric which is invariant to the group of transformations associated with those parameters, denoted by G . Let \mathcal{X} be the total space from which data is sampled. The group G acts on \mathcal{X} and instead of measuring distances between elements of \mathcal{X} , we want to measure distances between their orbits. The orbit of a point $x \in \mathcal{X}$ is the set of elements of \mathcal{X} to which x can be mapped by the elements of G , denoted by

$$Gx = \{g \circ x \mid g \in G\}. \quad (1.3)$$

The group action induces an equivalence relation on \mathcal{X} and the orbits are the equivalence classes, such that the equivalence class $[x]$ of $x \in \mathcal{X}$ is Gx . The invariant metric is a metric on the orbit space \mathcal{X}/G of equivalent classes.

One possible way of constructing the invariant metric d_G is through optimal alignment, given as

$$d_G([x_i], [x_j]) = \inf_{g_i, g_j \in G} d_E(g_i \circ x_i, g_j \circ x_j). \quad (1.4)$$

If the action of the group is an isometry, then

$$d_G([x_i], [x_j]) = \inf_{g \in G} d_E(x_i, g \circ x_j). \quad (1.5)$$

For example, if $\mathcal{X} = L^2(\mathbb{R}^3)$ and G is $O(3)$ (the group of 3×3 orthogonal matrices), then the left action

$$(g \circ f)(x) = f(g^{-1}x) \quad (1.6)$$

is an isometry, and

$$d_G^2([f_i], [f_j]) = \min_{g \in O(3)} \int_{\mathbb{R}^3} |f_i(x) - f_j(g^{-1}x)|^2 dx. \quad (1.7)$$

In this article we only consider groups that are either orthogonal and unitary, for three reasons. First, this condition guarantees that the GCL is symmetric (or Hermitian). Secondly, the action is an isometry and the invariant metric (1.5) is well defined. Thirdly, it is a compact group and the minimizer of (1.7) is well defined.

The invariant metric d_G can be used to define weights between data samples, for example, the Gaussian kernel gives

$$w_{ij} = e^{-\frac{d_G^2(x_i, x_j)}{2h}}. \quad (1.8)$$

While LE and DM with weights given in (1.2) correspond to diffusion over the original space \mathcal{X} , LE and DM with weights given in (1.8) correspond to diffusion over the orbit space \mathcal{X}/G . In VDM, the weights (1.8) are also accompanied by the optimal transformations

$$g_{ij} = \operatorname{argmin}_{g \in G} d_E(x_i, g \circ x_j). \quad (1.9)$$

VDM corresponds to diffusion over the vector bundle of the orbit space \mathcal{X}/G associated with the group action. The following existing examples demonstrate the usefulness of such a diffusion process in data analysis (see [12,23,25] for more applications):

- *Manifold learning:* Suppose we are given a point cloud randomly sampled from a d -dimensional/dimensional smooth manifold \mathbf{M} embedded in \mathbb{R}^p . Due to the smoothness of \mathbf{M} , the embedded tangent bundle of \mathbf{M} can be estimated by local principal component analysis (PCA) [33]. All bases of an embedded tangent plane at x form a group isomorphic to $O(d)$. Since the bases of the embedded tangent planes form the frame bundle $O(\mathbf{M})$, from this point cloud we obtain a set of samples from the frame bundle which form the total space $\mathcal{X} = O(\mathbf{M})$. Since the set of all the bases of an embedded tangent plane is invariant under the action of $O(d)$, for the purpose of learning the manifold \mathbf{M} , we take $O(d)$ as the nuisance group, and hence the orbit space is $\mathbf{M} = O(\mathbf{M})/O(d)$. As shown in [33], the generator of the diffusion process corresponding to VDM is the connection Laplacian associated with the tangent bundle. With the eigenvalues and eigenvectors of the connection Laplacian, the point cloud is embedded in an Euclidean space. We refer to the Euclidean distance in the embedded space as the *vector diffusion distance (VDD)*, which provides a metric for the point cloud. It is shown in [33] that VDD approximates the geodesic distance between nearby points on the manifold. Furthermore, by VDM, we extend the earlier spectral embedding theorem [6] by constructing a distance in a class of closed Riemannian manifolds with prescribed geometric conditions, which leads to a pre-compactness theorem on the class under consideration [40].
- *Orientability:* Suppose we are given a point cloud randomly sampled from a d -dimensional/dimensional smooth manifold \mathbf{M} and we want to learn its orientability. Since the frame bundle encodes whether or not the manifold is orientable, we take the nuisance group as \mathbb{Z}_2 defined as the determinant of the action $O(d)$ from the previous example. In other words, the orbit of each point on the manifold is \mathbb{Z}_2 , the total space \mathcal{X} is the \mathbb{Z}_2 bundle on \mathbf{M} following the orientation, and the orbit space is \mathbf{M} . With the nuisance group \mathbb{Z}_2 , *Orientable Diffusion Maps (ODM)* proposed in [32] can be considered as a variation of VDM in order to estimate the orientability of \mathbf{M} from a finite collection of random samples.

- *Cryo-EM*: The X-ray transform often serves as a mathematical model to many medical and biological imaging modalities, for example, in cryo-electron microscopy [15]. In cryo-electron microscopy, the 2-dimension/dimensional projection images of the 3-dimension/dimensional object are noisy and their projection directions are unknown. For the purpose of denoising, it is required to classify the images and average images with similar projection directions, a procedure known as class averaging. When the object of interest has no symmetry, the projection images have a one-to-one correspondence with a manifold diffeomorphic to $SO(3)$. Notice that $SO(3)$ can be viewed as the set of all right-handed bases of all tangent planes to S^2 , and the set of all right-handed bases of a tangent plane is isomorphic to $SO(2)$. Since the projection directions are parameterized by S^2 and the set of images with the same projection direction is invariant under the $SO(2)$ action, we learn the projection direction by taking $SO(2)$ as the nuisance group and S^2 as the orbit space. The VDD provides a metric for classification of the projection directions in S^2 , and this metric has been shown to outperform other classification methods [19,34,41].

The main contribution of this article is twofold. First, we use the mathematical framework of the *principal bundle* [8] in order to analyze the relationship between the nuisance group and the orbit space, and how their combination can be used to learn the dataset. In this setup, the total space is the principal bundle, the orbit space is the base manifold, and the orbit is the fiber. This principal bundle framework unifies LE, DM, ODM and VDM by providing a common mathematical language to all of them. Secondly, for data points that are independently sampled from the uniform distribution over a manifold, in addition to showing pointwise convergence of VDM in the general principal bundle setup, in Theorem 5.4 we prove that the algorithm converges in the spectral sense, that is, the eigenvalues and the eigenvectors computed by the algorithm converge to the eigenvalues and the eigen-vector-fields of the connection Laplacian of the associated vector bundle. Our pointwise and spectral convergence results also hold for manifolds with boundary, and in the case where data points are sampled independently from non-uniform distributions (that satisfy mild technical conditions). We also show spectral convergence of the GCL to the connection Laplacian of the associated tangent bundle in Theorem 6.2 when the tangent bundle is estimated from the point cloud. The importance of these spectral convergence results stem from the fact that they provide a theoretical guarantee in the limit of infinite number of data samples for the above listed problems, namely, estimating VDDs, determining the orientability of a manifold from a point cloud, and classifying the projection directions of cryo-EM images. In addition, we show that ODM can help reconstruct the orientable double covering of non-orientable manifolds by proving a symmetric version of Nash’s isometric embedding theorem [26,27].

The rest of the article is organized as follows. In Section 2, we review VDM and clarify the relationship between the point cloud sampled from the manifold and the bundle structure of the manifold. In Section 3, we introduce background material and set up the notations. In Section 4, we unify LE, DM, VDM and ODM by taking the principal bundle structure of the manifold into account. In Section 5, we prove the first spectral convergence result that assumes knowledge of the bundle structure. The non-empty boundary and non-uniform sampling effects are simultaneously handled. In Section 6, we prove the second spectral convergence result when the bundle information is missing and needs to be estimated directly from a finite random point cloud.

2 The graph connection Laplacian and vector diffusion maps

Consider an undirected affinity graph $\mathbb{G} = (\mathbb{V}, \mathbb{E})$, where $\mathbb{V} = \{x_i\}_{i=1}^n$ and fix a $q \in \mathbb{N}$. Suppose each edge $(i, j) \in \mathbb{E}$ is assigned a scalar value $w_{ij} > 0$ and a group element $g_{ij} \in O(q)$. We call w_{ij} the *affinity*

between x_i and x_j and g_{ij} the *connection group* between the *vector status* of x_i and x_j . We assume that $w_{ij} = w_{ji}$ and $g_{ij}^T = g_{ji}$. Construct the following $n \times n$ block matrix \mathbf{S}_n with $q \times q$ entries:

$$\mathbf{S}_n(i, j) = \begin{cases} w_{ij}g_{ij} & (i, j) \in \mathbb{E}, \\ 0_q & (i, j) \notin \mathbb{E}, \end{cases} \quad (2.1)$$

where 0_q is the $q \times q$ zero matrix. Notice that the square matrix \mathbf{S}_n is symmetric due to the assumption of w_{ij} and g_{ij} . Define

$$d_i = \sum_{(i, j) \in \mathbb{E}} w_{ij} \quad (2.2)$$

as the weighted degree of node i . Then define an $n \times n$ diagonal block matrix \mathbf{D}_n with $q \times q$ entries, where the diagonal blocks are scalar multiples of the identity given by

$$\mathbf{D}_n(i, i) = d_i \mathbf{l}_q, \quad (2.3)$$

where \mathbf{l}_q is the $q \times q$ identity matrix. The *un-normalized GCL* and the *normalized GCL* are defined in [2,33]

$$\mathbf{L}_n := \mathbf{D}_n - \mathbf{S}_n, \quad \mathcal{L}_n := \mathbf{l}_{qn} - \mathbf{D}_n^{-1} \mathbf{S}_n, \quad (2.4)$$

respectively. Given a $\mathbf{v} \in \mathbb{R}^{qn}$, we denote $\mathbf{v}[l] \in \mathbb{R}^q$ to be the l th component in the vector by saying that $\mathbf{v}[l] := [\mathbf{v}((l-1)q+1), \dots, \mathbf{v}(lq)]^T \in \mathbb{R}^q$ for all $l = 1, \dots, n$. The matrix $\mathbf{D}_n^{-1} \mathbf{S}_n$ is thus an operator acting on $\mathbf{v} \in \mathbb{R}^{qn}$ by

$$(\mathbf{D}_n^{-1} \mathbf{S}_n \mathbf{v})[i] = \frac{\sum_{j: (i, j) \in \mathbb{E}} w_{ij} g_{ij} \mathbf{v}[j]}{d_i}, \quad (2.5)$$

which suggests the interpretation of $\mathbf{D}_n^{-1} \mathbf{S}_n$ as a *generalized Markov chain* in the following sense, so that the random walker (e.g. diffusive particle) is characterized by a generalized status vector. Indeed, a particle at i is endowed with a q -dimension/dimensional vector status, and at each time step it hops from i to j with probability w_{ij}/d_i . In the absence of the group, these statuses are separately viewed as q functions defined on \mathbb{G} . Notice that the graph Laplacian arises as a special case for $q = 1$ and $g_{ij} = 1$. However, when $q > 1$ and g_{ij} are not identity matrices, in general the coordinates of the status vectors do not decouple into q independent processes due to the non-trivial effect of the group elements g_{ij} . Thus, if a particle with status $\mathbf{v}[i] \in \mathbb{R}^q$ moves along a path of length t from j_0 to j_t containing vertices $j_0, j_1, \dots, j_{t-1}, j_t$ so that $(j_l, j_{l+1}) \in \mathbb{E}$ for $0 = 1, \dots, t-1$, in the end it becomes

$$g_{j_{t-1}} \cdots g_{j_2 j_1} g_{j_1 i} \mathbf{v}[i]. \quad (2.6)$$

That is, when the particle arrives j , its vector status is influenced by a series of rotations along the path from i to j . In case there are more than two paths from i to j and the rotational groups on paths vary dramatically, we may get cancelation while adding transformations of different paths. Intuitively, ‘the closer two points are’ or ‘the less variance of the translational group on the paths is’, the more consistent the vector statuses are between i and j . We can thus define a new affinity between i and

j by the consistency between the vector statuses. Notice that the matrix $(\mathbf{D}_n^{-1}\mathbf{S}_n)^{2t}(i,j)$, where $t > 0$, contains the average of the rotational information over all paths of length $2t$ from i to j . Thus, the squared Hilbert–Schmidt norm, $\|(\mathbf{D}_n^{-1}\mathbf{S}_n)^{2t}(i,j)\|_{HS}^2$, can be viewed as a measure of not only the number of paths of length $2t$ from i to j , but also the amount of consistency of the vector statuses that propagated along different paths connecting i and j . This motivates to consider the notion of affinity between i and j as $\|(\mathbf{D}_n^{-1}\mathbf{S}_n)^{2t}(i,j)\|_{HS}^2$.

To understand $\|(\mathbf{D}_n^{-1}\mathbf{S}_n)^{2t}(i,j)\|_{HS}^2$, we consider the symmetric matrix $\tilde{\mathbf{S}}_n = \mathbf{D}_n^{-1/2}\mathbf{S}_n\mathbf{D}_n^{-1/2}$, which is similar to $\mathbf{D}_n^{-1}\mathbf{S}_n$. Since $\tilde{\mathbf{S}}_n$ is symmetric, it has a complete set of eigenvectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{nq}$ and eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_{nq}$, where the eigenvalues are the same as those of $\mathbf{D}_n^{-1}\mathbf{S}_n$. Order the eigenvalues so that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{nq}$. A direct calculation of the HS norm of $\tilde{\mathbf{S}}_n^{2t}(i,j)$ leads to:

$$\|\tilde{\mathbf{S}}_n^{2t}(i,j)\|_{HS}^2 = \sum_{l,r=1}^{nq} (\lambda_l \lambda_r)^{2t} \langle \mathbf{v}_l[i], \mathbf{v}_r[i] \rangle \langle \mathbf{v}_l[j], \mathbf{v}_r[j] \rangle. \quad (2.7)$$

The VDM V_t is defined as the following map from \mathbb{G} to $\mathbb{R}^{(nq)^2}$:

$$V_t : i \mapsto \left((\lambda_l \lambda_r)^t \langle \mathbf{v}_l[i], \mathbf{v}_r[i] \rangle \right)_{l,r=1}^{nq}. \quad (2.8)$$

We mention that when $q = 1$ and $g_{ij} \in SO(1)$ for all i, j , V_t is still different from the well-known DM [11], since DM is defined from \mathbb{G} to \mathbb{R}^n by

$$\Phi_t : i \mapsto (\lambda_l^t \mathbf{v}_l(i))_{l=1}^n. \quad (2.9)$$

This, we could view Φ_t as a restricted VDM. In general, there is no simple relationship between DM and VDM. With this map, $\|\tilde{\mathbf{S}}_n^{2t}(i,j)\|_{HS}^2$ becomes an inner product for a finite dimensional Hilbert space, that is,

$$\|\tilde{\mathbf{S}}_n^{2t}(i,j)\|_{HS}^2 = \langle V_t(i), V_t(j) \rangle, \quad (2.10)$$

which in practice is common considered as an affinity between i and j . The VDD between nodes i and j is defined as

$$d_i^{(VDD)}(i,j) := \|V_t(i) - V_t(j)\|^2. \quad (2.11)$$

Furthermore, $|\lambda_l| \leq 1$ due to the following identity:

$$\mathbf{v}^T (\mathbf{I}_n \pm \tilde{\mathbf{S}}_n) \mathbf{v} = \sum_{(i,j) \in \mathbb{E}} \left\| \frac{\mathbf{v}[i]}{\sqrt{d_i}} \pm \frac{w_{ij} g_{ij} \mathbf{v}[j]}{\sqrt{d_j}} \right\|^2 \geq 0, \quad (2.12)$$

for any $\mathbf{v} \in \mathbb{R}^{nq}$. By the above we cannot guarantee that the eigenvalues of $\tilde{\mathbf{S}}_n$ are non-negative, and that is the main reason we define V_t through $\|\tilde{\mathbf{S}}_n^{2t}(i,j)\|_{HS}^2$ rather than $\|\tilde{\mathbf{S}}_n^t(i,j)\|_{HS}^2$. On the other hand, we know that the unnormalized GCL is positive semi-definite because

$$\mathbf{v}^T (\mathbf{D}_n - \mathbf{S}_n) \mathbf{v} = \sum_{(i,j) \in \mathbb{E}} w_{ij} \|g_{ij} \mathbf{v}[j] - \mathbf{v}[i]\|^2 \geq 0. \quad (2.13)$$

We now come back to $D_n^{-1}\mathbf{S}_n$. The eigenvector of $D_n^{-1}\mathbf{S}_n$ associated with eigenvalue λ_i is $\mathbf{w}_i = D_n^{-1/2}\mathbf{v}_i$. This motivates the definition of another VDM from \mathbb{G} to $\mathbb{R}^{(nq)^2}$ as

$$V'_i : i \mapsto \left((\lambda_i \lambda_r)^t \langle \mathbf{w}_i[i], \mathbf{w}_r[i] \rangle \right)_{i,r=1}^{nq}, \quad (2.14)$$

so that $V'_i(i) = \frac{V_i(i)}{d_i}$. In other words, V'_i maps the data set in a Hilbert space upon proper normalization by the vertex degrees. The associated VDD is thus defined as $\|V'_i(i) - V'_i(j)\|^2$.

We mention that when $q = 1$ and $g_{ij} \in SO(1)$, that is, $g_{ij} = 1$ for all i, j , then the GCL is reduced to the well-known graph Laplacian. The introduction of the connection group leads to a fundamentally different meaning of the algorithm. For example, if $g_{ij} = O(1)$, that is, g_{ij} could be 1 or -1 , then the algorithm could reflect different topological structure of the underlying space, like the orientability if \mathbb{G} is constructed from a manifold. Another illustrative example to show how the connection group is fundamentally needed is the 2-dimension/dimensional sphere. Suppose \mathbb{G} is constructed from a 2-dimension/dimensional sphere and the connection group follows the connection structure of its frame bundle. Then the well-known ‘hairy ball theory’ is inevitable; that is, the smallest eigenvalue of \mathcal{L}_n is greater than 0 and the associated eigenvector is not constant on \mathbb{G} . However, if we ignore the connection structure of its frame bundle, and simply set $g_{ij} = \mathbf{I}_2$, then the smallest eigenvalue of the GCL is 0 and the associated eigenvector is constant on \mathbb{G} . This difference plays an essential role in all the applications. For further discussion of the motivation about VDM, VDD, other normalizations and its statistical properties, please see [14,33].

3 Notations, background and assumptions

In this section, we collect all notations and background facts about differential geometry needed throughout the article.

3.1 Notations and background of differential geometry

We refer the readers who are not familiar with the principal bundle structure to Appendix A for a quick introduction and [7,8] for a general treatment.

Denote \mathbf{M} to be a d -dimension/dimensional compact smooth manifold. If the boundary $\partial\mathbf{M}$ is non-empty, it is smooth. Denote $\iota : \mathbf{M} \hookrightarrow \mathbb{R}^p$ to be a smooth embedding of \mathbf{M} into \mathbb{R}^p and equip \mathbf{M} with the metric g induced from the canonical metric on \mathbb{R}^p via ι . With the metric g we have an induced measure, denoted as dV , on \mathbf{M} . Denote

$$\mathbf{M}_t := \left\{ x \in \mathbf{M} : \min_{y \in \partial\mathbf{M}} d(x, y) \leq t \right\}, \quad (3.1)$$

where $t \geq 0$ and $d(x, y)$ is the geodesic distance between x and y .

Denote $P(\mathbf{M}, G)$ to be the principal bundle with a connection 1-form ω , where G is a Lie group right acting on $P(\mathbf{M}, G)$ by \circ . Denote $\pi : P(\mathbf{M}, G) \rightarrow \mathbf{M}$ to be the canonical projection. We call \mathbf{M} the base space of the principal G bundle and G the structure group or the fiber of the principal bundle. From the view point of orbit space, $P(\mathbf{M}, G)$ is the total space, G is the group acting on $P(\mathbf{M}, G)$, and \mathbf{M} is the orbit space of $P(\mathbf{M}, G)$ under the action of G . In other words, when our interest is the parametrization of the orbit space, G becomes the nuisance group.

Denote ρ to be a representation of G into $O(q)$, where $q > 0$.¹ When there is no danger of confusion, we use the same symbol g to denote the Riemannian metric on \mathbf{M} and an element of G . Denote $\mathcal{E}(P(\mathbf{M}, G), \rho, \mathbb{R}^q)$, $q \geq 1$, to be the associated vector bundle with the fiber diffeomorphic to \mathbb{R}^q . By definition, $\mathcal{E}(P(\mathbf{M}, G), \rho, \mathbb{R}^q)$ is the quotient space $P(\mathbf{M}, G) \times \mathbb{R}^q / \sim$, where the equivalence relationship \sim is defined by the group action on $P(\mathbf{M}, G) \times \mathbb{R}^q$ by $g : (u, v) \rightarrow (g \circ u, \rho(g)^{-1}v)$, where $g \in G$, $u \in P(\mathbf{M}, G)$ and $v \in \mathbb{R}^q$. When there is no danger of confusion, we use \mathcal{E} to simplify the notation. Denote $\pi_{\mathcal{E}}$ to be the associated canonical projection and E_x to be the fiber of \mathcal{E} on $x \in \mathbf{M}$; that is, $E_x := \pi_{\mathcal{E}}^{-1}(x)$. Given a fiber metric $g^{\mathcal{E}}$ in \mathcal{E} , which always exists since \mathbf{M} is compact, we consider the metric connection under which the parallel displacement of fiber of \mathcal{E} is isometric related to $g^{\mathcal{E}}$. The metric connection on \mathcal{E} determined from ω is denoted as $\nabla^{\mathcal{E}}$. Note that by definition, each $u \in P(\mathbf{M}, G)$ turns out to be a linear mapping from \mathbb{R}^q to E_x preserving the inner product structure, where $x = \pi(u)$, and satisfies

$$(g \circ u)v = u(\rho(g)v) \in E_x, \quad (3.2)$$

where $u \in P(\mathbf{M}, G)$, $g \in G$ and $v \in \mathbb{R}^q$. We interpret the linear mapping u as finding the point $u(v) \in E_x$ possessing the coordinate $v \in \mathbb{R}^q$.

EXAMPLE 3.1 An important example is the frame bundle of the Riemannian manifold (\mathbf{M}, g) , denoted as $O(\mathbf{M}) = P(\mathbf{M}, O(d))$, and the tangent bundle $T\mathbf{M}$, which is the associated vector bundle of the frame bundle $O(\mathbf{M})$ if we take $\rho = id$ and $q = d$. The relationship among the principal bundle and its associated vector bundle can be better understood by considering the practical meaning of the relationship between the frame bundle and its associated tangent bundle. It is actually the change of coordinate (or change of variable linearly). In fact, if we view a point $u \in O(\mathbf{M})$ as the basis of the fiber $T_x\mathbf{M}$, where $x = \pi(u)$, then the coordinate of a point on the tangent plane $T_x\mathbf{M}$ changes, that is, $v \rightarrow g^{-1}v$, according to the changes of the basis, that is, $u \rightarrow g \circ u$, where $g \in O(d)$.

Denote $\Gamma(\mathcal{E})$ to be the set of sections, $C^k(\mathcal{E})$ to be the set of k th differentiable sections, where $k \geq 0$. Also denote $C(\mathcal{E}) := C^0(\mathcal{E})$ to be the set of continuous sections. Denote $L^p(\mathcal{E})$, $1 \leq p < \infty$ to be the set of L^p integrable sections, that is, $X \in L^p(\mathcal{E})$ iff $\int |g^{\mathcal{E}}(X, X)|^{p/2} dV < \infty$. Denote $\|X\|_{L^\infty}$ to be the L^∞ norm of X .

The covariant derivative $\nabla^{\mathcal{E}}$ of $X \in C^1(\mathcal{E})$ in the direction v at x is defined as

$$\nabla_{\dot{c}(0)}^{\mathcal{E}} X(x) = \lim_{h \rightarrow 0} \frac{1}{h} [u(0)u(h)^{-1}(X(c(h))) - X(c(0))], \quad (3.3)$$

where $c : [0, 1] \rightarrow \mathbf{M}$ is the curve on \mathbf{M} so that $c(0) = x$, $\dot{c}(0) = v$ and $u(h)$ is the horizontal lift of $c(h)$ to $P(\mathbf{M}, G)$ so that $\pi(u(0)) = x$. Let \parallel_y^x denote the parallel displacement from y to x . When y is in the cut locus of x , we set $\parallel_y^x X(y) = 0$; when h is small enough, $\parallel_{c(h)}^{c(0)} = u(0)u(h)^{-1}$ by definition. For a smooth section X , denote $X^{(l)}$, $l \in \mathbb{N}$, to be the l th order covariant derivatives of X .

EXAMPLE 3.2 We can better understand this definition in the frame bundle $O(\mathbf{M})$ and its associated tangent bundle. Take $X \in C^1(TM)$. The practical meaning of (3.3) is the following: find the coordinate

¹ We may also consider representing G into $U(q)$ if we take the fiber to be \mathbb{C}^q . However, to simplify the discussion, we focus ourselves on $O(q)$ and the real vector space.

of $X(c(h))$ by $u(h)^{-1}(X(c(h)))$, then view this coordinate to be associated with $T_x\mathbf{M}$, and map it back to the fiber $T_x\mathbf{M}$ by the basis $u(0)$. In this way we can compare two different ‘abstract fibers’ by comparing their coordinates.

Denote ∇^2 the connection Laplacian over \mathbf{M} with respect to \mathcal{E} . Denote by \mathcal{R} , Ric , and s the Riemannian curvature tensor, the Ricci curvature and the scalar curvature of (\mathbf{M}, g) , respectively. The second fundamental form of the embedding ι is denoted by II . Denote τ to be the largest positive number having the property: the open normal bundle about \mathbf{M} of radius r is embedded in \mathbb{R}^p for every $r < \tau$ [28]. Note that $1/\tau$ can be interpreted as the condition number of the manifold. Since \mathbf{M} is compact, $\tau > 0$ holds automatically. Denote $\text{inj}(\mathbf{M})$ to be the injectivity radius of \mathbf{M} .

3.2 Notations and background of numerical finite samples

When the range of a random vector Y is supported on a d -dimension/dimensional manifold \mathbf{M} embedded in \mathbb{R}^p via ι , where $d < p$, the notion of probability density function (p.d.f.) may not be defined. It is possible to discuss more general setups, but we restrict ourselves here to the following definition for the sake of the asymptotic analysis [10]. Consider a probability space (Ω, \mathcal{F}, P) , where Ω is the sample space, \mathcal{F} is the sigma algebra on Ω and P is a probability measure defined on \mathcal{F} . Let the random vector $Y : (\Omega, \mathcal{F}, P) \rightarrow \mathbb{R}^p$ be a measurable function defined on (Ω, \mathcal{F}, P) . Let $\tilde{\mathcal{B}}$ be the Borel sigma algebra of $\iota(\mathbf{M})$. Denote by $d\tilde{P}_Y$ the probability measure of Y , defined on $\tilde{\mathcal{B}}$, induced from the probability measure P . Assume that $d\tilde{P}_Y$ is absolutely continuous with respect to the volume measure on $\iota(\mathbf{M})$, that is, $d\tilde{P}_Y(x) = \mathbf{p}(\iota^{-1}(x))\iota_* dV(x)$.

DEFINITION 3.3 We call $\mathbf{p} : \mathbf{M} \rightarrow \mathbb{R}_+$ the p.d.f. of the p -dimension/dimensional random vector Y when its range is supported on a d -dimension/dimensional manifold $\iota(\mathbf{M})$, where $d < p$. When \mathbf{p} is constant, we say the sampling is *uniform*; otherwise *non-uniform*.

From now on we assume $\mathbf{p} \in C^4(\mathbf{M})$. With this definition, we can thus define the expectation and other moments. For example, if $f : \iota(\mathbf{M}) \rightarrow \mathbb{R}$ is an integrable function, we have

$$\begin{aligned} \mathbb{E}f(Y) &= \int_{\Omega} f(Y(\omega)) dP(\omega) = \int_{\iota(\mathbf{M})} f(x) d\tilde{P}_Y(x) \\ &= \int_{\iota(\mathbf{M})} f(x)\mathbf{p}(\iota^{-1}(x))\iota_* dV(x) = \int_{\mathbf{M}} f(\iota(x))\mathbf{p}(x) dV(\iota(x)), \end{aligned} \quad (3.4)$$

where the second equality follows from the fact that \tilde{P}_Y is the induced probability measure, and the last one comes from the change of variable. To simplify the notation, hereafter we will not distinguish between x and $\iota(x)$ and \mathbf{M} and $\iota(\mathbf{M})$, when there is no danger of ambiguity.

Suppose the data points $\mathcal{X} := \{x_1, x_2, \dots, x_n\} \subset \mathbb{R}^p$ are identically and independently (i.i.d.) sampled from Y . For each x_i we pick $u_i \in P(\mathbf{M}, G)$ so that $\pi(u_i) = x_i$. To simplify the notation, we denote $u_i := u_{x_i}$ when $x_i \in \mathcal{X}$ and $\|j^i := \|_{x_j}^{x_i}$ when $x_i, x_j \in \mathcal{X}$. Denote the nq -dimension/dimensional Euclidean vector spaces $V_{\mathcal{X}} := \bigoplus_{x_i \in \mathcal{X}} \mathbb{R}^q$ and $E_{\mathcal{X}} := \bigoplus_{x_i \in \mathcal{X}} E_{x_i}$, which represents the discretized vector bundle. Note that $V_{\mathcal{X}}$ is isomorphic to $E_{\mathcal{X}}$ since E_{x_i} is isomorphic to \mathbb{R}^q . Given a $\mathbf{w} \in E_{\mathcal{X}}$, we denote $\mathbf{w} = [\mathbf{w}[1], \dots, \mathbf{w}[n]]$ and $\mathbf{w}[l] \in E_{x_i}$ to be the l th component in the direct sum for all $l = 1, \dots, n$.

We need a map to realize the isomorphism between $V_{\mathcal{X}}$ and $E_{\mathcal{X}}$. Define operators $B_{\mathcal{X}} : V_{\mathcal{X}} \rightarrow E_{\mathcal{X}}$ and $B_{\mathcal{X}}^T : E_{\mathcal{X}} \rightarrow V_{\mathcal{X}}$ by

$$\begin{aligned} B_{\mathcal{X}}\mathbf{v} &:= [u_1\mathbf{v}[1], \dots, u_n\mathbf{v}[n]] \in E_{\mathcal{X}}, \\ B_{\mathcal{X}}^T\mathbf{w} &:= [u_1^{-1}\mathbf{w}[1], \dots, u_n^{-1}\mathbf{w}[n]] \in V_{\mathcal{X}}, \end{aligned} \quad (3.5)$$

where $\mathbf{w} \in E_{\mathcal{X}}$ and $\mathbf{v} \in V_{\mathcal{X}}$. Note that $B_{\mathcal{X}}^T B_{\mathcal{X}}\mathbf{v} = \mathbf{v}$ for all $\mathbf{v} \in V_{\mathcal{X}}$. We define $\delta_{\mathcal{X}} : X \in C(\mathcal{E}) \rightarrow E_{\mathcal{X}}$ by

$$\delta_{\mathcal{X}}X := [X(x_1), \dots, X(x_n)] \in E_{\mathcal{X}}. \quad (3.6)$$

Here $\delta_{\mathcal{X}}$ is interpreted as the operator finitely sampling the section X and $B_{\mathcal{X}}$ the discretization of the action of a section from $\mathbf{M} \rightarrow P(\mathbf{M}, G)$ on \mathbb{R}^q . Note that under the tangent bundle setup, the operator $B_{\mathcal{X}}^T$ can be understood as finding the coordinates of $\mathbf{w}[i]$ associated with u_i ; $B_{\mathcal{X}}$ can be understood as recovering the point on E_{x_i} from the coordinate $\mathbf{v}[i]$ associated with u_i . We can thus define

$$\mathbf{X} := B_{\mathcal{X}}^T \delta_{\mathcal{X}}X \in V_{\mathcal{X}}, \quad (3.7)$$

which is the coordinate of the discretized section X associated with the samples on the principal bundle if we are considering the tangent bundle setup.

Below, we follow the standard notation defined in [36] to discuss the Glivenko–Cantelli class.

DEFINITION 3.4 Take a probability space (Ω, \mathcal{F}, P) . For a pair of measurable functions $l : \Omega \rightarrow \mathbb{R}$ and $u : \Omega \rightarrow \mathbb{R}$, a bracket $[l, u]$ is the set of all measurable functions $f : \Omega \rightarrow \mathbb{R}$ with $l \leq f \leq u$. An ϵ -bracket in $L_1(P)$, where $\epsilon > 0$, is a bracket $[l, u]$ with $\int |u(y) - l(y)| dP(y) \leq \epsilon$. Given a class of measurable function \mathfrak{F} , the bracketing number $N_{[]}(\epsilon, \mathfrak{F}, L_1(P))$ is the minimum number of ϵ -brackets needed to cover \mathfrak{F} .

Define the empirical measure from the i.i.d. samples \mathcal{X} :

$$\mathbb{P}_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}. \quad (3.8)$$

For a given measurable vector-valued function $F : \mathbf{M} \rightarrow \mathbb{R}^m$ for $m \in \mathbb{N}$, define

$$\mathbb{P}_n F := \frac{1}{n} \sum_{i=1}^n F(x_i) \quad \text{and} \quad \mathbb{P} F := \int_{\mathbf{M}} F(x) \mathbf{p}(x) dV(x). \quad (3.9)$$

DEFINITION 3.5 Take a sequence of i.i.d. samples $\mathcal{X} := \{x_1, \dots, x_n\} \subset \mathbf{M}$ according to the p.d.f. \mathbf{p} . We call a class \mathfrak{F} of measurable functions a Glivenko–Cantelli class if

1. $\mathbb{P}f$ exists for all $f \in \mathfrak{F}$
2. $\sup_{f \in \mathfrak{F}} |\mathbb{P}_n f - \mathbb{P}f| \rightarrow 0$ almost surely when $n \rightarrow \infty$.

Next, we introduce the following notations regarding the kernel used throughout the article. Fix $h > 0$. Given a non-negative continuous kernel function $K : [0, \infty) \rightarrow \mathbb{R}_+$ decaying fast enough characterizing the affinity between two sampling points $x \in \mathbf{M}$ and $y \in \mathbf{M}$, we denote

$$K_h(x, y) := K\left(\frac{\|x - y\|_{\mathbb{R}^p}}{\sqrt{h}}\right) \in C(\mathbf{M} \times \mathbf{M}), \quad (3.10)$$

where $x, y \in \mathbf{M}$. For $0 \leq \alpha \leq 1$, we define the following functions

$$\begin{aligned} \mathbf{p}_h(x) &:= \int K_h(x, y) \mathbf{p}(y) dV(y) \in C(\mathbf{M}), & K_{h,\alpha}(x, y) &:= \frac{K_h(x, y)}{\mathbf{p}_h^\alpha(x) \mathbf{p}_h^\alpha(y)} \in C(\mathbf{M} \times \mathbf{M}), \\ d_{h,\alpha}(x) &:= \int K_{h,\alpha}(x, y) \mathbf{p}(y) dV(y) \in C(\mathbf{M}), & M_{h,\alpha}(x, y) &:= \frac{K_{h,\alpha}(x, y)}{d_{h,\alpha}(x)} \in C(\mathbf{M} \times \mathbf{M}), \end{aligned} \quad (3.11)$$

where $\mathbf{p}_h(x)$ is an estimation of the p.d.f. at x by the approximation of identify. Here, the practical meaning of $K_{h,\alpha}(x, y)$ is a new kernel function at (x, y) adjusted by the estimated p.d.f. at x and y ; that is, the kernel is normalized to reduce the influence of the non-uniform p.d.f. In practice, when we have only finite samples, we approximate the above terms by the following estimators:

$$\begin{aligned} \widehat{\mathbf{p}}_{h,n}(x) &:= \frac{1}{n} \sum_{k=1}^n K_h(x, x_k) \in C(\mathbf{M}), & \widehat{K}_{h,\alpha,n}(x, y) &:= \frac{K_h(x, y)}{\widehat{\mathbf{p}}_{h,n}^\alpha(x) \widehat{\mathbf{p}}_{h,n}^\alpha(y)} \in C(\mathbf{M} \times \mathbf{M}), \\ \widehat{d}_{h,\alpha,n}(x) &:= \frac{1}{n} \sum_{k=1}^n \widehat{K}_{h,\alpha,n}(x, x_k) \in C(\mathbf{M}), & \widehat{M}_{h,\alpha,n}(x, y) &:= \frac{\widehat{K}_{h,\alpha,n}(x, y)}{\widehat{d}_{h,\alpha,n}(x)} \in C(\mathbf{M} \times \mathbf{M}). \end{aligned} \quad (3.12)$$

Note that $\widehat{d}_{h,\alpha,n}$ is always positive if K is positive.

4 Unifying VDM, ODM, LE and DM from the principal bundle viewpoint

Before unifying these algorithms, we state some of the known results relevant to VDM, ODM, LE and DM. Most of the results that have been obtained are of two types: either they provide the topological information about the data which is global in nature, or they concern the geometric information which aims to recover the local information of the data. Fix the undirected affinity graph $\mathbb{G} = (\mathbb{V}, \mathbb{E})$. When it is built from a point cloud randomly sampled from a Riemannian manifold $\iota : \mathbf{M} \hookrightarrow \mathbb{R}^p$ with the induced metric g from the canonical metric of the ambient space, the main ingredient of LE and DM is the Laplace–Beltrami operator Δ_g of (\mathbf{M}, g) [11]. It is well known that the Laplace–Beltrami operator Δ_g provides some topology and geometry information about \mathbf{M} [16]. For example, the dimension of the null space of Δ_g is the number of connected components of \mathbf{M} ; the spectral embedding of \mathbf{M} into the Hilbert space [6] preserves the geometric information of \mathbf{M} . We can actually study LE and DM in the principal bundle framework. Indeed, Δ_g is associated with the trivial bundle $\mathcal{E}(P(\mathbf{M}, \{e\}), \rho, \mathbb{R})$, where ρ is the trivial representation of $\{e\}$ on \mathbb{R} . If we consider a non-trivial bundle, we obtain different Laplacian operators, which provide different geometric/topological information [16]. For example, the core of VDM in [33] is the connection Laplacian associated with the tangent bundle $T\mathbf{M}$, which provides not only the geodesic distance among nearby points (local information), but also the 1-Betti number

mixed with the Ricci curvature of the manifold. In addition, the notion of synchronization of vector fields on \mathbb{G} accompanied with translation group can be analyzed by the GCL [2].

4.1 Principal bundle setup

As the reader may have noticed, the appearance of VDM is similar to that of LE, DM and ODM. This is not a coincidence if we take the notion of principal bundle and its connection into account. Based on this observation, we are able to unify VDM, ODM, LE and DM in this section.

We make the following assumptions about the manifold setup.

ASSUMPTION 4.1 (A1) The manifold \mathbf{M} is d -dimensional/dimensional, smooth and smoothly embedded in \mathbb{R}^p via ι with the metric g induced from the canonical metric of \mathbb{R}^p . If the manifold is not closed, we assume that the boundary is smooth.

(A2) Fix a principal bundle $P(\mathbf{M}, G)$ with a connection 1-form ω . Denote ρ to be the representation of G into $O(q)$, where $q > 0$ depending on the application.² Denote $\mathcal{E} := \mathcal{E}(P(\mathbf{M}, G), \rho, \mathbb{R}^q)$ to be the associated vector bundle with a fiber metric $g^\mathcal{E}$ and the metric connection $\nabla^\mathcal{E}$.³

The following two special principal bundles and their associated vector bundles are directly related to ODM, LE and DM. The principal bundle for ODM is the non-trivial orientation bundle associated with the tangent bundle of a manifold \mathbf{M} , denoted as $P(\mathbf{M}, \mathbb{Z}_2)$, where $\mathbb{Z}_2 = \{-1, 1\}$. The construction of $P(\mathbf{M}, \mathbb{Z}_2)$ is shown in Example A5. Since \mathbb{Z}_2 is a discrete group, we take the connection as an assignment of the horizontal subspace of $TP(\mathbf{M}, \mathbb{Z}_2)$ as the simply tangent space of $P(\mathbf{M}, \mathbb{Z}_2)$; that is, $TP(\mathbf{M}, \mathbb{Z}_2)$. Its associated vector bundle is $\mathcal{E}^{\text{ODM}} = \mathcal{E}(P(\mathbf{M}, \mathbb{Z}_2), \rho, \mathbb{R})$, where ρ is the representation of \mathbb{Z}_2 so that ρ satisfies $\rho(g)x = gx$ for all $g \in \mathbb{Z}_2$ and $x \in \mathbb{R}$. Note that $\mathbb{Z}_2 \cong O(1)$. The principal bundle for LE and DM is $P(\mathbf{M}, \{e\})$, where $\{e\}$ is the identify group. Its construction can be found in Example A3 and we focus on the trivial connection. Its associated vector bundle is $\mathcal{E}^{\text{DM}} = \mathcal{E}(P(\mathbf{M}, \{e\}), \rho, \mathbb{R})$, where the representation ρ satisfies $\rho(e)x = x$ and $x \in \mathbb{R}$. In other words, \mathcal{E}^{DM} is the trivial line bundle on \mathbf{M} . Note that $\{e\} \cong SO(1)$.

Under the manifold setup assumption, we sample data from a random vector Y satisfying:

ASSUMPTION 4.2 (B1) The random vector Y has the range $\iota(\mathbf{M})$ satisfying Assumption 4.1. The p.d.f. $\mathfrak{p} \in C^4(\mathbf{M})$ of Y is uniformly bounded from below and above; that is, $0 < p_m \leq \mathfrak{p}(x) \leq p_M < \infty$ for all $x \in \mathbf{M}$.

(B2) The sample points $\mathcal{X} = \{x_i\}_{i=1}^n \subset M$ are sampled independently from Y .

(B3) For each $x_i \in \mathcal{X}$, pick $u_i \in P(\mathbf{M}, G)$ such that $\pi(u_i) = x_i$. Denote $\mathcal{G} = \{u_i : \mathbb{R}^q \rightarrow E_{x_i}\}_{i=1}^n$.

² We restrict ourselves to the orthogonal representation in order to obtain a symmetric matrix in the VDM algorithm. Indeed, if the translation of the vector status from x_i to x_j satisfies $u_j^{-1}u_i$, where $u_i, u_j \in P(\mathbf{M}, G)$ and $\pi(u_i) = x_i$ and $\pi(u_j) = x_j$, the translation from x_j back to x_i should satisfy $u_i^{-1}u_j$, which is the inverse of $u_j^{-1}u_i$. To have a symmetric matrix in the end, we thus need $u_j^{-1}u_i = (u_i^{-1}u_j)^T$, which is satisfied only when G is represented into the orthogonal group. We refer the reader to Appendix A for further details based on the notion of connection.

³ In general, ρ can be the representation of G into $O(q)$, which acts on the tensor space $T_s^r(\mathbb{R}^q)$ of type (r, s) or others. But we consider $\mathbb{R}^q = T_0^1(\mathbb{R}^q)$ to simplify the discussion.

The kernel and bandwidth used in the following sections satisfy:

ASSUMPTION 4.3 (K1) The kernel function $K \in C^2(\mathbb{R}_+)$ is a positive function satisfying that K and K' decay exponentially fast. Denote $\mu_{r,l}^{(k)} := \int_{\mathbb{R}^d} \|x\|^l \partial^k (K^r)(\|x\|) dx < \infty$, where $k = 0, 1, 2$, $l = 0, 1, 2, 3$, $r = 1, 2$ and ∂^k denotes the k th order derivative. We assume $\mu_{1,0}^{(0)} = 1$.

(K2) The bandwidth of the kernel, h , satisfies $0 < \sqrt{h} < \min\{\tau, \text{inj}(\mathbf{M})\}$.

4.2 Unifying VDM, ODM, LE and DM under the manifold setup

Suppose Assumption 4.1 is satisfied, and we are given \mathcal{X} and \mathcal{G} satisfying Assumption 4.2. The affinity graph $\mathbb{G} = (\mathbb{V}, \mathbb{E})$ is constructed in the following way. Take $\mathbb{V} = \mathcal{X}$ and $\mathbb{E} = \{(x_i, x_j) \mid x_i, x_j \in \mathcal{X}\}$. Under this construction \mathbb{G} is undirected and complete. The affinity between x_i and x_j is defined by

$$w_{ij} := \widehat{K}_{h,\alpha,n}(x_i, x_j), \quad (4.1)$$

where $0 \leq \alpha \leq 1$, K is the kernel function satisfying Assumption 4.3 and $\widehat{K}_{h,\alpha,n}(x_i, x_j)$ is defined in (3.12); that is, we define an affinity function $w : \mathbb{E} \rightarrow \mathbb{R}_+$. The connection group g_{ij} between x_i and x_j is constructed from \mathcal{G} by

$$g_{ij} := u_i^{-1} //_{j}^i u_j, \quad (4.2)$$

which form a group-valued function $g : \mathbb{E} \rightarrow O(q)$. We call (\mathbb{G}, w, g) a *connection graph*. With the connection graph, the GCL can be implemented. Define the following $n \times n$ block matrix $\mathbf{S}_{h,\alpha,n}$ with $q \times q$ block entries:

$$\mathbf{S}_{h,\alpha,n}(i, j) = \begin{cases} w_{ij} g_{ij} & (i, j) \in E, \\ 0_{q \times q} & (i, j) \notin E. \end{cases} \quad (4.3)$$

Notice that the square matrix $\mathbf{S}_{h,\alpha,n}$ is symmetric since $w_{ij} = w_{ji}$ and $g_{ij} = g_{ji}^T$. Then define an $n \times n$ diagonal block matrix \mathbf{D}_n with $q \times q$ entries, where the diagonal blocks are scalar multiples of the identity matrices given by

$$\mathbf{D}_{h,\alpha,n}(i, i) = \sum_{j:(i,j) \in E} w_{ij} \mathbf{1}_q = \widehat{d}_{h,\alpha,n}(x) \mathbf{1}_q. \quad (4.4)$$

Take $\mathbf{v} \in \mathbb{R}^{nq}$. The matrix $\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}$ is thus an operator acting on \mathbf{v} by

$$(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{v})[i] = \frac{\sum_{j=1}^n \widehat{K}_{h,\alpha,n}(x_i, x_j) g_{ij} \mathbf{v}[j]}{\sum_{j=1}^n \widehat{K}_{h,\alpha,n}(x_i, x_j)} = \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) g_{ij} \mathbf{v}[j], \quad (4.5)$$

where $\widehat{M}_{h,\alpha,n}(x_i, x_j)$ is defined in (3.12).

Recall the notation $\mathbb{X} := B_{\mathcal{X}}^T \delta_{\mathcal{X}} X$ defined in (3.7). Then, consider the following quantity:

$$\begin{aligned} \left(\frac{D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} - I_n}{h} \mathbb{X} \right) [i] &= \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) \frac{1}{h} (g_{ij} X[j] - X[i]) \\ &= \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) \frac{1}{h} (u_i^{-1} \parallel_j^i X(x_j) - u_i^{-1} X(x_i)). \end{aligned} \quad (4.6)$$

Note that geometrically g_{ij} is closely related to the parallel transport (3.3) from x_j to x_i . Indeed, rewrite the definition of the covariant derivative in (3.3) by

$$\nabla_{\dot{c}(0)} X(x_i) = \lim_{h \rightarrow 0} \frac{1}{h} [u(0)u(h)^{-1} X(c(h)) - X(c(0))], \quad (4.7)$$

where $c : [0, 1] \rightarrow \mathbf{M}$ is the geodesic on \mathbf{M} so that $c(0) = x_i$ and $c(h) = x_j$, and $u(h)$ is the horizontal lift of c to $P(\mathbf{M}, G)$ so that $\pi(u(0)) = x_i$. Next rewrite

$$u(0)^{-1} \nabla_{\dot{c}(0)} X = \lim_{h \rightarrow 0} \frac{1}{h} \{ u(h)^{-1} X(c(h)) - u(0)^{-1} X(c(0)) \}, \quad (4.8)$$

where the right-hand side is exactly the term appearing in (4.6) by the definition of parallel transport since $u(h)^{-1} = u(0)^{-1} \parallel_{c(h)}^{c(0)}$. As will be shown explicitly in the next section, the GCL reveals the information about the manifold by accumulating the local information via taking the covariant derivative into account.

Now we unify ODM, LE and DM. For ODM, we consider the orientation principal bundle $P(\mathbf{M}, \mathbb{Z}_2)$ and its associated vector bundle \mathcal{E}^{ODM} . In this case, \mathcal{G} is $\{u_i^{\text{ODM}}\}_{i=1}^n, u_i^{\text{ODM}} \in P(\mathbf{M}, \mathbb{Z}_2)$ and $u_i^{\text{ODM}} : \mathbb{R} \rightarrow E_i$, where E_i is the fiber of \mathcal{E}^{ODM} at $x_i \in \mathbf{M}$. Note that the fiber of \mathcal{E}^{ODM} is isomorphic to \mathbb{R} . The connection group g_{ij}^{ODM} between x_i and x_j is constructed by

$$g_{ij}^{\text{ODM}} = u_i^{\text{ODM}-1} u_j^{\text{ODM}}. \quad (4.9)$$

In practice, u_j^{ODM} comes from the orientation of the sample from the frame bundle. Indeed, given x_i and $u_i \in O(\mathbf{M})$ so that $\pi(u_i) = x_i$, g_{ij}^{ODM} is defined to be the orientation of $u_i^{-1} \parallel_j^i u_j$; that is, the determinant of $u_i^{-1} \parallel_j^i u_j \in O(d)$. Define an $n \times n$ matrix with scalar entries $\mathbf{S}_{h,\alpha,n}^{\text{ODM}}$, where

$$\mathbf{S}_{h,\alpha,n}^{\text{ODM}}(i, j) = \begin{cases} w_{ij} g_{ij}^{\text{ODM}} & (i, j) \in \mathbb{E}, \\ 0 & (i, j) \notin \mathbb{E} \end{cases} \quad (4.10)$$

and an $n \times n$ diagonal matrix $\mathbf{D}_{h,\alpha,n}^{\text{ODM}}$, where

$$\mathbf{D}_{h,\alpha,n}^{\text{ODM}}(i, i) = d_i. \quad (4.11)$$

It has been shown in [32, Section 2.3] that the orientability information of \mathbf{M} can be obtained from analyzing $\mathbf{D}_{h,1,n}^{\text{ODM}-1} \mathbf{S}_{h,1,n}^{\text{ODM}}$. When the manifold is orientable, we get the ODM by taking the higher eigenvectors of $\mathbf{D}_{h,1,n}^{\text{ODM}-1} \mathbf{S}_{h,1,n}^{\text{ODM}}$ into account; when the manifold is non-orientable, we can recover the orientable double covering of the manifold by the *modified diffusion maps* [32, Section 3]. In [32, Section 3], it is

conjectured that any smooth, closed non-orientable manifold (M, g) has an orientable double covering embedded symmetrically inside \mathbb{R}^p for some $p \in \mathbb{N}$. To make the unification self-contained, we will show in Appendix D that this conjecture is true by modifying the proof of the Nash embedding theorem [26,27]. This fact provides us with a better visualization of reconstructing the orientable double covering by the modified diffusion maps.

For LE and DM, we consider the trivial principal bundle $P(M, \{e\})$ and its associated trivial line bundle \mathcal{E}^{DM} . In this case, $q = 1$. Define an $n \times n$ matrix with scalar entries $\mathbf{S}_{h,\alpha,n}^{\text{DM}}$:

$$\mathbf{S}_{h,\alpha,n}^{\text{DM}}(i,j) = \begin{cases} w_{ij} & (i,j) \in \mathbb{E}, \\ 0 & (i,j) \notin \mathbb{E} \end{cases} \quad (4.12)$$

and an $n \times n$ diagonal matrix $\mathbf{D}_{h,\alpha,n}^{\text{DM}}$:

$$\mathbf{D}_{h,\alpha,n}^{\text{DM}}(i,i) = d_i. \quad (4.13)$$

Note that this is equivalent to ignoring the connection group in each edge in GCL. Indeed, when we study DM, we do not need the notion of connection group. This actually comes from the fact that functions defined on the manifold are actually sections of the trivial line bundle of M —since the fiber \mathbb{R} and M are decoupled, we can directly take the algebraic relationship of \mathbb{R} into consideration, so that it is not necessary to mention the bundle structure. With the well-known normalized graph Laplacian, $\mathbf{I}_n - \mathbf{D}_{h,0,n}^{\text{DM}}{}^{-1} \mathbf{S}_{h,0,n}^{\text{DM}}$, we can apply DM or LE for dimension reduction, spectral clustering, reparametrization, etc.

To sum up, we are able to unify the VDM, ODM, LE and DM by considering the principal bundle structure. In the following sections, we focus on the pointwise and spectral convergence of the corresponding operators.

5 Pointwise and spectral convergence of GCL

With the above setup, we now do the asymptotic analysis under Assumptions 4.1–4.3. In the asymptotical analysis, we will apply the big O notation. We will spell out details when we need the small o notation to avoid confusion. Recall the definition of the big O notation. For two functions f and g defined on $\{h \in \mathbb{R}; h \geq 0\}$, $f(h) = O(g(h))$, as $h \rightarrow 0$ means that there exists a positive constant C and $h_0 > 0$ so that $|f(h)| \leq C|g(h)|$ for all $h < h_0$. Here we call C the implied constant in the big O notation. From time to time, when we say that a quantity $f(h)$ depending on h is of order h^s when $h \rightarrow 0$, where $s \geq 0$, it means that $f(h)/h^s$ converges to a positive constant when $h \rightarrow 0$.

Throughout the proof, since \mathbf{p} , M and ι are fixed, and $\mathbf{p} \in C^4$, M , ∂M and ι are smooth and M is compact, we know that $\|\mathbf{p}^{(l)}\|_{L^\infty}$, $l = 0, 1, 2, 3, 4$, the volume of ∂M , the curvature of M and ∂M and the second fundamental form of the embedding ι , as well as their first few covariant derivatives are bounded independent of h and n . Thus, they will exist in the implied constant in the big O term and we will not explicitly mention them. However, when the implied constant in the big O term depends on a given section (or function), it will be precisely stated.

The pointwise convergence of the normalized GL can be found in [4,11,17,20], and the spectral convergence of the normalized GL when the sampling is uniform and the boundary is empty can be found in [5]. Here we take care of simultaneously the boundary, the non-uniform sampling and the bundle structure. Note that the asymptotical analysis of the normalized GL is a special case of the analysis in this article, since it is unified to the current framework based on the trivial principal bundle $P(M, \{e\})$ and

its associated trivial line bundle \mathcal{E}^{DM} . From a high level, except taking the possibly non-trivial bundle structure into account, the analysis is standard.

5.1 Pointwise convergence

DEFINITION 5.1 Define operators $T_{h,\alpha} : C(\mathcal{E}) \rightarrow C(\mathcal{E})$ and $\widehat{T}_{h,\alpha,n} : C(\mathcal{E}) \rightarrow C(\mathcal{E})$ as

$$\begin{aligned} T_{h,\alpha}X(y) &:= \int_{\mathbf{M}} M_{h,\alpha}(y,x) //_{x'}^y X(x) \mathbf{p}(x) dV(x), \\ \widehat{T}_{h,\alpha,n}X(y) &:= \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(y,x_j) //_{x_j'}^y X(x_j), \end{aligned} \quad (5.1)$$

where $X \in C(\mathcal{E})$, $0 \leq \alpha \leq 1$ and $M_{h,\alpha}$ and $\widehat{M}_{h,\alpha,n}$ are defined in (3.11) and (3.12), respectively.

First, we have the following theorem stating that the integral operator $T_{h,\alpha}$ is an approximation of identity, which allows us to obtain the connection Laplacian:

THEOREM 5.2 Suppose Assumptions 4.1 and 4.3 hold. Take $0 < \gamma < 1/2$. When $0 \leq \alpha \leq 1$, for all $x \notin \mathbf{M}_{h^\gamma}$ and $X \in C^4(\mathcal{E})$, we have

$$(T_{h,\alpha}X - X)(x) = h \frac{\mu_{1,2}^{(0)}}{2d} \left(\nabla^2 X(x) + \frac{2\nabla X(x) \cdot \nabla(\mathbf{p}^{1-\alpha})(x)}{\mathbf{p}^{1-\alpha}(x)} \right) + O(h^2), \quad (5.2)$$

where the implied constant in $O(h^2)$ depends on $\|X^{(\ell)}\|_{L^\infty}$, where $\ell = 0, 1, \dots, 4$; when $x \in \mathbf{M}_{h^\gamma}$, we have

$$(T_{h,\alpha}X - X)(x) = \sqrt{h} \frac{m_{h,1}}{m_{h,0}} //_{x_0}^x \nabla_{\partial_d} X(x_0) + O(h^{2\gamma}), \quad (5.3)$$

where the implied constant in $O(h^{2\gamma})$ depends on $\|X^{(\ell)}\|_{L^\infty}$, where $\ell = 0, 1, 2$, $x_0 = \operatorname{argmin}_{y \in \partial \mathbf{M}} d(x, y)$, $m_{h,1}$ and $m_{h,0}$ are constants of order 1 defined in (B.12), and ∂_d is the outer normal direction to the boundary at x_0 .

Note that near the boundary, the constant $m_{h,1}/m_{h,0}$ is of order 1, so the first term $\sqrt{h} \frac{m_{h,1}}{m_{h,0}}$ is of order \sqrt{h} . When $\gamma > 1/4$, the first term will asymptotically dominate the second term $O(h^{2\gamma})$.

Secondly, we show that when $n \rightarrow \infty$, asymptotically the matrix $\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} - \mathbf{I}$ behaves like the integral operator $T_{h,\alpha} - \mathbf{I}$. The main component in this asymptotical analysis is the stochastic fluctuation analysis of the GCL. As is shown in Theorem 5.2, the term we have interest in is the connection Laplacian (or Laplace–Beltrami operator when we consider GL), which is of order h , while the extra irrelevant terms are of higher order. Therefore the stochastic fluctuation incurred by the finite sampling points should be controlled to be much smaller than the connection Laplacian; otherwise the stochastic fluctuation will distort the object of interest.

THEOREM 5.3 Suppose Assumptions 4.1–4.3 hold and $X \in C(\mathcal{E})$.

Take $0 < \alpha \leq 1$. Suppose $h = h(n)$ so that $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2+s}} \rightarrow 0$, where $s \geq 0$, and $h \rightarrow 0$ as $n \rightarrow \infty$. With probability higher than $1 - 1/n^2$, for all $i = 1, \dots, n$,

$$(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X} - \mathbf{X})[i] = u_i^{-1}(T_{h,\alpha} X - X)(x_i) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right), \quad (5.4)$$

where \mathbf{X} is defined in (3.7).

Take $\alpha = 0$ and $1/4 < \gamma < 1/2$. Suppose $h = h(n)$ so that $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2}} \rightarrow 0$ and $h \rightarrow 0$ as $n \rightarrow \infty$. Then with probability higher than $1 - 1/n^2$, for all $x_i \notin \mathbf{M}_{h^\gamma}$ we have

$$(\mathbf{D}_{h,0,n}^{-1} \mathbf{S}_{h,0,n} \mathbf{X} - \mathbf{X})[i] = u_i^{-1}(T_{h,0} X - X)(x_i) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/2}}\right). \quad (5.5)$$

Suppose $h = h(n)$ so that $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2}} \rightarrow 0$ and $h \rightarrow 0$ as $n \rightarrow \infty$, with probability higher than $1 - 1/n^2$, for all $x_i \in \mathbf{M}_{h^\gamma}$:

$$(\mathbf{D}_{h,0,n}^{-1} \mathbf{S}_{h,0,n} \mathbf{X} - \mathbf{X})[i] = u_i^{-1}(T_{h,0} X - X)(x_i) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/4}}\right). \quad (5.6)$$

The proofs of Theorems 5.2 and 5.3 are postponed to the Appendix. Here $\sqrt{\log(n)}$ in the error term shows up due to the probability bound we are seeking and the union bound for all $i = 1, \dots, n$. When $\alpha > 0$, we need to estimate the p.d.f. from finite sampling points. This p.d.f. estimation dominates and slows down the convergence rate. Indeed, $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}/h^{1/2+s} \rightarrow 0$ when $h \rightarrow 0$, which only implies that the stochastic fluctuation incurred from the finite sampling points goes to zero faster than $h^{1/2+s}$, which might not be enough for us to recover the connection Laplacian we have interest in if $s < 1/2$.

The above two Theorems lead to the following pointwise convergence of the GCL. Here, the error term consists of the stochastic fluctuation (variance) when the number of samples is finite, and the error term in Theorem 5.2 is the bias term introduced by the kernel approximation.

COROLLARY 5.1 Suppose Assumptions 4.1–4.3 hold. Take $0 < \gamma < 1/2$ and $X \in C^4(\mathcal{E})$. Take $0 < \alpha \leq 1$. Suppose $h = h(n)$ so that $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1}} \rightarrow 0$ and $h \rightarrow 0$ as $n \rightarrow \infty$. Then with probability higher than $1 - 1/n^2$, the following holds for all $x_i \notin \mathbf{M}_{h^\gamma}$:

$$h^{-1}(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X} - \mathbf{X})[i] = \frac{\mu_{1,2}^{(0)}}{2d} u_i^{-1} \left\{ \nabla^2 X(x_i) + \frac{2\nabla X(x_i) \cdot \nabla(\mathbf{p}^{1-\alpha})(x_i)}{\mathbf{p}^{1-\alpha}(x_i)} \right\} + O(h) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1}}\right),$$

where $\nabla X(x_i) \cdot \nabla(\mathbf{p}^{1-\alpha})(x_i) := \sum_{l=1}^d \nabla_{\partial_l} X \nabla_{\partial_l}(\mathbf{p}^{1-\alpha})$ and $\{\partial_l\}_{l=1}^d$ is a normal coordinate around x_i ; the following holds for all $x_i \in \mathbf{M}_{h^\gamma}$:

$$(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X} - \mathbf{X})[i] = \sqrt{h} \frac{m_{h,1}}{m_{h,0}} u_i^{-1} \nabla_{\partial_d} X(x_0) + O(h^{2\gamma}) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right), \quad (5.7)$$

where $x_0 = \operatorname{argmin}_{y \in \partial \mathbf{M}} d(x_i, y)$, $m_{h,1}$ and $m_{h,0}$ are constants defined in (B.12), and ∂_d is the normal direction to the boundary at x_0 .

Take $\alpha = 0$. If $h = h(n)$ so that $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2}} \rightarrow 0$ and $h \rightarrow 0$ as $n \rightarrow \infty$, then with probability higher than $1 - 1/n^2$, the following holds for all $x_i \notin \mathbf{M}_{h^\gamma}$:

$$h^{-1}(\mathbf{D}_{h,0,n}^{-1} \mathbf{S}_{h,0,n} \mathbf{X} - \mathbf{X})[i] = \frac{\mu_{1,2}^{(0)}}{2d} u_i^{-1} \left\{ \nabla^2 X(x_i) + \frac{2\nabla X(x_i) \cdot \nabla \mathbf{p}(x_i)}{\mathbf{p}(x_i)} \right\} + O(h) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2}}\right);$$

the following holds for all $x_i \in \mathbf{M}_{h^\gamma}$:

$$(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X})[i] = u_i^{-1} \left(X(x) + \sqrt{h} \frac{m_{h,1}}{m_{h,0}} \parallel_{x_0}^{x_i} \nabla_{\partial_d} X(x_0) \right) + O(h^{2\gamma}) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/4}}\right). \quad (5.8)$$

We have several remarks for the above theorems and corollary.

REMARK 5.1 Several existing results regarding normalized GL and the estimation of Laplace–Beltrami operator are unified in Theorems 5.2, 5.3 and Corollary 5.1. Indeed, when the principal bundle structure is trivial, the above results are reduced to the case of the normalized GL. In particular, when $\alpha = 0$, the p.d.f. is uniform and the boundary does not exist, the results in [4,17] are recovered; when $\alpha = 0$, the p.d.f. is non-uniform and the boundary is not empty, we recover results in [11,31]; when $\alpha \neq 0$ and the boundary is empty, we recover results in [20].

REMARK 5.2 We now discuss how GCL converges from the discrete setup to the continuous setup, and the how to choose the optimal bandwidth under the assumption that $\partial \mathbf{M} = \emptyset$. Similar arguments hold when $\partial \mathbf{M} \neq \emptyset$. Take $\alpha = 0$. Asymptotically $h^{-1}(\mathbf{D}_{h,0,n}^{-1} \mathbf{S}_{h,0,n} \mathbf{X} - \mathbf{X})[i]$ converges to $\frac{\mu_{1,2}^{(0)}}{2d} u_i^{-1} \left\{ \nabla^2 X(x_i) + \frac{2\nabla X(x_i) \cdot \nabla \mathbf{p}(x_i)}{\mathbf{p}(x_i)} \right\}$ a.s. by the Borel–Cantelli Lemma. Note that based on the assumption about the relationship between n and h , we have $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2}} \rightarrow 0$ and $h \rightarrow 0$ as $n \rightarrow \infty$, but the convergence rate of $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2}} \rightarrow 0$ might be slower than $h \rightarrow 0$. If we want to balance the variance and squared bias, that is, $\frac{\log(n)}{nh^{d/2+1}}$ is of the same order of h^2 , then the number of samples we need should satisfy that $\frac{n}{\log(n)}$ is of the same order of $\frac{1}{h^{d/2+3}}$.

Take $\alpha \neq 0$. Similarly, $h^{-1}(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X} - \mathbf{X})[i]$ converges to $\frac{\mu_{1,2}^{(0)}}{2d} u_i^{-1} \left\{ \nabla^2 X(x_i) + \frac{2\nabla X(x_i) \cdot \nabla (\mathbf{p}^{1-\alpha})(x_i)}{\mathbf{p}^{1-\alpha}(x_i)} \right\}$ a.s. In this case, if we want to balance the variance and squared bias, the number of samples we need should satisfy that $\frac{n}{\log(n)}$ is of the same order of $\frac{1}{h^{d/2+4}}$. In conclusion, if we want to guarantee that the order of the estimation accuracy of the connection Laplacian is h when the p.d.f. is non-uniform and $\alpha = 1$, we need more points than that when the p.d.f. is uniform and $\alpha = 0$.

REMARK 5.3 In Theorem 5.2 and Corollary 5.1, the regularity of X and the p.d.f. \mathbf{p} are assumed to be C^4 . These conditions can be relaxed to C^3 and the proof remains almost the same, except that the bias term in Corollary 5.1 becomes $h^{1/2}$.

REMARK 5.4 A consequence of Corollary 5.1 and the above discussion about the error terms is that the eigenvectors of $\mathbf{D}_{h,1,n}^{-1} \mathbf{S}_{h,1,n} - \mathbf{I}_n$ are discrete approximations of the eigen-vector-fields of the connection

Laplacian operator with homogeneous Neumann boundary condition that satisfy

$$\begin{cases} \nabla^2 X(x) = -\lambda X(x), & \text{for } x \in \mathbf{M}, \\ \nabla_{\partial_d} X(x) = 0, & \text{for } x \in \partial\mathbf{M}. \end{cases} \quad (5.9)$$

Also note that the above results are pointwise in nature. The spectral convergence will be discussed in the coming section.

5.2 Spectral convergence

As informative as the pointwise convergence results in Corollary 5.1 are, they are not strong enough to guarantee the spectral convergence of our numerical algorithm, in particular those depending on the spectral structure of the underlying manifold. In this section, we explore this problem and provide the spectral convergence theorem.

It is well known that the spectrum of ∇^2 is discrete inside $\{x \leq 0\}$, and the only possible accumulation point is $-\infty$. Note that in general 0 might not be an eigenvalue of the connection Laplacian ∇^2 . For example, when the manifold is S^2 , the smallest eigenvalue of the connection Laplacian associated with the tangent bundle is strictly negative due to the vanishing theorem [7, p. 126]. When 0 is an eigenvalue, we denote the spectrum of ∇^2 by $\{-\lambda_l\}_{l=0}^\infty$, where $0 = \lambda_0 < \lambda_1 \leq \dots$, and the corresponding eigenspaces are denoted by $E_l := \{X \in L^2(\mathcal{E}) : \nabla^2 X = -\lambda_l X\}$, $l = 0, 1, \dots$; otherwise we denote the spectrum by $\{-\lambda_l\}_{l=1}^\infty$, where $0 < \lambda_1 \leq \dots$, and the eigenspaces by E_l . When 0 is not an eigenvalue, $E_0 = \emptyset$. It is well known [16] that $\dim(E_l) < \infty$, the eigen-vector-fields are smooth and form a basis for $L^2(\mathcal{E})$, that is, $L^2(\mathcal{E}) = \overline{\bigoplus_{l \in \mathbb{N} \cup \{0\}} E_l}$, where the over line means completion according to the measure associated with g . To simplify the statement and proof of the spectral convergence, we assume that λ_l for each l are simple and X_l is the normalized basis of E_l .⁴

The first theorem states the spectral convergence of $(\mathbf{D}_{h,1,n}^{-1} \mathbf{S}_{h,1,n})^{t/h}$ to $e^{t\nabla^2}$. Note that in the statement of the theorem, we use $\widehat{T}_{h,1,n}$ instead of $\mathbf{D}_{h,1,n}^{-1} \mathbf{S}_{h,1,n}$. As we will see in the proof, they are actually equivalent under pre transformation.

THEOREM 5.4 Suppose Assumptions 4.1–4.3 hold, and $2/5 < \gamma < 1/2$. Fix $t > 0$. Denote $\mu_{t,i,h,n}$ to be the i th eigenvalue of $\widehat{T}_{h,1,n}^{t/h}$ with the associated eigenvector $X_{t,i,h,n}$. Also denote $\mu_{t,i} > 0$ to be the i th eigenvalue of the heat kernel of the connection Laplacian $e^{t\nabla^2}$ with the associated eigen-vector field $X_{t,i}$. We assume that $\mu_{t,i}$ are simple, and both $\mu_{t,i,h,n}$ and $\mu_{t,i}$ decrease as i increases, respecting the multiplicity. Fix $i \in \mathbb{N}$. Then there exists a sequence $h_n \rightarrow 0$ such that in probability

$$\lim_{n \rightarrow \infty} \mu_{t,i,h,n} = \mu_{t,i} \quad \text{and} \quad \lim_{n \rightarrow \infty} \|X_{t,i,h,n} - X_{t,i}\|_{L^2(\mathcal{E})} = 0. \quad (5.10)$$

REMARK 5.5 Recall that for a finite integer n , as is discussed in (2.12), $\mu_{t,i,h,n}$ may be negative while $\mu_{t,i}$ is always non-negative. We mention that the existence of γ is for the sake of dealing with the boundary, whose effect is shown in (5.3). When the boundary is empty, we can ignore the γ assumption.

⁴ When any of the eigenvalues is not simple, the statement and proof are complicated by the need to introduce the notion of eigen-projection [9], while the proof is almost the same.

The second theorem states the spectral convergence of $h^{-1}(\mathbf{D}_{h,1,n}^{-1} \mathbf{S}_{h,1,n} - \mathbf{I}_{qn})$ to ∇^2 .

THEOREM 5.5 Suppose Assumptions 4.1–4.3 hold, and $2/5 < \gamma < 1/2$. Denote $-\lambda_{i,h,n}$ to be the i th eigenvalue of $h^{-1}(\widehat{T}_{h,1,n} - 1)$ with the associated eigenvector $X_{i,h,n}$. Also denote $-\lambda_i$, where $\lambda_i > 0$, to be the i th eigenvalue of the connection Laplacian ∇^2 with the associated eigen-vector field X_i . Assume that λ_i are simple, and both $\lambda_{i,h,n}$ and λ_i increase as i increases, respecting the multiplicity. Fix $i \in \mathbb{N}$. Then there exists a sequence $h_n \rightarrow 0$ such that in probability

$$\lim_{n \rightarrow \infty} \lambda_{i,h_n,n} = \lambda_i \quad \text{and} \quad \lim_{n \rightarrow \infty} \|X_{i,h_n,n} - X_i\|_{L^2(\mathcal{E})} = 0. \quad (5.11)$$

Note that the statement and proof hold for the special cases associated with DM and ODM. We prepare some bounds for the proof.

LEMMA 5.1 Take $0 \leq \alpha \leq 1$ and $h > 0$. Assume Assumptions 4.1–4.3 hold. Then the following uniform bounds hold

$$\begin{aligned} \delta &\leq \mathfrak{p}_h(x) \leq \|K\|_{L^\infty}, \quad \delta \leq \widehat{\mathfrak{p}}_{h,n}(x) \leq \|K\|_{L^\infty} \\ \frac{\delta}{\|K\|_{L^\infty}^{2\alpha}} &\leq K_{h,\alpha}(x, y) \leq \frac{\|K\|_{L^\infty}}{\delta^{2\alpha}}, \quad \frac{\delta}{\|K\|_{L^\infty}^{2\alpha}} \leq \widehat{K}_{h,\alpha,n}(x, y) \leq \frac{\|K\|_{L^\infty}}{\delta^{2\alpha}} \\ \frac{\delta}{\|K\|_{L^\infty}^{2\alpha}} &\leq d_{h,\alpha}(x) \leq \frac{\|K\|_{L^\infty}}{\delta^{2\alpha}}, \quad \frac{\delta}{\|K\|_{L^\infty}^{2\alpha}} \leq \widehat{d}_{h,\alpha,n}(x) \leq \frac{\|K\|_{L^\infty}}{\delta^{2\alpha}} \\ \frac{\delta^{1+2\alpha}}{\|K\|_{L^\infty}^{1+2\alpha}} &\leq M_{h,\alpha}(x, y) \leq \frac{\|K\|_{L^\infty}^{1+2\alpha}}{\delta^{1+2\alpha}}, \quad \frac{\delta^{1+2\alpha}}{\|K\|_{L^\infty}^{1+2\alpha}} \leq \widehat{M}_{h,\alpha,n}(x, y) \leq \frac{\|K\|_{L^\infty}^{1+2\alpha}}{\delta^{1+2\alpha}}, \end{aligned} \quad (5.12)$$

where $\delta := \inf_{t \in (0, D/\sqrt{h})} K(t)$ and $D := \max_{x, y \in \mathbf{M}} \|x - y\|_{\mathbb{R}^p}$.

Proof. By the assumption that the manifold \mathbf{M} is compact, there exists $D > 0$ so that $\|x - y\|_{\mathbb{R}^p} \leq D$ for all $x, y \in \mathbf{M}$. Under the assumption that the kernel function K is positive in Assumption 4.3, for a fixed $h > 0$, for all $n \in \mathbb{N}$ and $x, y \in \mathbf{M}$, we have

$$K_h(x, y) \geq \delta := \inf_{t \in (0, D/\sqrt{h})} K(t). \quad (5.13)$$

Then, for all $x, y \in \mathbf{M}$, the bounds in (5.12) hold immediately. \square

To prove Theorems 5.4 and 5.5, we need the following Lemma to take care of the pointwise convergence of a series of vector fields in the uniform norm on \mathbf{M} with the help of the notion of Glivenko–Cantelli class:

LEMMA 5.2 Take $0 \leq \alpha \leq 1$ and fix $h > 0$. Suppose Assumptions 4.1–4.3 are satisfied. Denote two functional classes

$$\mathcal{K}_h := \{K_h(x, \cdot); x \in \mathbf{M}\}, \quad \mathcal{K}_{h,\alpha} := \{K_{h,\alpha}(x, \cdot); x \in \mathbf{M}\}. \quad (5.14)$$

Then the above classes are Glivenko–Cantelli classes. Take $X \in C(\mathcal{E})$ and a measurable section $q_0 : \mathbf{M} \rightarrow P(\mathbf{M}, G)$, and denote

$$X \circ \mathcal{M}_{h,\alpha} := \left\{ M_{h,\alpha}(x, \cdot) q_0(x)^T \int^x X(\cdot); x \in \mathbf{M} \right\}. \quad (5.15)$$

Then the above classes satisfy

$$\sup_{W \in X \circ \mathcal{M}_{h,\alpha}} \|\mathbb{P}_n W - \mathbb{P}W\|_{\mathbb{R}^q} \rightarrow 0 \quad (5.16)$$

a.s. when $n \rightarrow \infty$.

Note that $W_x \in X \circ \mathcal{M}_{h,\alpha}$ is an \mathbb{R}^q -valued function defined on \mathbf{M} . Also recall that when y is in the cut locus of x , we set $\int_y^x W_x(y) = 0$. The above notations are chosen to be compatible with the matrix notation used in the VDM algorithm.

Proof. We prove (5.16). The proof for \mathcal{K}_h and $\mathcal{K}_{h,\alpha}$ can be found in [37, Proposition 11]. Take $W_x \in X \circ \mathcal{M}_{h,\alpha}$. Since $X \in C(\mathcal{E})$, \mathbf{M} is compact, $\nabla^{\mathcal{E}}$ is metric and $q(x) : \mathbb{R}^q \rightarrow E_x$ preserving the inner product, we know

$$\|W_x\|_{L^\infty} \leq \frac{\|K\|_{L^\infty}^{1+2\alpha}}{\delta^{1+2\alpha}} \|q(x)^{-1} \int^x X(\cdot)\|_{L^\infty} = \frac{\|K\|_{L^\infty}^{1+2\alpha}}{\delta^{1+2\alpha}} \|X\|_{L^\infty}, \quad (5.17)$$

where the first inequality holds by the bound in Lemma 5.1. Under Assumption 4.1, g_x is isometric pointwisely, so $X \circ \mathcal{M}_{h,\alpha}$ is uniformly bounded.

We now tackle the vector-valued function W_x component by component. Rewrite a vector-valued function W_x as $W_x = (W_{x,1}, \dots, W_{x,q})$. Consider

$$\mathcal{M}_{h,\alpha}^{(j)} := \left\{ M_{h,\alpha}(x, \cdot) W_{x,j}(\cdot), x \in \mathbf{M} \right\}, \quad (5.18)$$

where $j = 1, \dots, q$. Fix $\epsilon > 0$. Since \mathbf{M} is compact and W_x is uniformly bounded over x , we can choose finite ϵ -brackets $[l_{j,i}, u_{j,i}]$, where $i = 1, \dots, N(j, \epsilon)$, so that its union contains $\mathcal{M}_{h,\alpha}^{(j)}$ and $\mathbb{P}|u_{j,i} - l_{j,i}| < \epsilon$ for all $i = 1, \dots, N(j, \epsilon)$. Then, for every $f \in \mathcal{M}_{h,\alpha}^{(j)}$, there is an ϵ -bracket $[l_{j,l}, u_{j,l}]$ in $L^1(P)$ such that $l_{j,l} \leq f \leq u_{j,l}$, and hence

$$\begin{aligned} |\mathbb{P}_n f - \mathbb{P}f| &\leq |\mathbb{P}_n f - \mathbb{P}u_{j,l}| + |\mathbb{P}u_{j,l}(y) - f(y)| \leq |\mathbb{P}_n u_{j,l} - \mathbb{P}u_{j,l}| + |\mathbb{P}u_{j,l} - f| \\ &\leq |\mathbb{P}_n u_{j,l} - \mathbb{P}u_{j,l}| + \mathbb{P}|u_{j,l} - l_{j,l}| \leq |\mathbb{P}_n u_{j,l} - \mathbb{P}u_{j,l}| + \epsilon. \end{aligned} \quad (5.19)$$

Hence we have

$$\sup_{f \in \mathcal{M}_{h,\alpha}^{(j)}} |\mathbb{P}_n f - \mathbb{P}f| \leq \max_{l=1, \dots, N(j, \epsilon)} |\mathbb{P}_n u_{j,l} - \mathbb{P}u_{j,l}| + \epsilon, \quad (5.20)$$

where the right-hand side converges a.s. to ϵ when $n \rightarrow \infty$ by the strong law of large numbers and the fact that $N(j, \epsilon)$ is finite. As a result, we have

$$|\mathbb{P}_n W_x - \mathbb{P} W_x| \leq \sum_{l=1}^q \sup_{f \in \mathcal{M}_{h,\alpha}^{(j)}} |\mathbb{P}_n f - \mathbb{P} f| \leq \sum_{j=1}^q \max_{l=1, \dots, N(j, \epsilon)} |\mathbb{P}_n u_{j,l} - \mathbb{P} u_{j,l}| + q\epsilon, \quad (5.21)$$

so that $\limsup_{W_x \in X_{\circ} \circ \mathcal{M}_{h,\alpha}} |\mathbb{P}_n W_x - \mathbb{P} W_x|$ is bounded by $q\epsilon$ a.s. as $n \rightarrow \infty$. Since q is fixed and ϵ is arbitrary, we conclude the proof. \square

With these Lemmas, we now prove Theorems 5.4 and 5.5. The proof is long and is divided into several steps. First, we study the relationship between the normalized GCL $D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}$ and an integral operator $\widehat{T}_{h,\alpha,n}$. Secondly, for a given fixed bandwidth $h > 0$, we show a.s. spectral convergence of $\widehat{T}_{h,\alpha,n}$ to $T_{h,\alpha}$ when $n \rightarrow \infty$, the spectral convergence of $T_{h,1}^{t/h}$ to $e^{t\nabla^2}$ and $h^{-1}(T_{h,1} - 1)$ to ∇^2 in $L^2(\mathcal{E})$ as $h \rightarrow 0$ is provided. Finally, we put all ingredients together and finish the proof. Essentially the proof follows [5,11,37], while we take care simultaneously the non-empty boundary, the non-uniform sampling and the non-trivial bundle structure. Note that when we work with the trivial principal bundle, that is, we work with the normalized GL, $\alpha = 0$, the p.d.f. is uniform and the boundary is empty, then we recover the result in [5].

Proof of Theorems 5.4 and 5.5. Step 1: Relationship between $D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}$ and $\widehat{T}_{h,\alpha,n}$.

We immediately have that

$$(B_{\mathcal{X}}^T \delta_{\mathcal{X}} \widehat{T}_{h,\alpha,n} X)[i] = \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) u_i^{-1} \llbracket_j^i X(x_j) = (D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} X)[i], \quad (5.22)$$

which leads to the relationship between the eigen-structure of $h^{-1}(\widehat{T}_{h,\alpha,n} - 1)$ and $h^{-1}(D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} - 1)$. Suppose X is an eigen-section of $h^{-1}(\widehat{T}_{h,\alpha,n} - 1)$ with eigenvalue λ . We claim that $X = B_{\mathcal{X}}^T \delta_{\mathcal{X}} X$ is an eigenvector of $D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}$ with eigenvalue λ . Indeed, for all $i = 1, \dots, n$,

$$\begin{aligned} h^{-1}[(D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} - 1)X][i] &= \frac{1}{hn} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) u_i^{-1} [\llbracket_j^i X(x_j) - X(x_i)] \\ &= u_i^{-1} \frac{1}{hn} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) [\llbracket_j^i X(x_j) - X(x_i)] = u_i^{-1} h^{-1}(\widehat{T}_{h,\alpha,n} - 1)X(x_i) = \lambda u_i^{-1} X(x_i) = \lambda X[i]. \end{aligned} \quad (5.23)$$

On the other hand, consider an eigenvector \mathbf{v} of $h^{-1}(D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} - 1_{nd})$ with eigenvalue λ , that is,

$$(D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{v})[i] = (1 + h\lambda)\mathbf{v}[i]. \quad (5.24)$$

When $0 \geq h\lambda > -1$, we show that there is an eigen-vector field of $h^{-1}(\widehat{T}_{h,\alpha,n} - 1)$ with eigenvalue λ . In order to show this fact, we note that if X is an eigen-vector field of $h^{-1}(\widehat{T}_{h,\alpha,n} - 1)$ with eigenvalue λ so

that $0 \geq h\lambda > -1$, it should satisfy

$$\begin{aligned} X(x_i) &= \frac{\widehat{T}_{h,\alpha,n} X(x_i)}{1+h\lambda} = \frac{\frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) \mathbb{I}_j^i X(x_j)}{1+h\lambda} \\ &= \frac{\frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) \mathbb{I}_j^i u_j^{-1} X(x_j)}{1+h\lambda} = \frac{\frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) \mathbb{I}_j^i u_j X[j]}{1+h\lambda}. \end{aligned} \quad (5.25)$$

The relationship in (5.25) leads us to consider the vector field

$$X_v(x) := \frac{\frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x, x_j) \mathbb{I}_{x_j}^x u_j v[j]}{1+h\lambda} \quad (5.26)$$

to be the related eigen-vector field of $h^{-1}(\widehat{T}_{h,\alpha,n} - 1)$ associated with v . To show this, we directly calculate:

$$\begin{aligned} \widehat{T}_{h,\alpha,n} X_v(y) &= \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(y, x_j) \mathbb{I}_{x_j}^y X_v(x_j) = \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(y, x_j) \mathbb{I}_{x_j}^y \left(\frac{\frac{1}{n} \sum_{k=1}^n \widehat{M}_{h,\alpha,n}(x_j, x_k) \mathbb{I}_{x_k}^{x_j} u_k v[k]}{1+h\lambda} \right) \\ &= \frac{1}{1+h\lambda} \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(y, x_j) \mathbb{I}_{x_j}^y (1+h\lambda) u_j v[j] = (1+h\lambda) X_v(y), \end{aligned} \quad (5.27)$$

where the third equality comes from the expansion (5.22) and the last equality comes from the definition of X_v . Thus we conclude that X_v is the eigen-vector field of $h^{-1}(\widehat{T}_{h,\alpha,n} - 1)$ with eigenvalue λ since $0 \geq h\lambda > -1$.

The above one to one relationship between eigenvalues and eigenfunctions of $h^{-1}(\widehat{T}_{h,\alpha,n} - 1)$ and $h^{-1}(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} - 1)$ when $0 \geq h\lambda > -1$ allows us to analyze the spectral convergence of $h^{-1}(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} - 1)$ by analyzing the spectral convergence of $h^{-1}(\widehat{T}_{h,\alpha,n} - 1)$ to $h^{-1}(T_{h,\alpha} - 1)$. A similar argument shows that when the eigenvalue of $\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}$ is between $(0, 1]$, the eigen-structures of $\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}$ and $\widehat{T}_{h,\alpha,n}$ are again related. Note that in general the eigenvalues of $\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}$ might be negative when n is finite, as is shown in (2.12).

Step 2: Compact convergence of $\widehat{T}_{h,\alpha,n}$ to $T_{h,\alpha}$ a.s. when $n \rightarrow \infty$ and h is fixed.

Recall the definition of compact convergence of a series of operators in the Banach space $C(\mathcal{E})$ with the L^∞ norm [9, p. 122]. We say that a sequence of operators $T_n : C(\mathcal{E}) \rightarrow C(\mathcal{E})$ compactly converges to $T : C(\mathcal{E}) \rightarrow C(\mathcal{E})$ if and only if

- (C1) T_n converges to T pointwisely, that is, for all $X \in C(\mathcal{E})$, we have $\|T_n X - T X\|_{L^\infty(\mathcal{E})} \rightarrow 0$;
- (C2) for any uniformly bounded sequence $\{X_l : \|X_l\|_{L^\infty} \leq 1\}_{l=1}^\infty \subset C(\mathcal{E})$, the sequence $\{(T_n - T)X_l\}_{l=1}^\infty$ is relatively compact.

Now we show (C1)—the pointwise convergence of $\widehat{T}_{h,\alpha,n}$ to $T_{h,\alpha}$ a.e. when h is fixed and $n \rightarrow \infty$. By a simple bound we have

$$\begin{aligned} \|\widehat{T}_{h,\alpha,n} X - T_{h,\alpha} X\|_{L^\infty(\mathcal{E})} &= \sup_{y \in \mathbf{M}} |\mathbb{P}_n \widehat{M}_{h,\alpha,n}(y, \cdot) \mathbb{I}^y X(\cdot) - \mathbb{P} M_{h,\alpha}(y, \cdot) \mathbb{I}^y X(\cdot)| \\ &\leq \sup_{y \in \mathbf{M}} |\mathbb{P}_n \widehat{M}_{h,\alpha,n}(y, \cdot) \mathbb{I}^y X(\cdot) - \mathbb{P}_n \widehat{M}_{h,\alpha,n}^{(d_{h,\alpha})}(y, \cdot) \mathbb{I}^y X(\cdot)| \end{aligned} \quad (5.28)$$

$$+ \sup_{y \in \mathbf{M}} |\mathbb{P}_n \widehat{\mathcal{M}}_{h,\alpha,n}^{(d_{h,\alpha})}(y, \cdot) //^y X(\cdot) - \mathbb{P}_n \mathcal{M}_{h,\alpha}(y, \cdot) //^y X(\cdot)| \quad (5.29)$$

$$+ \sup_{y \in \mathbf{M}} |\mathbb{P}_n \mathcal{M}_{h,\alpha}(y, \cdot) //^y X(\cdot) - \mathbb{P} \mathcal{M}_{h,\alpha}(y, \cdot) //^y X(\cdot)|, \quad (5.30)$$

where $\widehat{\mathcal{M}}_{h,\alpha,n}^{(d_{h,\alpha})}(x, y) := \frac{K_{h,\alpha}(x,y)}{d_{h,\alpha,n}(x)} \in C(\mathbf{M} \times \mathbf{M})$.

Rewrite (5.30) as $\sup_{W \in \mathcal{X} \circ \mathcal{M}_{h,\alpha}} \|\mathbb{P}_n W - \mathbb{P} W\|_{\mathbb{R}^m}$. Since u_i preserves the inner product structure, by Lemma 5.2, (5.30) converges to 0 a.s. when $n \rightarrow \infty$. Next, by a direct calculation and the bound in Lemma 5.1, we have

$$\begin{aligned} \sup_{y \in \mathbf{M}} |\mathbb{P}_n \widehat{\mathcal{M}}_{h,\alpha,n}(y, \cdot) //^y X(\cdot) - \mathbb{P}_n \widehat{\mathcal{M}}_{h,\alpha,n}^{(d_{h,\alpha})}(y, \cdot) //^y X(\cdot)| &\leq \|X\|_{L^\infty} \sup_{x,y \in \mathbf{M}} \left| \frac{\widehat{K}_{h,\alpha,n}(x,y) - K_{h,\alpha}(x,y)}{\widehat{d}_{h,\alpha,n}(x)} \right| \\ &\leq \|X\|_{L^\infty} \frac{\|K\|_{L^\infty}^{2\alpha}}{\delta} \sup_{x,y \in \mathbf{M}} |\widehat{K}_{h,\alpha,n}(x,y) - K_{h,\alpha}(x,y)| \\ &\leq \|X\|_{L^\infty} \frac{\|K\|_{L^\infty}^{2\alpha+1}}{\delta} \sup_{x,y \in \mathbf{M}} \left| \frac{1}{\widehat{\mathfrak{p}}_{h,n}^\alpha(x) \widehat{\mathfrak{p}}_{h,n}^\alpha(y)} - \frac{1}{p_h^\alpha(x) p_h^\alpha(y)} \right| \\ &\leq \frac{2\|X\|_{L^\infty} \|K\|_{L^\infty}^{2\alpha+1}}{\delta^{\alpha+1}} \sup_{y \in \mathbf{M}} \left| \frac{1}{\widehat{\mathfrak{p}}_{h,n}^\alpha(y)} - \frac{1}{p_h^\alpha(y)} \right| \leq \frac{2\|X\|_{L^\infty} \|K\|_{L^\infty}^{2\alpha+1}}{\delta^{3\alpha+1}} \sup_{y \in \mathbf{M}} |\widehat{\mathfrak{p}}_{h,n}^\alpha(y) - p_h^\alpha(y)| \\ &\leq \frac{2\alpha \|X\|_{L^\infty} \|K\|_{L^\infty}^{2\alpha+1}}{\delta^{2\alpha+2}} \sup_{f \in \mathcal{K}_h} \|(\mathbb{P}_n f) - (\mathbb{P} f)\|, \end{aligned} \quad (5.31)$$

where the last inequality holds due to the fact that when $A, B \geq c > 0$, $|A^\alpha - B^\alpha| \leq \frac{\alpha}{c^{1-\alpha}} |A - B|$ and $\widehat{\mathfrak{p}}_{h,n}(y), \mathfrak{p}_h(y) > \delta$ by Lemma 5.1. Note that since h is fixed, δ is fixed. Thus, the term (5.28) converges to 0 a.s. as $n \rightarrow \infty$ by Lemma 5.2. The convergence of (5.29) follows the same line:

$$\begin{aligned} \sup_{y \in \mathbf{M}} |\mathbb{P}_n \widehat{\mathcal{M}}_{h,\alpha,n}^{(d_{h,\alpha})}(y, \cdot) //^y X(\cdot) - \mathbb{P}_n \mathcal{M}_{h,\alpha}(y, \cdot) //^y X(\cdot)| &\leq \|X\|_{L^\infty} \|K\|_{L^\infty} \sup_{x \in \mathbf{M}} \left| \frac{1}{\widehat{d}_{h,\alpha,n}(x)} - \frac{1}{d_{h,\alpha}(x)} \right| \\ &\leq \|X\|_{L^\infty} \|K\|_{L^\infty}^{3-2\alpha} \sup_{x \in \mathbf{M}} |\widehat{d}_{h,\alpha,n}(x) - d_{h,\alpha}(x)|, \end{aligned} \quad (5.32)$$

where the last term is bounded by

$$\begin{aligned} \sup_{x \in \mathbf{M}} |\widehat{d}_{h,\alpha,n}(x) - d_{h,\alpha}(x)| &\leq \sup_{x \in \mathbf{M}} |\widehat{d}_{h,\alpha,n}(x) - \widehat{d}_{h,\alpha,n}^{(\mathfrak{p}_h)}(x)| + \sup_{x \in \mathbf{M}} |\widehat{d}_{h,\alpha,n}^{(\mathfrak{p}_h)}(x) - d_{h,\alpha}(x)| \\ &\leq \frac{\|K\|_{L^\infty}}{\delta^{3\alpha}} \sup_{x \in \mathbf{M}} |\widehat{\mathfrak{p}}_{h,n}^\alpha(x) - p_h^\alpha(x)| + \|K\|_{L^\infty} \sup_{f \in \mathcal{K}_{h,\alpha}} \|\mathbb{P}_n f - \mathbb{P} f\|, \end{aligned} \quad (5.33)$$

where $\widehat{d}_{h,\alpha,n}^{(\mathfrak{p}_h)}(x) := \frac{1}{n} \sum_{k=1}^n K_{h,\alpha}(x, x_k) \in C(\mathbf{M})$, which again converges to 0 a.s. as $n \rightarrow \infty$ by Lemma 5.2. We thus conclude the pointwise convergence of $\widehat{T}_{h,\alpha,n}$ to $T_{h,\alpha}$ a.e. as $n \rightarrow \infty$.

Next we check the condition (C2). Since $T_{h,\alpha}$ is compact, the problem is reduced to show that $\widehat{T}_{h,\alpha,n} X_n$ is pre-compact for any given sequence of vector fields $\{X_1, X_2, \dots\} \subset C(\mathcal{E})$ so that $\|X_l\|_{L^\infty} \leq 1$ for all

$l \in \mathbb{N}$. We count on the Arzela–Ascoli theorem [13, IV.6.7] to finish the proof. By Lemma 5.1, a direct calculation leads to

$$\sup_{n \geq 1} \|\widehat{T}_{h,\alpha,n} X_n\|_{L^\infty} = \sup_{n \geq 1, y \in \mathbb{M}} \left| \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(y, x_j) //_{x_j}^y X_n(x_j) \right| \leq \frac{\|K\|_{L^\infty}^{2\alpha+1}}{\delta^{2\alpha+1}}, \quad (5.34)$$

which guarantees the uniform boundedness. Next we show the equi-continuity of $\widehat{T}_{h,\alpha,n} X_n$. For a given pair of close points $x \in \mathbb{M}$ and $y \in \mathbb{M}$, a direct calculation leads to

$$\begin{aligned} |\widehat{T}_{h,\alpha,n} X_n(y) - //_{x}^y \widehat{T}_{h,\alpha,n} X_n(x)| &= |\mathbb{P}_n \widehat{M}_{h,\alpha,n}(y, \cdot) //_{x}^y X_n(\cdot) - //_{x}^y \mathbb{P}_n \widehat{M}_{h,\alpha,n}(x, \cdot) //_{x}^y X_n(\cdot)| \\ &\leq \|X_n\|_{L^\infty} \sup_{z \in \mathbb{M}} |\mathbb{P}_n \widehat{M}_{h,\alpha,n}(y, z) - \mathbb{P}_n \widehat{M}_{h,\alpha,n}(x, z)| \leq \sup_{z \in \mathbb{M}} |\widehat{M}_{h,\alpha,n}(y, z) - \widehat{M}_{h,\alpha,n}(x, z)| \\ &\leq \frac{\|K\|_{L^\infty}^{4\alpha}}{\delta^2} \sup_{z \in \mathbb{M}} |\widehat{d}_{h,\alpha,n}(y) \widehat{K}_{h,\alpha,n}(x, z) - \widehat{d}_{h,\alpha,n}(x) \widehat{K}_{h,\alpha,n}(y, z)| \\ &\leq \frac{\|K\|_{L^\infty}^{4\alpha+1}}{\delta^{2+2\alpha}} \left(\sup_{z \in \mathbb{M}} |\widehat{K}_{h,\alpha,n}(x, z) - \widehat{K}_{h,\alpha,n}(y, z)| + |\widehat{d}_{h,\alpha,n}(y) - \widehat{d}_{h,\alpha,n}(x)| \right) \\ &\leq \frac{\|K\|_{L^\infty}^{4\alpha+1}}{\delta^{2+2\alpha}} \left(\sup_{z \in \mathbb{M}} |\widehat{K}_{h,\alpha,n}(x, z) - \widehat{K}_{h,\alpha,n}(y, x)| + |\widehat{d}_{h,\alpha,n}(y) - \widehat{d}_{h,\alpha,n}^{(p_n)}(y)| \right. \\ &\quad \left. + |\widehat{d}_{h,\alpha,n}^{(p_n)}(y) - \widehat{d}_{h,\alpha,n}^{(p_n)}(x)| + |\widehat{d}_{h,\alpha,n}^{(p_n)}(x) - \widehat{d}_{h,\alpha,n}(x)| \right) \\ &\leq \frac{\|K\|_{L^\infty}^{4\alpha+1}}{\delta^{2+2\alpha}} \left(\sup_{z \in \mathbb{M}} |\widehat{K}_{h,\alpha,n}(x, z) - \widehat{K}_{h,\alpha,n}(y, z)| + |\widehat{d}_{h,\alpha,n}^{(p_n)}(y) - \widehat{d}_{h,\alpha,n}^{(p_n)}(x)| + 2\|\widehat{d}_{h,\alpha,n}^{(p_n)} - \widehat{d}_{h,\alpha,n}\|_{L^\infty} \right), \end{aligned} \quad (5.35)$$

where the last term is further controlled by $|\widehat{d}_{h,\alpha,n}^{(p_n)}(y) - \widehat{d}_{h,\alpha,n}^{(p_n)}(x)| \leq \sup_{z \in \mathbb{M}} |K_{h,\alpha}(y, z) - K_{h,\alpha}(x, z)|$,

$$\begin{aligned} &\sup_{z \in \mathbb{M}} |\widehat{K}_{h,\alpha,n}(x, z) - \widehat{K}_{h,\alpha,n}(y, z)| \\ &\leq \sup_{z \in \mathbb{M}} \frac{1}{\widehat{\mathfrak{p}}_{h,n}^\alpha(x) \widehat{\mathfrak{p}}_{h,n}^\alpha(y) \widehat{\mathfrak{p}}_{h,n}^\alpha(z)} |\widehat{\mathfrak{p}}_{h,n}^\alpha(y) K_h(x, z) - \widehat{\mathfrak{p}}_{h,n}^\alpha(x) K_h(y, z)| \\ &\leq \frac{1}{\delta^{3\alpha}} \left(\sup_{z \in \mathbb{M}} \widehat{\mathfrak{p}}_{h,n}^\alpha(y) |K_h(x, z) - K_h(y, z)| + \sup_{z \in \mathbb{M}} K_h(y, z) |\widehat{\mathfrak{p}}_{h,n}^\alpha(y) - \widehat{\mathfrak{p}}_{h,n}^\alpha(x)| \right) \\ &\leq \frac{\|K\|_{L^\infty}}{\delta^{3\alpha}} \left(\sup_{z \in \mathbb{M}} |K_h(x, z) - K_h(y, z)| + \sup_{z \in \mathbb{M}} \frac{\alpha}{\delta^{1-\alpha}} |\widehat{\mathfrak{p}}_{h,n}(y) - \widehat{\mathfrak{p}}_{h,n}(x)| \right) \\ &\leq \frac{\|K\|_{L^\infty}}{\delta^{3\alpha}} \left(\sup_{z \in \mathbb{M}} |K_h(x, z) - K_h(y, z)| + \frac{\alpha}{\delta^{1-\alpha}} \sup_{z \in \mathbb{M}} |K_h(y, z) - K_h(x, z)| \right), \end{aligned} \quad (5.36)$$

and similarly

$$\|\widehat{d}_{h,\alpha,n}^{(p_h)} - \widehat{d}_{h,\alpha,n}\|_{L^\infty} = \sup_{z \in \mathbb{M}} \left| \frac{1}{n} \sum_{k=1}^n \left(\frac{K_h(z, x_k)}{\widehat{\mathfrak{p}}_{h,n}^\alpha(z) \widehat{\mathfrak{p}}_{h,n}^\alpha(x_k)} - \frac{K_h(z, x_k)}{\mathfrak{p}_h^\alpha(z) \mathfrak{p}_h^\alpha(x_k)} \right) \right| \quad (5.37)$$

$$\begin{aligned}
&\leq \frac{\|K\|_{L^\infty}}{\delta^\alpha} \sup_{z \in \mathbb{M}} \left| \frac{1}{\widehat{\mathbf{p}}_{h,n}^\alpha(z) \widehat{\mathbf{p}}_{h,n}^\alpha(x_k)} - \frac{1}{\mathbf{p}_h^\alpha(z) \mathbf{p}_h^\alpha(x_k)} \right| \leq \frac{\|K\|_{L^\infty}}{\delta^{3\alpha}} \sup_{z \in \mathbb{M}} |\widehat{\mathbf{p}}_{h,n}^\alpha(z) - \mathbf{p}_h^\alpha(z)| \\
&\leq \frac{\|K\|_{L^\infty}}{\delta^{3\alpha}} \frac{\alpha}{\delta^{1-\alpha}} \|\widehat{\mathbf{p}}_{h,n} - \mathbf{p}_h\|_{L^\infty}.
\end{aligned}$$

As a result, we have the following bound

$$\begin{aligned}
|\widehat{T}_{h,\alpha,n} X_n(y) - \widehat{T}_{h,\alpha,n} X_n(x)| &\leq \frac{\|K\|_{L^\infty}^{4\alpha+2}}{\delta^{2+5\alpha}} \left(\left(1 + \frac{\alpha}{\delta^{1-\alpha}}\right) \sup_{z \in \mathbb{M}} |K_h(x, z) - K_h(y, z)| \right. \\
&\quad \left. + \frac{\delta^{3\alpha}}{\|K\|_{L^\infty}} \sup_{z \in \mathbb{M}} |K_{h,\alpha}(y, z) - K_{h,\alpha}(x, z)| + \frac{\alpha}{\delta^{1-\alpha}} \|\widehat{\mathbf{p}}_{h,n} - \mathbf{p}_h\|_{L^\infty} \right). \quad (5.38)
\end{aligned}$$

Thus, when $y \rightarrow x$, $\sup_{z \in \mathbb{M}} |K_h(x, z) - K_h(y, z)|$ and $\sup_{z \in \mathbb{M}} |K_{h,\alpha}(y, z) - K_{h,\alpha}(x, z)|$ both converge to 0 since K_h and $K_{h,\alpha}$ are both continuous. Also, $\|\widehat{\mathbf{p}}_{h,n} - \mathbf{p}_h\|_{L^\infty}$ converges to 0 a.s. as $n \rightarrow \infty$ by the Glivenko–Cantali property; that is, for a given small $\epsilon > 0$, we can find $N > 0$ so that $\|\widehat{\mathbf{p}}_{h,n} - \mathbf{p}_h\|_{L^\infty} \leq \epsilon$ a.s. for all $n \geq N$. Thus, by the Arzela–Ascoli theorem, we have the compact convergence of $\widehat{T}_{h,\alpha,n}$ to $T_{h,\alpha}$ a.s. when $n \rightarrow \infty$.

Since the compact convergence implies the spectral convergence (see [9] or Proposition 6 in [37]), we get the spectral convergence of $\widehat{T}_{h,\alpha,n}$ to $T_{h,\alpha}$ a.s. when $n \rightarrow \infty$.

Step 3: Spectral convergence of $T_{h,1}^{t/h}$ to $e^{t\nabla^2}$ and $h^{-1}(T_{h,1} - 1)$ to ∇^2 in $L^2(\mathcal{E})$ as $h \rightarrow 0$.

First we consider the case when $\partial\mathbb{M} = \emptyset$. We assume $\frac{\mu_2}{d} = 1$ to simplify the notation. To show the spectral convergence, we restrict the operator to a finite dimensional subspace determined by the first few eigenvector fields. To do so, fix $l_0 \geq 0$ and consider the finite dimensional subspace $\bigoplus_{k \leq l_0} E_k$. For all $x \in \mathbb{M}$, by Theorem 5.2, we have uniformly

$$\frac{T_{h,1} X_l(x) - X_l(x)}{h} = \nabla^2 X_l(x) + O(h), \quad (5.39)$$

where the implied constant in $O(h)$ depends on $\|X_l^{(k)}\|_{L^\infty(\mathcal{E})}$, where $k = 0, 1, 2, 3$. To control the $O(h)$ term, by the Sobolev embedding theorem [30, Theorem 9.2], for all $l \leq l_0$ we have

$$\|X_l^{(3)}\|_{L^\infty(\mathcal{E})} \lesssim \|X_l\|_{H^{d/2+4}(\mathcal{E})} \lesssim 1 + \|(\nabla^2)^{d/4+2} X_l\|_{L^2(\mathcal{E})} = 1 + \lambda_l^{d/4+2}, \quad (5.40)$$

where we choose $d/2 + 4$ for convenience. Similar bounds hold for $\|X_l\|_{L^\infty(\mathcal{E})}$, $\|X_l^{(1)}\|_{L^\infty(\mathcal{E})}$ and $\|X_l^{(2)}\|_{L^\infty(\mathcal{E})}$. Thus, for all $l \leq l_0$, since $\lambda_l \leq \lambda_{l_0}$ by assumption, we have

$$\left\| \frac{T_{h,1} X_l - X_l}{h} - \nabla^2 X_l \right\|_{L^2(\mathcal{E})} \lesssim \left(1 + \lambda_{l_0}^{d/4+2}\right) h. \quad (5.41)$$

Thus, if we choose h small enough so that $(1 + \lambda_{l_0}^{d/4+2})h \leq h^{1/2}$, that is, $\lambda_{l_0} \leq (h^{-1/2} - 1)^{4/(d+8)}$, we reach the fact that

$$\left\| \frac{T_{h,1} - 1}{h} - \nabla^2 \right\|_{L^2(\mathcal{E})} \lesssim h^{1/2} \quad (5.42)$$

on $\overline{\oplus_{k \leq l_0} E_k}$. Note that $\overline{\oplus_{k \leq l_0} E_k} = \overline{\oplus_{I_h} E_k}$, where $I_h := \{k; \lambda_k \leq (h^{-1/2} - 1)^{4/(d+8)}\}$, and $\overline{\oplus_{I_h} E_k}$ approaches $L^2(\mathcal{E})$ when h decreases. As a result, when $h \rightarrow 0$, $h^{-1}(T_{h,1} - 1)$ spectrally converges to ∇^2 in the boundary-free case.

Next we show the spectral convergence of $T_{h,1}^{t/h}$ to the heat semigroup $e^{t\nabla^2}$ for a fixed $t > 0$ as $h \rightarrow 0$. Again, fix $l_0 \geq 0$ and consider the finite dimensional subspace $\overline{\oplus_{k \leq l_0} E_k}$. First, we study the difference between $(I + h\nabla^2)^{t/h}$ and $T_{h,1}^{t/h}$. Note that on $\overline{\oplus_{k \leq l_0} E_k}$, from (5.41) we have

$$T_{h,1} = I + h\nabla^2 + E_h, \quad (5.43)$$

where $\|E_h\|_{L^2(\mathcal{E})} \lesssim (1 + \lambda_{l_0}^{d/4+2})h^2$. When $h < \frac{1}{2\lambda_{l_0}}$ is small enough, we have $1/2 \leq \|I + h\nabla^2\|_{L^2(\mathcal{E})} \leq 1$ and $(1 + \lambda_{l_0}^{d/4+2})h^2 < 1/2$. Thus, by the binomial expansion, we have

$$\begin{aligned} \|T_{h,1}^{t/h} - (I + h\nabla^2)^{t/h}\|_{L^2(\mathcal{E})} &\leq \frac{t}{h} \|I + h\nabla^2\|_{L^2(\mathcal{E})}^{t/h-1} \|E_h\|_{L^2(\mathcal{E})} \\ &\quad + \frac{1}{2} \frac{t}{h} \left(\frac{t}{h} - 1 \right) \|I + h\nabla^2\|_{L^2(\mathcal{E})}^{t/h-2} \|E_h\|_{L^2(\mathcal{E})}^2 + \dots \\ &= (1 + \|E_h\|_{L^2(\mathcal{E})}^2)^{t/h} - 1. \end{aligned} \quad (5.44)$$

When $t/h \leq 1$, then clearly by the binomial approximation, $\|T_{h,1}^{t/h} - (I + h\nabla^2)^{t/h}\|_{L^2(\mathcal{E})} \leq 2\frac{t}{h} \|E_h\|_{L^2(\mathcal{E})}^2 \lesssim (1 + \lambda_{l_0}^{d/4+2})th$; when $t/h > 1$, h could be chosen further small, if needed, so that $\|E_h\|_{L^2(\mathcal{E})}^2 < 2^{1/(t/h-1)} - 1$, which leads to $\|T_{h,1}^{t/h} - (I + h\nabla^2)^{t/h}\|_{L^2(\mathcal{E})} \leq 2\frac{t}{h} \|E_h\|_{L^2(\mathcal{E})}^2 \lesssim (1 + \lambda_{l_0}^{d/4+2})th$. To sum up, for a chosen l_0 , we could find $h > 0$ small enough so that

$$\|T_{h,1}^{t/h} - (I + h\nabla^2)^{t/h}\|_{L^2(\mathcal{E})} \leq 2\frac{t}{h} \|E_h\|_{L^2(\mathcal{E})}^2 \lesssim (1 + \lambda_{l_0}^{d/4+2})th. \quad (5.45)$$

Secondly, we take a careful look at the difference between $(I + h\nabla^2)^{t/h}$ and $e^{t\nabla^2}$. When $0 < h < \frac{1}{2\lambda_{l_0}}$, $I + h\nabla^2$ is invertible on $\overline{\oplus_{k \leq l_0} E_k}$ with norm $\frac{1}{2} \leq \|I + h\nabla^2\| \leq 1$. So, for all $l \leq l_0$ we have

$$(I + h\nabla^2)^{t/h} X_l = (1 - h\lambda_l)^{t/h} X_l \quad (5.46)$$

and

$$e^{t\nabla^2} X_l = e^{-t\lambda_l} X_l. \quad (5.47)$$

By the binomial expansion, we have the following bound

$$\begin{aligned} &|(1 - h\lambda_l)^{t/h} - e^{-t\lambda_l}| \\ &= \left| \left[1 - \frac{t}{h}(h\lambda_l) + \frac{1}{2} \frac{t}{h} \left(\frac{t}{h} - 1 \right) (h\lambda_l)^2 - \frac{1}{3!} \frac{t}{h} \left(\frac{t}{h} - 1 \right) \left(\frac{t}{h} - 2 \right) (h\lambda_l)^3 + \dots \right] \right. \\ &\quad \left. - \left[1 - t\lambda_l + \frac{1}{2} (t\lambda_l)^2 - \frac{1}{3!} (t\lambda_l)^3 + \dots \right] \right| \end{aligned}$$

$$\begin{aligned}
&= \lambda_t^2 th \left| -\frac{1}{2} - \frac{1}{3!}(-3t + 2h) + \frac{1}{4!}(-6t^2 + 11th - 6h^2) - \dots \right| \\
&\lesssim \lambda_t^2 th,
\end{aligned} \tag{5.48}$$

where the last inequality holds since the denominator is factorial and the numerator is polynomial. Therefore, when $0 < h < \frac{1}{2\lambda_{l_0}}$, on $\overline{\oplus_{k \leq l_0} E_k}$ the following holds

$$\|e^{t\nabla^2} - (I + h\nabla^2)^{t/h}\|_{L^2(\mathcal{E})} \lesssim \lambda_{l_0}^2 th. \tag{5.49}$$

Now, we put the above results together. On $\overline{\oplus_{k \leq l_0} E_k}$, as $d \geq 1$, by (5.45) and (5.49), we have

$$\begin{aligned}
\|T_{h,1}^{t/h} - e^{t\nabla^2}\|_{L^2(\mathcal{E})} &\leq \|T_{h,1}^{t/h} - (I + h\nabla^2)^{t/h}\|_{L^2(\mathcal{E})} + \|e^{t\nabla^2} - (I + h\nabla^2)^{t/h}\|_{L^2(\mathcal{E})} \\
&\lesssim (1 + \lambda_{l_0}^{d/4+2})th.
\end{aligned} \tag{5.50}$$

Thus, if we choose h small enough, which depends on t , so that $(1 + \lambda_{l_0}^{d/4+2})th \leq h^{1/2}$, that is, $\lambda_{l_0} \leq (h^{-1/2}t^{-1} - 1)^{4/(d+8)}$, we reach the fact that

$$\|T_{h,1}^{t/h} - e^{t\nabla^2}\|_{L^2(\mathcal{E})} \lesssim h^{1/2} \tag{5.51}$$

on $\overline{\oplus_h E_k}$. As a result, when $h \rightarrow 0$, $T_{h,1}^{t/h}$ spectrally converges to $e^{t\nabla^2}$ in the boundary-free case.

When $\partial M \neq \emptyset$, the proof is exactly the same, except that we have to take the boundary effect (5.3) and the Neuman's condition into account. We skip the details.

Final step: Putting everything together.

We now finish the Proof of Theorem 5.4 here. The proof holds when the boundary is empty or non-empty. Fix i and denote $\mu_{t,i,h}$ to be the i th eigenvalue of $T_{h,1}$ with the associated eigenvector $Y_{t,i,h}$. By Step 1, we know that all the eigenvalues inside $(-1/h, 0]$ of $\widehat{T}_{h,1,n}$ and $D_{h,1,n}^{-1} \mathcal{S}_{h,1,n}$ are the same and their eigenvectors are related. By Step 2, since we have the spectral convergence of $\widehat{T}_{h,1,n}$ to $T_{h,1}$ almost surely as $n \rightarrow \infty$, for each $j \in \mathbb{N}$ large enough, we have by the definition of convergence in probability that for $h_j = 1/j$, we can find $n_j \in \mathbb{N}$ so that

$$P\{\|Y_{t,i,h_j} - Y_{t,i,h_j,n_j}\|_{L^2(\mathcal{E})} \geq 1/j\} \leq 1/j. \tag{5.52}$$

Take n_j as an increasing sequence. By step 3, for each $j \in \mathbb{N}$, there exists $j' \geq j$ so that

$$\|Y_{t,i} - Y_{t,i,h_{j'}}\|_{L^2(\mathcal{E})} < 1/2j'. \tag{5.53}$$

Arrange j' as an increasing sequence. As j is chosen as an increasing sequence toward ∞ , j' is also an increasing sequence toward ∞ . Thus, for the increasing sequence $\{j'\} \subset \mathbb{N}$, we could find an increasing sequence $\{n_{j'}\} \subset \mathbb{N}$ so that

$$P\{\|Y_{t,i} - Y_{t,i,h_{j'},n_{j'}}\|_{L^2(\mathcal{E})} \geq 1/j'\} \leq P\{\|Y_{t,i,h_{j'}} - Y_{t,i,h_{j'},n_{j'}}\|_{L^2(\mathcal{E})} \geq 1/2j'\} \leq 1/2j'. \tag{5.54}$$

Therefore, we conclude the convergence of the eigenvectors in probability. Similar statements hold for the eigenvalue, $\mu_{t,i,h}$. Since the proof for Theorem 5.5 is the same, we skip it. \square

6 Extract more topological/geometric information from a point cloud

In Section 2, we understand VDM under the assumption that we have an access to the principal bundle structure of the manifold. However, in practice the knowledge of the bundle structure is not always available and we may only have access to the point cloud sampled from the manifold. Is it possible to obtain any principal bundle under this situation? The answer is yes if we restrict ourselves to a special principal bundle, the frame bundle.

The main ingredient added in this section is the estimation of the frame bundle from the point cloud. Recall that the frame bundle is composed of two components—the bundle itself, and the connection between the fibers. The estimation of the frame bundle thus depends on two algorithms—the local PCA algorithm is applied to estimate the frame bundle, while the rotational alignment algorithm is applied to estimate the connection between fibers. The theoretical analysis of these algorithms have been detailed in [33], so we will just summarize the analysis result. However, to have the spectral convergence proof of the algorithm, we have to better quantify the probability of getting the satisfactory estimation from the finite sampling points. Below, we will start from summarizing the algorithm, and provide the spectral convergence theory and its proof.

We summarize the proposed reconstruction algorithm considered in [33] below. Take a point cloud $\mathcal{X} = \{x_i\}_{i=1}^n$ sampled from \mathbf{M} under Assumptions 4.1 (A1), 4.2 (B1) and 4.2 (B2). The algorithm consists of the following three steps:

- (Step a) Reconstruct the frame bundle from \mathcal{X} . It is possible since locally a manifold can be well approximated by an affine space up to second order [1,18,22,24,33,38,39]. Thus, the embedded tangent bundle is estimated by local PCA with the kernel bandwidth $h_{\text{pca}} > 0$. Indeed, the top d eigenvectors, $v_{x,k} \in \mathbb{R}^p$, $k = 1, \dots, d$, of the covariance matrix of the dataset near $x \in \mathbf{M}$, $\mathcal{N}_x := \{x_j \in \mathcal{X}; \|x - x_j\|_{\mathbb{R}^p} \leq \sqrt{h_{\text{pca}}}\}$, are chosen to form the estimated basis of the embedded tangent plane $\iota_* T_x \mathbf{M}$. Denote O_x to be a $p \times d$ matrix, whose k th column is $v_{x,k}$. Note that x may or may not be in \mathcal{X} . Here O_x can be viewed as an estimation of a point u_x of the frame bundle such that $\pi(u_x) = x$. When $x = x_i \in \mathcal{X}$, we use O_i to denote O_{x_i} . See [33] for details.
- (Step b) Estimate the connection (parallel transport) between tangent planes by aligning O_x and O_y by

$$O_{x,y} = \operatorname{argmin}_{O \in O(d)} \|O - O_x^T O_y\|_{HS} \in O(d), \quad (6.1)$$

where $\|\cdot\|_{HS}$ is the Hilbert–Schmidt norm. It is proved that $O_{x,y}$ is an approximation of the parallel transport from y to x when x and y are close enough in the following sense [33, (B.6)]:

$$O_{x,y} \bar{X}_y \approx O_x^T \iota_* \parallel_y^x X(y), \quad (6.2)$$

where $X \in C(TM)$ and $\bar{X}_y = O_y^T \iota_* X(y) \in \mathbb{R}^d$ is the coordinate of $X(y)$ with related to the estimated basis. Note that x and y may or may not be in \mathcal{X} . When $x = x_i \in \mathcal{X}$ and $y = x_j \in \mathcal{X}$, we use O_{ij} to denote O_{x_i, x_j} and \bar{X}_j to denote \bar{X}_{x_j} .

(Step c) Build GCL mentioned in Section 2 based on the connection graph from \mathcal{X} and $\{O_{ij}\}$. We build up a block matrix $\mathbf{S}_{h,\alpha,n}^{\circ}$ with $d \times d$ entries, where $h > h_{\text{pca}}$:

$$\mathbf{S}_{h,\alpha,n}^{\circ}(i,j) = \begin{cases} \widehat{K}_{h,\alpha,n}(x_i, x_j) O_{ij} & (i,j) \in E, \\ 0_{d \times d} & (i,j) \notin E, \end{cases} \quad (6.3)$$

where $0 \leq \alpha \leq 1$ and the kernel K satisfies Assumption 4.3, and an $n \times n$ diagonal block matrix $\mathbf{D}_{h,\alpha,n}$ with $d \times d$ entries defined in (4.4). Denote operators $O_{\mathcal{X}}^T : TM_{\mathcal{X}} \rightarrow V_{\mathcal{X}}$, $O_{\mathcal{X}} : V_{\mathcal{X}} \rightarrow TM_{\mathcal{X}}$

$$\begin{aligned} O_{\mathcal{X}} \mathbf{v} &:= [i_*^T O_1 \mathbf{v}[1], \dots, i_n^T O_n \mathbf{v}[n]] \in TM_{\mathcal{X}}, \\ O_{\mathcal{X}}^T \mathbf{w} &:= [(O_1^T \iota_* \mathbf{w}[1])^T, \dots, (O_n^T \iota_* \mathbf{w}[n])^T]^T \in V_{\mathcal{X}}, \end{aligned} \quad (6.4)$$

where $\mathbf{w} \in TM_{\mathcal{X}}$ and $\mathbf{v} \in V_{\mathcal{X}}$. Here $V_{\mathcal{X}}$ means the coordinates of a set of embedded tangent vectors on \mathbf{M} with related to the estimated basis of the embedded tangent plane. The pointwise convergence of GCL has been shown in [33, Theorem 5.3]; that is, a.s. we have

$$\lim_{h \rightarrow 0} \lim_{n \rightarrow \infty} \frac{1}{h} (\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}^{\circ} \bar{\mathbf{X}} - \bar{\mathbf{X}})[i] = \frac{\mu_{1,2}^{(0)}}{2d} O_i^T \iota_* \left\{ \nabla^2 X(x_i) + \frac{2 \nabla X(x_i) \cdot \nabla(\mathbf{p}^{1-\alpha})(x_i)}{\mathbf{p}^{1-\alpha}(x_i)} \right\}, \quad (6.5)$$

where $X \in C^4(TM)$ and $\bar{\mathbf{X}} = O_{\mathcal{X}}^T \delta_{\mathcal{X}} X$. This means that by taking $\alpha = 1$, we reconstruct the connection Laplacian associated with the tangent bundle TM .

Note that the errors introduced in (a) and (b) may accumulate and influence spectral convergence of the GCL. In this section we study the spectral convergence under this setup, which answers our question in the beginning and affirms that we are able to extract further geometric/topological information simply from the point cloud.

DEFINITION 6.1 Define operators $\widetilde{T}_{h,\alpha,n}^{\circ} : C(TM) \rightarrow C(TM)$ as

$$\widetilde{T}_{h,\alpha,n}^{\circ} X(y) = i_*^T O_y \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(y, x_j) O_{y,x_j} O_j^T \iota_* X(x_j). \quad (6.6)$$

The main result of this section is the following spectral convergence theorems stating the spectral convergence of $(\mathbf{D}_{h,1,n}^{-1} \mathbf{S}_{h,1,n}^{\circ})^{t/h}$ to $e^{t\nabla^2}$ and $h^{-1}(\mathbf{D}_{h,1,n}^{-1} \mathbf{S}_{h,1,n}^{\circ} - \mathbf{I}_{dn})$ to ∇^2 . Note that except the estimated parallel transport, the statements of Theorems 6.2 and 6.3 are the same as those of Theorems 5.4 and 5.5.

THEOREM 6.2 Assume Assumptions 4.1 (A1), 4.2 (B1), 4.2 (B2) and 4.3 hold. Estimate the parallel transport and construct the GCL by Step a, Step b and Step c. Fix $t > 0$. Denote $\widetilde{\mu}_{t,i,h,n}$ to be the i th eigenvalue of $(\widetilde{T}_{h,1,n}^{\circ})^{t/h}$ with the associated eigenvector $\widetilde{Y}_{t,i,h,n}$. Also denote $\mu_{t,i} > 0$ to be the i th eigenvalue of the heat kernel of the connection Laplacian $e^{t\nabla^2}$ with the associated eigen-vector field $Y_{t,i}$.

We assume that both $\mu_{i,i,h,n}$ and $\mu_{i,i}$ decrease as i increases, respecting the multiplicity. Fix $i \in \mathbb{N}$. Then there exists a sequence $h_n \rightarrow 0$ such that

$$\lim_{n \rightarrow \infty} \tilde{\mu}_{i,i,h,n} = \mu_{i,i} \quad \text{and} \quad \lim_{n \rightarrow \infty} \|\tilde{Y}_{i,i,h,n} - Y_{i,i}\|_{L^2(TM)} = 0 \quad (6.7)$$

in probability.

THEOREM 6.3 Assume Assumptions 4.1 (A1), 4.2 (B1), 4.2 (B2) and 4.3 hold. Estimate the parallel transport and construct the GCL by Step a, Step b and Step c. Denote $-\tilde{\lambda}_{i,h,n}$ to be the i th eigenvalue of $h^{-1}(\widehat{T}_{h,1,n}^O - 1)$ with the associated eigenvector $\tilde{X}_{i,h,n}$. Also denote $-\lambda_i$, where $\lambda_i > 0$, to be the i th eigenvalue of the connection Laplacian ∇^2 with the associated eigen-vector field X_i . We assume that both $\lambda_{i,h,n}$ and λ_i increase as i increases, respecting the multiplicity. Fix $i \in \mathbb{N}$. Then there exists a sequence $h_n \rightarrow 0$ such that

$$\lim_{n \rightarrow \infty} \tilde{\lambda}_{i,h,n} = \lambda_i \quad \text{and} \quad \lim_{n \rightarrow \infty} \|\tilde{X}_{i,h,n} - X_i\|_{L^2(TM)} = 0 \quad (6.8)$$

in probability.

The proofs of Theorems 6.2 and 6.3 are essentially the same as those of Theorems 5.4 and 5.5, except the fact that we lack the knowledge of the parallel transport. Indeed, in (4.2) the parallel transport is assumed to be accessible to the data analyst, while in this section we only have access to the point cloud. Thus, the key ingredient of the proofs of Theorems 6.2 and 6.3 is controlling the error terms coming from two estimations, the estimation of the frame bundle and the estimation of the connection, while the other comments and details are the same as those in Section 5.

To better appreciate the role of these two estimations, we consider an intermediate scenario. We assume that we only have an access to the embedding ι and the knowledge of the embedded tangent bundle, which are represented as affine spaces inside \mathbb{R}^p , but the parallel transport is not accessible to us. Denote the basis of the embedded tangent plane $\iota_* T_{x_i} \mathbf{M}$ to be a $p \times d$ matrix Q_i . By [33, (B.68)], we can approximate the parallel transport from x_i to x_j from Q_i and Q_j with a tolerable error; that is,

$$\|_j^i X(x_j) \approx \iota_*^T Q_i Q_{ij} Q_j^T \iota_* X(x_j), \quad (6.9)$$

where $Q_{ij} := \operatorname{argmin}_{O \in O(d)} \|O - Q_i^T Q_j\|_{\text{HS}}$. Notice that even we know bases of these embedded tangent planes, the optimization step to obtain Q_{ij} is still needed since in general $Q_i^T Q_j$ is not orthogonal due to the curvature. In this intermediate scenario, to get the spectral convergence, we only need to control the error incurred by the estimation of the connection.

With the above discussion, we know that if the embedded tangent bundle information is further missing and we have to estimate it from the point cloud, another resource of error comes to play. Indeed, denote the estimated embedded tangent plane by a $p \times d$ matrix O_x . In [33], it has been shown that

$$O_x^T \iota_* X(x) \approx Q_x^T \iota_* X(x). \quad (6.10)$$

This approximation is possible due to the following two facts. First, by definition locally a manifold is isomorphic to the Euclidean space up to a second order error depending on the curvature. Secondly, the embedding ι is smooth so locally the manifold is distorted up to the Jacobian of ι . We point out that

in [33] we focus on the pointwise convergence so the error terms in [33] were simplified by the big O notations.

*Proof of Theorems 6.2 and 6.3. **Step 1: Estimate the frame bundle and connection.***

We show the proof when the boundary is empty. When the boundary is not empty, the proof is exactly the same, except that the convergence rate is different near the boundary. Here we give an outline of the proof and indicate how the error terms look like. We refer the reader to [33] for the other details. Recall the following results in [33, Theorem B.1]: with the kernel bandwidth h_{pca} , which is chosen so that $h_{\text{pca}}/h \rightarrow 0$ as $h \rightarrow 0$, with high probability we have

$$O_i^T t_* X(x_i) = Q_i^T t_* X(x_i) + O(h^{3/2}), \quad (6.11)$$

where $x_i \in \mathcal{X}$ and the $O(h^{3/2})$ term contains both the bias error and variance originating from the finite sample. Here, the implied constant in $O(h^{3/2})$ solely depends on the curvatures of the manifold and their covariant derivatives. To show the spectral convergence, we have to further quantify this result.

For a fixed x_i , the covariance matrix \mathcal{E}_i built up in the local PCA step is

$$\mathcal{E}_i = \frac{1}{n-1} \sum_{j \neq i}^n F_{ij} \mathcal{X}_{\|t(x_i) - t(x_j)\| \leq \sqrt{h_{\text{pca}}}}, \quad (6.12)$$

where F_{ij} are i.i.d. random matrix of size $p \times p$

$$F_{ij} = K \left(\frac{\|t(x_i) - t(x_j)\|_{\mathbb{R}^p}}{\sqrt{h_{\text{pca}}}} \right) (t(x_j) - t(x_i))(t(x_j) - t(x_i))^T, \quad (6.13)$$

so that its (k, l) th entry

$$F_{ij}(k, l) = K \left(\frac{\|t(x_i) - t(x_j)\|_{\mathbb{R}^p}}{\sqrt{h_{\text{pca}}}} \right) \langle t(x_j) - t(x_i), v_k \rangle \langle t(x_j) - t(x_i), v_l \rangle, \quad (6.14)$$

where v_l is the unit column vector with the l th entry 1. Since F_{ij} are i.i.d. random matrices for all $j \neq i$, we could view them as an i.i.d. sample from a random matrix F_i . To simplify the discussion, we assume that for some $C_{k,l} > 0$ depending on the second fundamental form of ι , $F_i(k, l)$ is bounded by $C_{k,l} h_{\text{pca}}$ when $k, l = 1, \dots, d$, bounded by $C_{k,l} h_{\text{pca}}^2$ when $k, l = d+1, \dots, p$, and bounded by $C_{k,l} h_{\text{pca}}^{3/2}$ for the other cases. Note that when the manifold is flat around x_i , when h_{pca} is small enough, $C_{k,l}$ when $k > d$ or $l > d$. In this case, the proof of the bound is trivial.

The expectation of $F_i(k, l)$ could be directly evaluated

$$\mathbb{E}F_i(k, l) = \int_B \mathcal{K}_{h_{\text{pca}}}(x_i, y) \langle t(y) - t(x_i), v_k \rangle \langle t(y) - t(x_i), v_l \rangle \mathbf{p}(y) dV(y), \quad (6.15)$$

and the variance could be evaluated in a similar way. It has been shown in [33, (B.33)–(B.35)] that expectation of $F_i(k, l)$ is of order $h_{\text{pca}}^{d/2+1}$ when $l, k = 1, \dots, d$ and is $O(h_{\text{pca}}^{d/2+2})$ for the other cases;

the variance of $F_i(k, l)$, denoted as $\sigma_{k,l}^2$, is $O(h_{\text{pca}}^{d/2+2})$ when $l, k = 1, \dots, d$, $O(h_{\text{pca}}^{d/2+4})$ and when $l, k = d + 1, \dots, p$, and $O(h_{\text{pca}}^{d/2+3})$ for the other cases. To simplify the discussion, we assume that there exists $c_{k,l} > 0$ so that $\sigma_{k,l}^2 = c_{k,l} h_{\text{pca}}^{d/2+2}$, when $l, k = 1, \dots, d$; that is, $\sigma_{k,l}^2$ is of order $h_{\text{pca}}^{d/2+2}$. Similarly, we assume that $\sigma_{k,l}^2 = c_{k,l} h_{\text{pca}}^{d/2+4}$ when $l, k = 1, \dots, d$, and $\sigma_{k,l}^2 = h_{\text{pca}}^{d/2+3}$ for the other cases. When the variance is of higher order, the deviation could be evaluated similarly and we skip the details. Also note that when the manifold is flat around x_i , when h_{pca} is small enough, $c_{k,l} = 0$ and when $k > d$ or $l > d$, and the deviation bound is trivial.

Clearly the variance is much smaller than the bound, so we could apply Bernstein's inequality to control the deviation. For $\beta > 0$, we have

$$\Pr \{ |\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| > \beta \} \leq \exp \left\{ - \frac{(n-1)\beta^2}{c_{k,l} h_{\text{pca}}^{d/2+2} + C_{k,l} h_{\text{pca}} \beta} \right\}, \quad (6.16)$$

when $k, l = 1, \dots, d$;

$$\Pr \{ |\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| > \beta \} \leq \exp \left\{ - \frac{(n-1)\beta^2}{c_{k,l} h_{\text{pca}}^{d/2+4} + C_{k,l} h_{\text{pca}}^2 \beta} \right\}, \quad (6.17)$$

when $k, l = d + 1, \dots, p$;

$$\Pr \{ |\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| > \beta \} \leq \exp \left\{ - \frac{(n-1)\beta^2}{c_{k,l} h_{\text{pca}}^{d/2+3} + C_{k,l} h_{\text{pca}}^{3/2} \beta} \right\}, \quad (6.18)$$

for the other cases. β should be chosen so that $\beta/h_{\text{pca}}^{d/2+1} \rightarrow 0$ as $h_{\text{pca}} \rightarrow 0$ when $k, l = 1, \dots, d$, and $\beta/h_{\text{pca}}^{d/2+2} \rightarrow 0$ as $h_{\text{pca}} \rightarrow 0$ for the other cases; that is, $\mathbb{E}F_i(k, l)$ could be well approximated when h_{pca} is small enough and when $k, l = 1, \dots, d$, and for the other k, l , $\mathcal{E}_i(k, l)$ should be no larger than $h_{\text{pca}}^{d/2+2}$. These lead to $\sigma_{k,l}^2 + C_{k,l} h_{\text{pca}} \beta \leq 2\sigma_{k,l}^2$ for all k, l , so that $\frac{(n-1)\beta^2}{\sigma_{k,l}^2 + C_{k,l} h_{\text{pca}} \beta} \geq \frac{(n-1)\beta^2}{2\sigma_{k,l}^2}$. To guarantee that the deviation greater than β happens with probability less than $\frac{1}{3d^2 n^3}$, n should satisfy $\frac{n}{\log(n)} \geq 2\sigma_{k,l}^2 \beta^{-2}$. Choose $\beta_1 > 0$ to be of order $\frac{\log(n) h_{\text{pca}}^{d/4+1}}{n^{1/2}}$ so that with probability greater than $1 - \frac{1}{3d^2 n^3}$, $|\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| \leq \beta_1$ for all $k, l = 1, \dots, d$; choose $\beta_2 > 0$ to be of order $\frac{\log(n) h_{\text{pca}}^{d/4+2}}{n^{1/2}}$ so that with probability greater than $1 - \frac{1}{3(p-d)^2 n^3}$, $|\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| \leq \beta_2$ for all $k, l = d + 1, \dots, p$; choose $\beta_3 > 0$ to be of order $\frac{\log(n) h_{\text{pca}}^{d/4+3/2}}{n^{1/2}}$ so that with probability greater than $1 - \frac{1}{3p(p-d)n^3}$, $|\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| \leq \beta_3$ for the other cases. Note that $\beta_1/h_{\text{pca}}^{d/2+1} \rightarrow 0$ as $h_{\text{pca}} \rightarrow 0$ for all $k, l = 1, \dots, d$; $\beta_2/h_{\text{pca}}^{d/2+2} \rightarrow 0$ as $h_{\text{pca}} \rightarrow 0$ for all $k, l = d + 1, \dots, p$; $\beta_3/h_{\text{pca}}^{d/2+2} \rightarrow 0$ as $h_{\text{pca}} \rightarrow 0$ for the other cases.

Denote $\Omega_{n, \beta_1, \beta_2, \beta_3}$ to be the event space that for all $i = 1, \dots, n$, $|\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| \leq \beta_1$ for all $k, l = 1, \dots, d$, $|\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| \leq \beta_2$ for all $k, l = d + 1, \dots, p$, $|\mathcal{E}_i(k, l) - \mathbb{E}F_i(k, l)| \leq \beta_3$ for all $k = 1, \dots, d, l = d + 1, \dots, p$ and $l = 1, \dots, d, k = d + 1, \dots, p$. By a direct calculation, we know

that the probability of $\Omega_{n,\beta_1,\beta_2,\beta_3}$ is bounded from below by

$$1 - n \left(d^2 \exp \left\{ -\frac{(n-1)\beta_1^2}{c_{k,l}h_{\text{pca}}^{d/2+2} + C_{k,l}h_{\text{pca}}\beta_1} \right\} + (p-d)^2 \exp \left\{ -\frac{(n-1)\beta_2^2}{c_{k,l}h_{\text{pca}}^{d/2+4} + C_{k,l}h_{\text{pca}}^2\beta_2} \right\} \right. \\ \left. + p(p-d) \exp \left\{ -\frac{(n-1)\beta_3^2}{c_{k,l}h_{\text{pca}}^{d/2+3} + C_{k,l}h_{\text{pca}}^{3/2}\beta_3} \right\} \right) \geq 1 - 1/n^2. \quad (6.19)$$

As a result, when conditional on $\Omega_{n,\beta_1,\beta_2,\beta_3}$ and a proper chosen h_{pca} , that is, $h_{\text{pca}} = O(n^{-2/(d+2)})$ [33, Theorem B.1], we have

$$O_i^T \iota_* X(x) = Q_i^T \iota_* X(x_i) + h_{\text{pca}}^{3/2} b_1 \iota_* X(x_i), \quad (6.20)$$

where $b_1 : \mathbb{R}^p \rightarrow \mathbb{R}^d$ is a bounded operator.

With the above probability control of $\Omega_{n,\beta_1,\beta_2,\beta_3}$, by [33, (B.76)], when conditional on $\Omega_{n,\beta_1,\beta_2,\beta_3}$, we have

$$O_i^T O_i = Q_i^T Q_i + (h^{3/2} + h_{\text{pca}}^{3/2}) b_2, \quad (6.21)$$

and hence [33, Theorem B.2]

$$\iota_*^T O_i O_{ij} B_i^T X(x_j) = \parallel_j^i X(x_j) + (h^{3/2} + h_{\text{pca}}^{3/2}) \tilde{b}_3 X(x_j), \quad (6.22)$$

where $b_2 : \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $\tilde{b}_3 : T_{x_j} \mathbf{M} \rightarrow T_{x_i} \mathbf{M}$ are bounded operators. It is shown in [33] that h_{pca} should be chosen so that $h_{\text{pca}}/h \rightarrow 0$ as $h \rightarrow 0$, we could combine the error introduced by local PCA step with the error introduced by parallel transport estimate, and obtain

$$\iota_*^T O_i O_{ij} B_i^T X(x_j) = \parallel_j^i X(x_j) + h^{3/2} b_3 X(x_j), \quad (6.23)$$

where $b_3 = 2\tilde{b}_3$. We emphasize that both O_i and O_{ij} are random in nature, and they are dependent to some extent. When conditional on $\Omega_{n,\beta_1,\beta_2,\beta_3}$, the randomness is bounded and we are able to proceed.

Define operators $Q_{\mathcal{X}}^T : TM_{\mathcal{X}} \rightarrow V_{\mathcal{X}}$ and $Q_{\mathcal{X}} : V_{\mathcal{X}} \rightarrow TM_{\mathcal{X}}$ by

$$Q_{\mathcal{X}} \mathbf{v} := [\iota_*^T Q_1^T \mathbf{v}[1], \dots, \iota_*^T Q_n^T \mathbf{v}[n]] \in TM_{\mathcal{X}}, \\ Q_{\mathcal{X}}^T \mathbf{w} := [(Q_1 \iota_* \mathbf{w}[1])^T, \dots, (Q_n \iota_* \mathbf{w}[n])^T]^T \in V_{\mathcal{X}}, \quad (6.24)$$

where $\mathbf{w} \in TM_{\mathcal{X}}$ and $\mathbf{v} \in V_{\mathcal{X}}$.

Note that $Q_{\mathcal{X}}^T D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} X$ is exactly the same as $B_{\mathcal{X}}^T D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} X$, so its behavior has been understood in Theorem 5.4. Therefore, if we can control the difference between $Q_{\mathcal{X}}^T D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} X$ and $O_{\mathcal{X}}^T D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}^O X$, where $\mathbf{S}_{h,\alpha,n}$ is defined in (4.3) when the frame bundle information can be fully accessed, by some modification of the proof of Theorem 5.4, we can conclude the theorem. By Lemma C1, we know that conditional on the event space Ω_{ρ} , which has probability higher than $1 - 1/n^2$, we have

$\widehat{p}_{h,n} > p_m/4$. Thus, while conditional on $\Omega_{n,\beta_1,\beta_2,\beta_3} \cap \Omega_p$, by (6.23), for all $i = 1, \dots, n$,

$$\begin{aligned} \left| Q_{\mathcal{X}}^T D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X}[i] - O_{\mathcal{X}}^T D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n}^O \mathbf{X}[i] \right| &= \left| \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) (\|j^i - \iota_*^T O_i O_{ij} B_j^T) X(x_j) \right| \\ &= h^{3/2} \left| \frac{1}{n} \sum_{j=1}^n \widehat{M}_{h,\alpha,n}(x_i, x_j) b_3 X(x_j) \right| = O(h^{3/2}), \end{aligned} \quad (6.25)$$

where the last inequality holds due to the fact that $\widehat{p}_{h,n} > p_m/4$ and $O(h^{3/2})$ depends on $\|X\|_{L^\infty}$. As a result, when conditional on $\Omega_{n,\beta_1,\beta_2,\beta_3} \cap \Omega_p$, the error introduced by the frame bundle estimation is of order high enough so that the object of interest, the connection Laplacian, is not influenced if we focus on a proper subspace of $L^2(\mathcal{E})$ depending on h .

Step 2: Spectral convergence

Based on the analysis on Step 1, when conditional on $\Omega_{n,\beta_1,\beta_2,\beta_3} \cap \Omega_p$, we can directly study $Q_{\mathcal{X}}^T D_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X}$ with the price of a negligible error. Clearly all steps in the proof of Theorem 5.4 hold for $Q_{\mathcal{X}}^T D_{h,1,n}^{-1} \mathbf{S}_{h,1,n}$. As a result, conditional on $\Omega_{n,\beta_1,\beta_2,\beta_3} \cap \Omega_p$, by the perturbation theory, the eigenvectors of $O_{\mathcal{X}}^T D_{h,1,n}^{-1} \mathbf{S}_{h,1,n}^O$ is deviated from the eigenvectors of $Q_{\mathcal{X}}^T D_{h,1,n}^{-1} \mathbf{S}_{h,1,n}$ by an error of order $h^{3/2}$, and we have finished the proof. \square

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REFERENCES

1. ARIAS-CASTRO, E., LERMAN, G. & ZHANG, T. (2014) Spectral clustering based on local PCA. arXiv:1301.2007.
2. BANDEIRA, A. S., SINGER, A. & SPIELMAN, D. A. (2013) A cheeger inequality for the graph connection Laplacian. *SIAM J. Matrix Anal. Appl.*, **34**, 1611–1630.
3. BELKIN, M. & NIYOGI, P. (2003) Laplacian eigenmaps for dimensionality reduction and data representation. *Neural Comput.*, **15**, 1373–1396.
4. BELKIN, M. & NIYOGI, P. (2005) Towards a theoretical foundation for Laplacian-based manifold methods. *Proceedings of the 18th Conference on Learning Theory (COLT)* (A. Peter and M. Ron eds). Bertinoro, Italy: COLT, pp. 486–500.
5. BELKIN, M. & NIYOGI, P. (2007) Convergence of Laplacian eigenmaps, vol. 19. *Proceedings of the 2006 Conference on Advances in Neural Information Processing Systems*. Cambridge, MA, USA: The MIT Press, p. 129.
6. BÉRARD, P., BESSON, G. & GALLOT, S. (1994) Embedding Riemannian manifolds by their heat kernel. *Geom. Funct. Anal.*, **4**, 373–398.

7. BERLINE, N., GETZLER, E. & VERGNE, M. (2004) *Heat Kernels and Dirac Operators*. Berlin: Springer.
8. BISHOP, R. L. & CRITTENDEN, R. J. (2001) *Geometry of Manifolds*. Providence, RI: American Mathematical Society.
9. CHATELIN, F. (2011) *Spectral Approximation of Linear Operators*. Philadelphia: SIAM.
10. CHENG, M.-Y. & WU, H.-T. (2013) Local linear regression on manifolds and its geometric interpretation. *J. Am. Stat. Assoc.*, **108**, 1421–1434.
11. COIFMAN, R. R. & LAFON, S. (2006) Diffusion maps. *Appl. Comput. Harmon. Anal.*, **21**, 5–30.
12. DSILVA, C. J., LIM, B., LU, H., SINGER, A., KEVREKIDIS, I. G. & SHVARTSMAN, S. Y. (2015) Temporal ordering and registration of images in studies of developmental dynamics. *Development*, **142**, 1717–1724.
13. DUNFORD, N. & SCHWARTZ, J. T. (1958) *Linear Operators*, vol. 1. New York: Wiley-Interscience.
14. EL KAROUI, N. & WU, H.-T. (2015) Connection graph Laplacian methods can be made robust to noise. *Ann. Stat.*, **44**, 346–372.
15. FRANK, J. (2006) *Three-Dimensional Electron Microscopy of Macromolecular Assemblies: Visualization of Biological Molecules in their Native State*, 2nd edn. New York: Oxford University Press.
16. GILKEY, P. (1974) *The Index Theorem and the Heat Equation*. Princeton: Princeton University Press.
17. GINÉ, E. & KOLTCHINSKII, V. (2006) Empirical graph Laplacian approximation of Laplace–Beltrami operators: large sample results. *IMS Lecture Notes* (A. Bonato & J. Janssen eds), vol. 51. Monograph Series. Beachwood, Ohio, USA: The Institute of Mathematical Statistics, pp. 238–259.
18. GONG, D., ZHAO, X. & MEDIONI, G. (2012) Robust multiple manifolds structure learning. *Proceedings of the 29th International Conference on Machine Learning (ICML-12)* (J. Langford and J. Pineau eds). New York, NY, USA: Omnipress, pp. 321–328.
19. HADANI, R. & SINGER, A. (2011) Representation theoretic patterns in three-dimensional cryo-electron microscopy II: the class averaging problem. *Found. Comput. Math.*, **11**, 589–616.
20. HEIN, M., AUDIBERT, J. & VON LUXBURG, U. (2005) From graphs to manifolds—weak and strong pointwise consistency of graph Laplacians. *Proceedings of the 18th Conference on Learning Theory (COLT)* (P. Auer and R. Meir eds). Heidelberg: Springer-Verlag Berlin, pp. 470–485.
21. HUETTEL, S. A., SONG, A. W. & MCCARTHY, G. (2008) *Functional Magnetic Resonance Imaging*, 2nd edn. Sunderland, MA: Sinauer Associates.
22. KASLOVSKY, D. & MEYER, F. (2014) Non-Asymptotic analysis of tangent space perturbation. *Inf. Inference*, **3**, 134–187.
23. LIN, C.-Y., MINASIAN, A., & WU, H.-T. (2016) Vector nonlocal median and diffusion on the principal bundle. Submitted.
24. LITTLE, A., JUNG, Y.-M. & MAGGIONI, M. (2009) Multiscale estimation of intrinsic dimensionality of data sets. *Manifold Learning and its Applications: Papers from the AAAI Fall Symposium (FS-09-04)*, pp. 26–33.
25. MARCHESINI, S., TU, Y.-C. & WU, H.-T. (2015) Alternating projection, ptychographic imaging and phase synchronization. *Appl. Comput. Harmon. Anal.*, **41**, 815–851.
26. NASH, J. (1954) C^1 Isometric imbeddings. *Ann. Math.*, **60**, 383–396.
27. NASH, J. (1956) The imbedding problem for Riemannian manifolds. *Ann. Math.*, **63**, 20–63.
28. NIYOGI, P., SMALE, S. & WEINBERGER, S. (2009) *Finding the Homology of Submanifolds with High Confidence from Random Samples*. Twentieth Anniversary Volume. New York: Springer, pp. 1–23.
29. OVSJANIKOV, M., BEN-CHEN, M., SOLOMON, J., BUTSCHER, A. & GUIBAS, L. (2012) Functional maps: a flexible representation of maps between shapes. *ACM Trans. Graphics*, **4**, 30:1–30:11.
30. PALAIS, R. S. (1968) *Foundations of Global Non-linear Analysis*. New York: W.A. Benjamin, Inc.
31. SINGER, A. (2006) From graph to manifold Laplacian: the convergence rate. *Appl. Comput. Harmon. Anal.*, **21**, 128–134.
32. SINGER, A. & WU, H.-T. (2011) Orientability and diffusion map. *Appl. Comput. Harmon. Anal.*, **31**, 44–58.
33. SINGER, A. & WU, H.-T. (2012) Vector diffusion maps and the connection Laplacian. *Comm. Pure Appl. Math.*, **65**, 1067–1144.
34. SINGER, A., ZHAO, Z., SHKOLNISKY, Y. & HADANI, R. (2011) Viewing angle classification of cryo-electron microscopy images using eigenvectors. *SIAM J. Imaging Sci.*, **4**, 723–759.

35. STERNBERG, S. (1999) *Lectures on Differential Geometry*. Providence: American Mathematical Society.
36. VAN DER VAART, A. & WELLNER, J. (1996) *Weak Convergence and Empirical Processes*. New York: Springer.
37. VON LUXBURG, U., BELKIN, M. & BOUSQUET, O. (2008) Consistency of spectral clustering. *Ann. Stat.*, **36**, 555–586.
38. WANG, X., SLAVAKIS, K. & LERMAN, G. (2014) Riemannian multi-manifold modeling. arXiv:1410.0095.
39. WANG, Y., JIANG, Y., WU, Y. & ZHOU, Z.-H. (2011) Spectral clustering on multiple manifolds. *IEEE Trans. Neural Netw.*, **22**, 1149–1161.
40. WU, H.-T. (2017) Embedding Riemannian manifolds by the heat kernel of the connection Laplacian. *Adv. Math.* **304**, 1055–1079.
41. ZHAO, Z. & SINGER, A. (2014) Rotationally invariant image representation for viewing direction classification in Cryo-EM. *J. Struct. Biol.*, **186**, 153–166.

Appendix A. An introduction to principal bundle

In this Appendix, we collect relevant and self-contained facts about the mathematical framework *principal bundle* which are used in the main text. We refer the readers to, for example [7,8], for more general definitions which are not used in this article.

We start from discussing the notion of *group action*, *orbit* and *orbit space*. Consider a set Y and a group G with the identity element e . The left group action of G on Y is a map from $G \times Y$ onto Y

$$G \times Y \rightarrow Y, \quad (g, x) \mapsto g \circ x \quad (\text{A.1})$$

so that $(gh) \circ x = g \circ (h \circ x)$ is satisfied for all $g, h \in G$ and $x \in Y$ and $e \circ x = x$ for all x . The right group action can be defined in the same way. Note that we can construct a right action by composing with the inverse group operation, so in some scenarios it is sufficient to discuss only left actions. There are several types of group action. We call an action *transitive* if for any $x, y \in Y$, there exists a $g \in G$ so that $g \circ x = y$. In other words, under the group action we can jump between any pair of two points on Y , or $Y = G \circ x$ for any $x \in Y$. We call an action *effective* for any $g, h \in G$, there exists x so that $g \circ x \neq h \circ x$. In other words, different group elements induce different permutations of Y . We call an action *free* if $g \circ x = x$ implies $g = e$ for all g . In other words, there is no fixed points under the G action, and hence the name free. If Y is a topological space, we call an action *totally discontinuous* if, for every $x \in Y$, there is an open neighborhood U such that $(g \circ U) \cap U = \emptyset$ for all $g \in G, g \neq e$.

The *orbit* of a point $x \in Y$ is the set

$$Gx := \{g \circ x; g \in G\}. \quad (\text{A.2})$$

The group action induces an equivalence relation. We say $x \sim y$ if and only if there exists $g \in G$ so that $g \circ x = y$ for all pairs of $x, y \in Y$. Clearly the set of orbits form a partition of Y , and we denote the set of all orbits as Y/\sim or Y/G . We can thus define a projection map π by

$$Y \rightarrow Y/G, \quad x \mapsto Gx. \quad (\text{A.3})$$

We call Y the *total space* or the *left G -space*, G the *structure group*, Y/G the *quotient space*, the *base space* or the *orbit space* of Y under the action of G and π the *canonical projection*.

We define a principal bundle as a special G -space which satisfies more structure. Note that the definitions given here are not the most general ones, but are enough for our purpose.

DEFINITION A1 (Fiber bundle) Let \mathcal{F} and \mathbf{M} be two smooth manifolds and π a smooth map from \mathcal{F} to \mathbf{M} . We say that \mathcal{F} is a *fiber bundle* with fiber F over \mathbf{M} if there is an open covering of \mathbf{M} , denoted as

$\{U_i\}$, and diffeomorphisms $\{\psi_i : \pi^{-1}(U_i) \rightarrow U_i \times F\}$ so that $\pi : \pi^{-1}(U_i) \rightarrow U_i$ is the composition of ψ_i with projection onto U_i .

By definition, $\pi^{-1}(x)$ is diffeomorphic to F for all $x \in \mathbf{M}$. We call \mathcal{F} the total space of the fiber bundle, \mathbf{M} is the base space, π the canonical projection, and F the fiber of \mathcal{F} . With the above algebraic setup, in a nutshell, the principal bundle is a special fiber bundle accompanied by a group action.

DEFINITION A2 (Principal bundle) Let \mathbf{M} be a smooth manifold and G a Lie group. A *principal bundle over \mathbf{M} with structure group G* is a fiber bundle $P(\mathbf{M}, G)$ with fiber diffeomorphic to G , a smooth right action of G , denoted as \circ , on the fibers and a canonical projection $\pi : P \rightarrow \mathbf{M}$ so that

1. π is smooth and $\pi(g \circ p) = \pi(p)$ for all $p \in P$ and $g \in G$;
2. G acts freely and transitively;
3. the diffeomorphism $\psi_i : \pi^{-1}(U_i) \rightarrow U_i \times G$ satisfies $\psi_i(p) = (\pi(p), \phi_i(p)) \in U_i \times G$ such that $\phi_i : \pi^{-1}(U_i) \rightarrow G$ satisfying $\phi_i(pg) = \phi_i(p)g$ for all $p \in \pi^{-1}(U_i)$ and $g \in G$.

Note that $\mathbf{M} = P(\mathbf{M}, G)/G$, where the equivalence relation is induced by G . From the view point of orbit space, $P(\mathbf{M}, G)$ is the total space, G is the structure group and \mathbf{M} is the orbit space of $P(\mathbf{M}, G)$ under the action of G . Intuitively, $P(\mathbf{M}, G)$ is composed of a bunch of sets diffeomorphic to G , all of which are pulled together under some rules.⁵ We give some examples here:

EXAMPLE A3 Consider $P(\mathbf{M}, G) = \mathbf{M} \times G$ so that G acts by $g \circ (x, h) = (x, hg)$ for all $(x, h) \in \mathbf{M} \times G$ and $g \in G$. We call such principal bundle *trivial*. In particular, when $G = \{e\}$, the trivial group, $P(\mathbf{M}, \{e\})$ is the principal bundle, which we choose to unify the graph Laplacian and diffusion map.

EXAMPLE A4 A particular important example of the principal bundle is the *frame bundle*, denoted as $GL(\mathbf{M})$, which is the principal $GL(d, \mathbb{R})$ -bundle with the base manifold a d -dimensional/dimensional smooth manifold \mathbf{M} . We construct $GL(\mathbf{M})$ for the purpose of completeness. Denote B_x to be the set of bases of the tangent space $T_x\mathbf{M}$, that is, $B_x \cong GL(d, \mathbb{R})$ and $u_x \in B_x$ is a basis of $T_x\mathbf{M}$. Let $GL(\mathbf{M})$ be the set consisting of all bases at all points of \mathbf{M} , that is, $GL(\mathbf{M}) := \{u_x; u_x \in B_x, x \in \mathbf{M}\}$. Let $\pi : GL(\mathbf{M}) \rightarrow \mathbf{M}$ by $u_x \mapsto x$ for all $u_x \in B_x$ and $x \in \mathbf{M}$. Define the right $GL(d, \mathbb{R})$ action on $GL(\mathbf{M})$ by $g \circ u_x = v_x$, where $g = [g_{ij}]_{i,j=1}^d \in GL(d, \mathbb{R})$, $u_x = (X_1, \dots, X_d) \in B_x$ and $v_x = (Y_1, \dots, Y_d) \in B_x$ with $Y_i = \sum_{j=1}^d g_{ij}X_j$. By a direct calculation, $GL(d, \mathbb{R})$ acts on $GL(\mathbf{M})$ from the right freely and transitively, and $\pi(g \circ u_x) = \pi(u_x)$. In a coordinate neighborhood U , $\pi^{-1}(U)$ is 1–1 corresponding with $U \times GL(d, \mathbb{R})$, which induces a differentiable structure on $GL(\mathbf{M})$. Thus $GL(\mathbf{M})$ is a principal $GL(d, \mathbb{R})$ -bundle.

EXAMPLE A5 Another important example is the *orientation principal bundle*, which we choose to unify the orientable diffusion map. The construction is essentially the same as that of the frame bundle. First, let $P(\mathbf{M}, O(1))$ be the set of all orientations at all points of \mathbf{M} and let π be the canonical projection from $P(\mathbf{M}, O(1))$ to \mathbf{M} , where $O(1) \cong \mathbb{Z}_2 \cong \{1, -1\}$. In other words, $P(\mathbf{M}, O(1)) := \{u_x; u_x \in \{1, -1\}, x \in \mathbf{M}\}$, where \mathbb{Z}_2 stands for the possible orientation of each point x . The $O(1) \cong \{1, -1\}$ group acts on $P(\mathbf{M}, O(1))$ simply by $u \rightarrow ug$, where $u \in P(\mathbf{M}, O(1))$ and $g \in \{1, -1\}$. The differentiable structure in $P(\mathbf{M}, O(1))$ is introduced in the following way. Take (x^1, \dots, x^d) as a local coordinate system in a coordinate neighborhood U in \mathbf{M} . Since \mathbb{Z}_2 is a discrete group, we take $\pi^{-1}(U)$ as two disjoint sets

⁵ These rules are referred to as *transition functions*.

$U \times \{1\}$ and $U \times \{-1\}$ and take (x^1, \dots, x^d) as their coordinate systems. Clearly $P(\mathbf{M}, O(1))$ is a principal fiber bundle and we call it the orientation principal bundle.

If we are given a left G -space F , we can form a *fiber bundle* from $P(\mathbf{M}, G)$ so that its fiber is diffeomorphic to F and its base manifold is \mathbf{M} in the following way. By denoting the left G action on F by \cdot , we have

$$\mathcal{E}(P(\mathbf{M}, G), \cdot, F) := P(\mathbf{M}, G) \times_G F := P(\mathbf{M}, G) \times F/G, \quad (\text{A.4})$$

where the equivalence relation is defined as

$$(g \circ p, g^{-1} \cdot f) \sim (p, f) \quad (\text{A.5})$$

for all $p \in P(\mathbf{M}, G)$, $g \in G$ and $f \in F$. The canonical projection from $\mathcal{E}(P(\mathbf{M}, G), \cdot, F)$ to \mathbf{M} is denoted as $\pi_{\mathcal{E}}$:

$$\pi_{\mathcal{E}} : (p, f) \mapsto \pi(p), \quad (\text{A.6})$$

for all $p \in P(\mathbf{M}, G)$ and $f \in F$. We call $\mathcal{E}(P(\mathbf{M}, G), \cdot, F)$ the *fiber bundle associated with $P(\mathbf{M}, G)$ with standard fiber F* or the *associated fiber bundle* whose differentiable structure is induced from \mathbf{M} . Given $p \in P(\mathbf{M}, G)$, denote pf to be the image of $(p, f) \in P(\mathbf{M}, G) \times F$ onto $\mathcal{E}(P(\mathbf{M}, G), \cdot, F)$. By definition, p is a diffeomorphism from F to $\pi_{\mathcal{E}}^{-1}(\pi(p))$ and

$$(g \circ p)f = p(g \cdot f). \quad (\text{A.7})$$

Note that the associated fiber bundle $\mathcal{E}(P(\mathbf{M}, G), \cdot, F)$ is a special fiber bundle and its fiber is diffeomorphic to F . When there is no danger of confusion, we denote $\mathcal{E} := \mathcal{E}(P(\mathbf{M}, G), \cdot, F)$ to simply the notation.

EXAMPLE A6 When $F = V$ is a vector space and the left G action on F is a linear representation, the associated fiber bundle is called the *vector bundle associated with the principal bundle $P(\mathbf{M}, G)$ with fiber V* , or simply called the *vector bundle* if there is no danger of confusion. For example, take $F = \mathbb{R}^q$, denote ρ to be a representation of G into $GL(q, \mathbb{R})$ and assume G acts on \mathbb{R}^q via the representation ρ . A particular example of interest is the tangent bundle $T\mathbf{M} := \mathcal{E}(P(\mathbf{M}, GL(d, \mathbb{R})), \rho, \mathbb{R}^d)$, when \mathbf{M} is a d -dimensional smooth manifold and the representation ρ is identity. The practical meaning of the frame bundle and its associated tangent bundle is change of coordinate. That is, if we view a point $u_x \in GL(\mathbf{M})$ as the basis of the fiber $T_x\mathbf{M}$, where $x = \pi(u_x)$, then the coordinate of a point on the tangent plane $T_x\mathbf{M}$ changes, that is, $v_x \rightarrow g \cdot v_x$ where $g \in GL(d, \mathbb{R})$ and $v_x \in \mathbb{R}^d$, according to the changes of the basis, that is, $g \rightarrow g \circ u_x$. Also notice that we can view a basis of $T_x\mathbf{M}$ as an invertible linear map from \mathbb{R}^d to $T_x\mathbf{M}$ by definition. Indeed, if we take $e_i, i = 1, \dots, d$ to be the natural basis of \mathbb{R}^d ; that is, e_i is the unit vector with 1 in the i th entry, a linear frame $u_x = (X_1, \dots, X_d)$ at x can be viewed as a linear mapping $u_x : \mathbb{R}^d \rightarrow T_x\mathbf{M}$ such that $u_x e_i = X_i, i = 1, \dots, d$.

A (global) *section* of a fiber bundle \mathcal{E} with fiber F over \mathbf{M} is a map

$$s : \mathbf{M} \rightarrow \mathcal{E} \quad (\text{A.8})$$

so that $\pi(s(x)) = x$ for all $x \in \mathbf{M}$. We denote $\Gamma(\mathcal{E})$ to be the set of sections; $C^l(\mathcal{E})$ to be the space of all sections with the l th regularity, where $l \geq 0$. An important property of the principal bundle is that a principal bundle is trivial if and only if $C^0(P(\mathbf{M}, G)) \neq \emptyset$. In other words, all sections on a non-trivial principal bundle are discontinuous. On the other hand, there always exists a continuous section on the associated vector bundle \mathcal{E} .

Let V be a vector space. Denote $GL(V)$ to be the group of all invertible linear maps on V . If V comes with an inner product, then define $O(V)$ to be the group of all orthogonal maps on V with related to the inner product. From now on we focus on the vector bundle, with fiber being a vector space V and the action \cdot being a representation $\rho : G \rightarrow GL(V)$, that is, $\mathcal{E}(P(\mathbf{M}, G), \rho, V)$.

To introduce the notion of *covariant derivative* on the vector bundle \mathcal{E} , we have to introduce the notion of *connection*. Note that the fiber bundle \mathcal{E} is a manifold. Denote $T\mathcal{E}$ to be the tangent bundle of \mathcal{E} and $T^*\mathcal{E}$ to be the cotangent bundle of \mathcal{E} . We call a tangent vector X on \mathcal{E} *vertical* if it is tangential to the fibers; that is, $X(\pi_*f) = 0$ for all $f \in C^\infty(\mathbf{M})$. Note that π_*f is a function defined on \mathcal{E} which is constant on each fiber, so we call X vertical when $X(\pi_*f) = 0$ for all $f \in C^\infty(\mathbf{M})$. Denote the bundle of vertical vectors as $V\mathcal{E}$, which is referred to as *the vertical bundle*, and is a subbundle of $T\mathcal{E}$. We call a vector field vertical if it is a section of the vertical bundle. Clearly the quotient of $T\mathcal{E}$ by its subbundle $V\mathcal{E}$ is isomorphic to π^*TM , and hence we have a short exact sequence of vector bundles:

$$0 \rightarrow V\mathcal{E} \rightarrow T\mathcal{E} \rightarrow \pi^*TM \rightarrow 0. \quad (\text{A.9})$$

However, there is no canonical splitting of this short exact sequence. A chosen splitting is called a *connection*. In other words, a connection is a G -invariant distribution $H \subset T\mathcal{E}$ complementary to $V\mathcal{E}$.

DEFINITION A7 (Connection 1-form) Let $P(\mathbf{M}, G)$ be a principal bundle. A connection 1-form on $P(\mathbf{M}, G)$ is a \mathfrak{g} -valued 1-form $\omega \in \Gamma(T^*P(\mathbf{M}, G) \otimes VP(\mathbf{M}, G))$ so that $\omega(X) = X$ for any $X \in \Gamma(VP(\mathbf{M}, G))$ and is invariant under the action of G . The kernel of ω is called the *horizontal bundle* and is denoted as $HP(\mathbf{M}, G)$.

Note that $HP(\mathbf{M}, G)$ is isomorphic to π^*TM . Clearly, a connection 1-form determines a splitting of (A.9), or the connection on $P(\mathbf{M}, G)$. In other words, as a linear subspace, the horizontal subspace $H_pP(\mathbf{M}, G) \subset T_pP(\mathbf{M}, G)$ is cut out by $\dim G$ linear equations defined on $T_pP(\mathbf{M}, G)$.

We call a section X_p of $HP(\mathbf{M}, G)$ a *horizontal vector field*. Given $X \in \Gamma(TM)$, we say that X_p is the *horizontal lift* with respect to the connection on $P(\mathbf{M}, G)$ of X if $X = \pi_*X_p$. Given a smooth curve $\tau := c(t)$, $t \in [0, 1]$ on \mathbf{M} and a point $u(0) \in P(\mathbf{M}, G)$, we call a curve $\tau^* = u(t)$ on $P(\mathbf{M}, G)$ the (*horizontal*) *lift* of $c(t)$ if the vector tangent to $u(t)$ is horizontal and $\pi(u(t)) = c(t)$ for $t \in [0, 1]$. The existence of τ^* is an important property of the connection theory. We call $u(t)$ the *parallel displacement* of $u(0)$ along the curve τ on \mathbf{M} .

With the connection on $P(\mathbf{M}, G)$, the connection on an associated vector bundle \mathcal{E} with fiber V is determined. As a matter of fact, we define the connection, or $H\mathcal{E}$, to be the image of $HP(\mathbf{M}, G)$ under the natural projection $P(\mathbf{M}, G) \times V \rightarrow \mathcal{E}(P(\mathbf{M}, G), \rho, V)$. Similarly, we call a section $X_\mathcal{E}$ of $H\mathcal{E}$ a *horizontal vector field*. Given $X \in \Gamma(TM)$, we say that $X_\mathcal{E}$ is the *horizontal lift* with respect to the connection on \mathcal{E} of X if $X = \pi_{\mathcal{E}*}X_\mathcal{E}$. Given a smooth curve $c(t)$, $t \in [0, 1]$ on \mathbf{M} and a point $v_0 \in \mathcal{E}$, we call a curve v_t on \mathcal{E} the (*horizontal*) *lift* of $c(t)$ if the vector tangent to v_t is horizontal and $\pi_\mathcal{E}(v_t) = c(t)$ for $t \in [0, 1]$. The existence of such horizontal lift holds in the same way as that of the principal bundle. We call v_t the *parallel displacement* of v_0 along the curve τ on \mathbf{M} . Note that we have interest in this connection on the vector bundle since it leads to the *covariant derivative* we have interest.

DEFINITION A8 (Covariant derivative) Take a vector bundle \mathcal{E} associated with the principal bundle $P(\mathbf{M}, G)$ with fiber V . The covariant derivative $\nabla^{\mathcal{E}}$ of a smooth section $X \in C^1(\mathcal{E})$ at $x \in \mathbf{M}$ in the direction \dot{c}_0 is defined as

$$\nabla_{\dot{c}_0}^{\mathcal{E}} X = \lim_{h \rightarrow 0} \frac{1}{h} [\parallel_{c(h)}^{c(0)} X(c(h)) - X(x)], \quad (\text{A.10})$$

where $c : [0, 1] \rightarrow \mathbf{M}$ is a curve on \mathbf{M} so that $c(0) = x$ and $\parallel_{c(h)}^{c(0)}$ denotes the parallel displacement of X from $c(h)$ to $c(0)$.

Note that in general, although all fibers of \mathcal{E} are isomorphic to V , the notion of comparison among them is not provided. An explicit example demonstrating the derived problem is given in the appendix of [33]. However, with the parallel displacement based on the notion of connection, we are able to compare among fibers, and hence define the derivative. With the fact that

$$\parallel_{c(h)}^{c(0)} X(c(h)) = u(0)u(h)^{-1}X(c(h)), \quad (\text{A.11})$$

where $u(h)$ is the horizontal lift of $c(h)$ to $P(\mathbf{M}, G)$ so that $\pi(u(0)) = x$, the covariant derivative (A.10) can be represented in the following format:

$$\nabla_{\dot{c}_0}^{\mathcal{E}} X = \lim_{h \rightarrow 0} \frac{1}{h} [u(0)u(h)^{-1}(X(c(h))) - X(c(0))], \quad (\text{A.12})$$

which is independent of the choice of $u(0)$. To show (A.11), set $v := u(h)^{-1}(X(c(h))) \in V$. Clearly $u(t)(v)$, $t \in [0, h]$, is a horizontal curve in \mathcal{E} by definition. It implies that $u(0)v = u(0)u(h)^{-1}(X(c(h)))$ is the parallel displacement of $X(c(h))$ along $c(t)$ from $c(h)$ to $c(0)$. Thus, although the covariant derivatives defined in (A.10) and (A.12) are different in their appearances, they are actually equivalent. We can understand this definition in the frame bundle $GL(\mathbf{M}^d)$ and its associated tangent bundle. First, we find the coordinate of a point on the fiber $X(c(h))$, which is denoted as $u(h)^{-1}(X(c(h)))$, and then we put this coordinate $u(h)^{-1}(X(c(h)))$ to $x = c(0)$ and map it back to the fiber $T_x \mathbf{M}$ by the basis $u(0)$. In this way we can compare two different ‘abstract fibers’ by comparing their coordinates. A more abstract definition of the covariant derivative, yet equivalent to the above, is the following. A covariant derivative of \mathcal{E} is a differential operator

$$\nabla^{\mathcal{E}} : C^\infty(\mathcal{E}) \rightarrow C^\infty(T^* \mathbf{M} \otimes \mathcal{E}) \quad (\text{A.13})$$

so that the Leibniz’s rule is satisfied, that is, for $X \in C^\infty(\mathcal{E})$ and $f \in C^\infty(\mathbf{M})$, we have

$$\nabla^{\mathcal{E}}(fX) = df \otimes X + f \nabla^{\mathcal{E}} X, \quad (\text{A.14})$$

where d is the exterior derivative on \mathbf{M} . Denote $\Lambda^k T^* M$ (resp $\Lambda T^* M$) to be the bundle of k th exterior differentials (resp. the bundle of exterior differentials), where $k \geq 1$. Given two vector bundles \mathcal{E}_1 and \mathcal{E}_2 on M with the covariant derivatives $\nabla^{\mathcal{E}_1}$ and $\nabla^{\mathcal{E}_2}$, we construct a covariant derivative on $\mathcal{E}_1 \otimes \mathcal{E}_2$ by

$$\nabla^{\mathcal{E}_1 \otimes \mathcal{E}_2} := \nabla^{\mathcal{E}_1} \otimes 1 + 1 \otimes \nabla^{\mathcal{E}_2}. \quad (\text{A.15})$$

A fiber metric $g^{\mathcal{E}}$ in a vector bundle \mathcal{E} is a positive-definite inner-product in each fiber V that varies smoothly on \mathbf{M} . For any \mathcal{E} , if \mathbf{M} is paracompact, $g^{\mathcal{E}}$ always exists. A connection in $P(\mathbf{M}, G)$, and also its associated vector bundle \mathcal{E} , is called metric if

$$dg^{\mathcal{E}}(X_1, X_2) = g^{\mathcal{E}}(\nabla^{\mathcal{E}} X_1, X_2) + g^{\mathcal{E}}(X_1, \nabla^{\mathcal{E}} X_2), \quad (\text{A.16})$$

for all $X_1, X_2 \in C^\infty(\mathcal{E})$. We mainly focus on metric connection in this work. It is equivalent to say that the parallel displacement of \mathcal{E} preserves the fiber metric. An important fact about the metric connection is that if a connection on $P(\mathbf{M}, G)$ is metric, given a fiber metric $g^{\mathcal{E}}$, then the covariant derivative on the associated vector bundle \mathcal{E} can be equally defined from a sub-bundle $Q(\mathbf{M}, H)$ of $P(\mathbf{M}, G)$, which is defined as

$$Q(\mathbf{M}, H) := \{p \in P(\mathbf{M}, G) : g^{\mathcal{E}}(p(u), p(v)) = (u, v)\}, \quad (\text{A.17})$$

where (\cdot, \cdot) is an inner product on V and the structure group H is a closed subgroup of G . In other words, $p \in Q(\mathbf{M}, H)$ is a linear map from V to $\pi_{\mathcal{E}}^{-1}(\pi(p))$ which preserves the inner product. A direct verification shows that the structure group of $Q(\mathbf{M}, H)$ is

$$H := \{g \in G : \rho(g) \in O(V)\} \subset G. \quad (\text{A.18})$$

Since orthogonal property is needed in our analysis, when we work with a metric connection on a principal bundle $P(\mathbf{M}, G)$ given a fiber metric $g^{\mathcal{E}}$ on $\mathcal{E}(P(\mathbf{M}, G), \rho, V)$, we implicitly assume we work with its sub bundle $Q(\mathbf{M}, H)$. With the covariant derivative, we now define the connection Laplacian. Assume \mathbf{M} is a d -dimensional/dimensional smooth Riemannian manifold with the metric g . With the metric g we have an induced measure on M , denoted as dV .⁶ Denote $L^p(\mathcal{E})$, $1 \leq p < \infty$ to be the set of L^p integrable sections, that is, $X \in L^p(\mathcal{E})$ if and only if

$$\int |g_x^{\mathcal{E}}(X(x), X(x))|^{p/2} dV(x) < \infty. \quad (\text{A.19})$$

Denote \mathcal{E}^* to be the dual bundle of \mathcal{E} , which is paired with \mathcal{E} by $g^{\mathcal{E}}$, that is, the pairing between \mathcal{E} and \mathcal{E}^* is $\langle X, Y \rangle := g^{\mathcal{E}}(X, Y)$, where $X \in C^\infty(\mathcal{E})$ and $Y \in C^\infty(\mathcal{E}^*)$. The connection on the dual bundle \mathcal{E}^* is thus defined by

$$d\langle X, Y \rangle = g^{\mathcal{E}}(\nabla^{\mathcal{E}} X, Y) + g^{\mathcal{E}}(X, \nabla^{\mathcal{E}^*} Y). \quad (\text{A.20})$$

Recall that the Riemannian manifold (M, g) possesses a canonical connection referred to as the Levi-Civita connection ∇ [7, p. 31]. Based on ∇ , we define the connection $\nabla^{T^*M \otimes \mathcal{E}}$ on the tensor product bundle $T^*M \otimes \mathcal{E}$.

DEFINITION A9 Take the Riemannian manifold (M, g) , the vector bundle $\mathcal{E} := \mathcal{E}(P(\mathbf{M}, G), \rho, V)$ and its connection $\nabla^{\mathcal{E}}$. The connection Laplacian on \mathcal{E} is defined as $\nabla^2 : C^\infty(\mathcal{E}) \rightarrow C^\infty(\mathcal{E})$ by

$$\nabla^2 := -\text{tr}(\nabla^{T^*M \otimes \mathcal{E}} \nabla^{\mathcal{E}}), \quad (\text{A.21})$$

where $\text{tr} : C^\infty(T^*M \otimes T^*M \otimes \mathcal{E}) \rightarrow C^\infty(\mathcal{E})$ by contraction with the metric g .

⁶ To obtain the most geometrically invariant formulations, we may consider the density bundles as is considered in [7, Chapter 2]. We choose not to do that in order to simplify the discussion.

If we take the normal coordinate $\{\partial_i\}_{i=1}^d$ around $x \in \mathbf{M}$, for $X \in C^\infty(\mathcal{E})$, we have

$$\nabla^2 X(x) = - \sum_{i=1}^d \nabla_{\partial_i} \nabla_{\partial_i} X(x). \quad (\text{A.22})$$

Given compactly supported smooth sections $X, Y \in C^\infty(\mathcal{E})$, a direct calculation leads to

$$\begin{aligned} & \text{tr}[\nabla(g^\mathcal{E}(\nabla^\mathcal{E} X, Y))] \\ &= \text{tr}[g^\mathcal{E}(\nabla^{T^*M \otimes \mathcal{E}} \nabla^\mathcal{E} X, Y) + g^\mathcal{E}(\nabla^\mathcal{E} X, \nabla^\mathcal{E} Y)] \\ &= g^\mathcal{E}(\nabla^2 X, Y) + \text{tr} g^\mathcal{E}(\nabla^\mathcal{E} X, \nabla^\mathcal{E} Y). \end{aligned} \quad (\text{A.23})$$

By the divergence theorem, the left-hand side disappears after integration over \mathbf{M} , and we obtain $\nabla^2 = -\nabla^{\mathcal{E}*} \nabla^\mathcal{E}$. Similarly we can show that ∇^2 is self-adjoint. We refer the readers to [16] for further properties of ∇^2 , for example the ellipticity, its heat kernel and its application to the index theorem.

Appendix B. Proof of Theorem 5.2

The proof is a generalization of [33, Theorem B.4] to the general principal bundle structure. Note that in [33, Theorem B.4] dependence of the error terms on a given section is not explicitly shown. In order to prove the spectral convergence, we have to make this dependence explicit. Denote $\tilde{B}_t(x) := \iota^{-1}(B_t^{\mathbb{R}^p}(x) \cap \iota(\mathbf{M}))$, where $t \geq 0$.

LEMMA B1 Assume Assumptions 4.1 and 4.3 hold. Suppose $X \in L^\infty(\mathcal{E})$ and $0 < \gamma < 1/2$. Then, when h is small enough, for all $x \in \mathbf{M}$ the following holds:

$$\left| \int_{\mathbf{M} \setminus \tilde{B}_{h^\gamma}(x)} h^{-d/2} K_h(x, y) \int_y^x X(y) dV(y) \right| = O(h^2), \quad (\text{B.1})$$

where the implied constant in $O(h^2)$ depends on $\|X\|_{L^\infty}$.

Proof. We immediately have

$$\begin{aligned} & \left| \int_{\mathbf{M} \setminus \tilde{B}_{h^\gamma}(x)} h^{-d/2} K_h(x, y) \int_y^x X(y) dV(y) \right| \leq \|X\|_{L^\infty} \left| \int_{\mathbf{M} \setminus \tilde{B}_{h^\gamma}(x)} h^{-d/2} K_h(x, y) dV(y) \right| \\ &= \|X\|_{L^\infty} \left| \int_{s^{d-1}} \int_{h^\gamma}^\infty h^{-d/2} \left[K\left(\frac{t}{\sqrt{h}}\right) + K'\left(\frac{t}{\sqrt{h}}\right) \frac{\|\Pi(\theta, \theta)\| t^3}{24\sqrt{h}} + O\left(\frac{t^6}{h}\right) \right] \right. \\ & \quad \left. \times [t^{d-1} + \text{Ric}(\theta, \theta) t^{d+1} + O(t^{d+2})] dt d\theta \right| \\ &= \|X\|_{L^\infty} \left[\int_{h^{\gamma-1/2}}^\infty K(s) (s^{d-1} + h s^{d+1}) ds + h \int_{h^{\gamma-1/2}}^\infty K'(s) s^{d+2} ds \right] + O(h^2) = O(h^2), \end{aligned} \quad (\text{B.2})$$

where the implied constant in $O(h^2)$ depends on $\|X\|_{L^\infty}$ and the last inequality holds by the fact that K and K' decay exponentially. Indeed, $h^{(d-1)(\gamma-1/2)} e^{-h^{\gamma-1/2}} < h^2$ when h is small enough. \square

We need the next Lemma to handle the points near the boundary. Note that when x is near the boundary, the integral domain is no longer symmetric, so its proof is different from the points away from the boundary. In particular, the first order term cannot be canceled. In order to fully understand the first order term, we have to take care of the possible nonlinearity of the manifold.

LEMMA B2 Assume Assumption 4.1. Take $0 < \gamma < 1/2$ and $x \in \mathbf{M}_{h^\gamma}$. Suppose $\min_{y \in \partial \mathbf{M}} d(x, y) = \tilde{h}$. Fix a normal coordinate $\{\partial_1, \dots, \partial_d\}$ on the geodesic ball $B_{h^\gamma}(x)$ around x so that $x_0 = \exp_x(\tilde{h}\partial_d(x))$. Divide $\exp_x^{-1}(B_{h^\gamma}(x))$ into slices S_η defined by

$$S_\eta = \{(\mathbf{u}, \eta) \in \mathbb{R}^d; \exp_x(\mathbf{u}, \eta) \in B_{h^\gamma}(x), \|(u_1, \dots, u_{d-1}, \eta)\| < h^\gamma\}, \quad (\text{B.3})$$

where $\eta \in [-h^\gamma, h^\gamma]$ and $\mathbf{u} = (u_1, \dots, u_{d-1}) \in \mathbb{R}^{d-1}$; that is, $\exp_x^{-1}(B_{h^\gamma}(x)) = \cup_{\eta \in [-h^\gamma, h^\gamma]} S_\eta \subset \mathbb{R}^d$. Define the symmetrization of S_η by

$$\tilde{S}_\eta := \cap_{i=1}^{d-1} (R_i S_\eta \cap S_\eta), \quad (\text{B.4})$$

where R_i is the reflective operator satisfying $R_i(u_1, \dots, u_i, \dots, u_{d-1}, \eta) = (u_1, \dots, -u_i, \dots, u_{d-1}, \eta)$ and $i = 1, \dots, d-1$. Then, we have

$$\left| \int_{S_\eta} \int_{-h^\gamma}^{h^\gamma} d\eta d\mathbf{u} - \int_{\tilde{S}_\eta} \int_{-h^\gamma}^{h^\gamma} d\eta d\mathbf{u} \right| = O(h^{2\gamma}). \quad (\text{B.5})$$

Proof. Note that in general the slice S_η is not symmetric with related to $(0, \dots, 0, \eta)$, while the symmetrization \tilde{S}_η is. Recall the following relationship [33, (B.23)] when $y = \exp_x(t\theta)$:

$$\partial_l(\exp_x(t\theta)) = \int_x^y \partial_l(x) + \frac{t^2}{6} \int_x^y (\mathcal{R}(\theta, \partial_l(x))\theta) + O(t^3), \quad (\text{B.6})$$

where $\theta \in T_x \mathbf{M}$ is of unit norm and t when t is small enough, which leads to

$$\int_x^{x_0} \partial_l(x) = \partial_l(x_0) + O(\tilde{h}^2), \quad (\text{B.7})$$

for all $l = 1, \dots, d$. Also note that up to error $O(\tilde{h}^3)$, we can express $\partial \mathbf{M} \cap B_{h^\gamma}(x)$ by a homogeneous degree 2 polynomial with variables $\{\int_x^{x_0} \partial_1(x), \dots, \int_x^{x_0} \partial_{d-1}(x)\}$. Thus the difference between \tilde{S}_η and S_η is $O(h^{2\gamma})$ since $\tilde{h} \leq h^\gamma$. \square

Next we elaborate the error term in the kernel approximation.

LEMMA B3 Assume Assumptions 4.1 and 4.3 hold. Take $0 < \gamma < 1/2$. Fix $x \notin \mathbf{M}_{h^\gamma}$ and denote C_x to be the cut locus of x . Take a vector-valued function $F : \mathbf{M} \rightarrow \mathbb{R}^q$, where $q \in \mathbb{N}$ and $F \in C^4(\mathbf{M} \setminus C_x) \cap L^\infty(\mathbf{M})$. Then, when h is small enough, we have

$$\int_{\mathbf{M}} h^{-d/2} K_h(x, y) F(y) dV(y) = F(x) + h \frac{\mu_{1,2}^{(0)}}{d} \left(\frac{\Delta F(x)}{2} + w(x)F(x) \right) + O(h^2), \quad (\text{B.8})$$

where $w(x) = s(x) + \frac{\mu_{1,3}^{(1)}z(x)}{24|S^{d-1}|}$, $s(x)$ is the scalar curvature at x , and $z(x) = \int_{S^{d-1}} \|\Pi(\theta, \theta)\| d\theta$ and the error term depends on $\|F^{(\ell)}\|_{L^\infty}$, where $\ell = 0, 1, \dots, 4$.

Fix $x \in \mathbf{M}_{h^\gamma}$. Then, when h is small enough, we have

$$\int_{\mathbf{M}} h^{-d/2} K_h(x, y) F(y) dV(y) = m_{h,0} F(x) + \sqrt{h} m_{h,1} \nabla_{\partial_d} F(x) + O(h^{2\gamma}), \quad (\text{B.9})$$

where the implied constant in $O(h^{2\gamma})$ depends on $\|F\|_{L^\infty}$, $\|F^{(1)}\|_{L^\infty}$ and $\|F^{(2)}\|_{L^\infty}$ and $m_{h,0}$ and $m_{h,1}$ are of order 1 and defined in (B.12).

Proof. By Lemma B1, we can focus our analysis on $\tilde{\mathbf{B}}_{h^\gamma}(x)$ since F is a section of the trivial bundle. Also, we can view F as q functions defined on \mathbf{M} with the same regularity. Then, the proof is exactly the same as that of [11, Lemma 8], except the explicit dependence of the error term on F . Since the main point is the uniform bound of the third derivative of the embedding function ι and F on \mathbf{M} , we simply list the calculation steps:

$$\begin{aligned} \int_{\tilde{\mathbf{B}}_{h^\gamma}(x)} K_h(x, y) F(y) dV(y) &= \int_{\tilde{\mathbf{B}}_{h^\gamma}(x)} K\left(\frac{\|x - y\|_{\mathbb{R}^p}}{\sqrt{h}}\right) F(y) dV(y) \\ &= \int_{S^{d-1}} \int_0^{h^\gamma} \left[K\left(\frac{t}{\sqrt{h}}\right) + K'\left(\frac{t}{\sqrt{h}}\right) \frac{\|\Pi(\theta, \theta)\| t^3}{24\sqrt{h}} + O\left(\frac{t^6}{h}\right) \right] \\ &\quad \times \left[F(x) + \nabla_\theta F(x) t + \nabla_{\theta, \theta}^2 F(x) \frac{t^2}{2} + \nabla_{\theta, \theta, \theta}^3 F(x) \frac{t^3}{6} + O(t^3) \right] \\ &\quad \times [t^{d-1} + \text{Ric}(\theta, \theta) t^{d+1} + O(t^{d+2})] dt d\theta. \end{aligned} \quad (\text{B.10})$$

By a direct expansion, the regularity assumption and the compactness of \mathbf{M} , we conclude the first part of the proof.

Next, suppose $x \in \mathbf{M}_{h^\gamma}$. By Taylor's expansion and Lemma B2, we obtain

$$\begin{aligned} &\int_{\mathbf{B}_{h^\gamma}(x)} h^{-d/2} K_h(x, y) F(y) dV(y) \\ &= \int_{S_\eta} \int_{-h^\gamma}^{h^\gamma} h^{-d/2} \left[K\left(\frac{\sqrt{\|\mathbf{u}\|^2 + \eta^2}}{\sqrt{h}}\right) + K'\left(\frac{\sqrt{\|\mathbf{u}\|^2 + \eta^2}}{\sqrt{h}}\right) \frac{\|\Pi((\mathbf{u}, \eta), (\mathbf{u}, \eta))\| (\|\mathbf{u}\|^2 + \eta^2)^{3/2}}{24\sqrt{h}} \right. \\ &\quad \left. + O\left(\frac{(\|\mathbf{u}\|^2 + \eta^2)^3}{h}\right) \right] \left(F(x) + \sum_{i=1}^{d-1} u_i \nabla_{\partial_i} F(x) + \eta \nabla_{\partial_d} F(x) + O(\tilde{h}^2) \right) d\eta d\mathbf{u} \\ &= \int_{\tilde{S}_\eta} \int_{-h^\gamma}^{h^\gamma} h^{-d/2} K\left(\frac{\sqrt{\|\mathbf{u}\|^2 + \eta^2}}{\sqrt{h}}\right) \left(F(x) + \sum_{i=1}^{d-1} u_i \nabla_{\partial_i} F(x) + \eta \nabla_{\partial_d} F(x) + O(\tilde{h}^2) \right) d\eta d\mathbf{u} + O(h^{2\gamma}) \\ &= \int_{\tilde{S}_\eta} \int_{-h^\gamma}^{h^\gamma} h^{-d/2} K\left(\frac{\sqrt{\|\mathbf{u}\|^2 + \eta^2}}{\sqrt{h}}\right) \left(F(x) + \eta \nabla_{\partial_d} F(x) + O(\tilde{h}^2) \right) d\eta d\mathbf{u} + O(h^{2\gamma}) \\ &= m_{h,0} F(x) + \sqrt{h} m_{h,1} \nabla_{\partial_d} F(x) + O(h^{2\gamma}), \end{aligned} \quad (\text{B.11})$$

where the third equality holds due to the symmetry of the kernel and

$$\begin{cases} m_{h,0} := \int_{\tilde{S}_\eta} \int_{-h^\gamma}^{h^\gamma} h^{-d/2} K \left(\frac{\sqrt{\|u\|^2 + \eta^2}}{\sqrt{h}} \right) d\eta dx \\ m_{h,1} := \int_{\tilde{S}_\eta} \int_{-h^\gamma}^{h^\gamma} h^{-d/2-1/2} K \left(\frac{\sqrt{\|u\|^2 + \eta^2}}{\sqrt{h}} \right) \eta d\eta dx. \end{cases} \quad (\text{B.12})$$

□

With the above Lemmas, we are able to finish the Proof of Theorem 5.2.

Proof of Theorem 5.2. Take $0 < \gamma < 1/2$. By Lemma B1, we can focus our analysis of the numerator and denominator of $T_{h,\alpha}X$ on $\tilde{B}_{h^\gamma}(x)$, no matter x is away from the boundary or close to the boundary. Suppose $x \notin M_{h^\gamma}$. By Lemma B3, we get

$$\mathbf{p}_h(y) = \mathbf{p}(y) + h \frac{\mu_{1,2}^{(0)}}{d} \left(\frac{\Delta \mathbf{p}(y)}{2} + w(y)\mathbf{p}(y) \right) + O(h^{3/2}), \quad (\text{B.13})$$

which leads to

$$\frac{\mathbf{p}(y)}{p_h^\alpha(y)} = \mathbf{p}^{1-\alpha}(y) \left[1 - \alpha h \frac{\mu_{1,2}^{(0)}}{d} \left(w(y) + \frac{\Delta \mathbf{p}(y)}{2\mathbf{p}(y)} \right) \right] + O(h^{3/2}). \quad (\text{B.14})$$

Plug (B.14) into the numerator of $T_{h,\alpha}X(x)$:

$$\begin{aligned} & \int_{\tilde{B}_{h^\gamma}(x)} K_{h,\alpha}(x, y) \mathbb{I}_y^x X(y) \mathbf{p}(y) dV(y) \\ &= \mathbf{p}_h^{-\alpha}(x) \int_{\tilde{B}_{h^\gamma}(x)} K_h(x, y) \mathbb{I}_y^x X(y) \mathbf{p}_h^{-\alpha}(y) \mathbf{p}(y) dV(y) \\ &= \mathbf{p}_h^{-\alpha}(x) \int_{\tilde{B}_{h^\gamma}(x)} K_h(x, y) \mathbb{I}_y^x X(y) \mathbf{p}^{1-\alpha}(y) \left[1 - \alpha h \frac{\mu_{1,2}^{(0)}}{d} \left(w(y) + \frac{\Delta \mathbf{p}(y)}{2\mathbf{p}(y)} \right) \right] dV(y) + O(h^{d/2+3/2}) \\ &:= \mathbf{p}_h^{-\alpha}(x) \left(A - h \frac{\alpha \mu_{1,2}^{(0)}}{d} B \right) + O(h^{d/2+3/2}), \end{aligned} \quad (\text{B.15})$$

where

$$\begin{cases} A := \int_{\tilde{B}_{h^\gamma}(x)} K_h(x, y) \mathbb{I}_y^x X(y) \mathbf{p}^{1-\alpha}(y) dV(y), \\ B := \int_{\tilde{B}_{h^\gamma}(x)} K_h(x, y) \mathbb{I}_y^x X(y) \mathbf{p}^{1-\alpha}(y) \left(w(y) + \frac{\Delta \mathbf{p}(y)}{2\mathbf{p}(y)} \right) dV(y). \end{cases} \quad (\text{B.16})$$

When we evaluate A and B , the odd monomials in the integral vanish because the kernel we use has the symmetry property. By Taylor's expansion, A becomes

$$\begin{aligned}
A &= \int_{S^{d-1}} \int_0^{h^\gamma} \left[K\left(\frac{t}{\sqrt{h}}\right) + K'\left(\frac{t}{\sqrt{h}}\right) \frac{\|\Pi(\theta, \theta)\| t^3}{24\sqrt{h}} + O\left(\frac{t^6}{h}\right) \right] \\
&\quad \times \left[X(x) + \nabla_\theta X(x)t + \nabla_{\theta, \theta}^2 X(x) \frac{t^2}{2} + \nabla_{\theta, \theta, \theta}^3 X(x) \frac{t^3}{6} + O(t^4) \right] \\
&\quad \times \left[\mathbf{p}^{1-\alpha}(x) + \nabla_\theta(\mathbf{p}^{1-\alpha})(x)t + \nabla_{\theta, \theta}^2(\mathbf{p}^{1-\alpha})(x) \frac{t^2}{2} + \nabla_{\theta, \theta, \theta}^3(\mathbf{p}^{1-\alpha})(x) \frac{t^3}{6} + O(t^3) \right] \\
&\quad \times [t^{d-1} + \text{Ric}(\theta, \theta)t^{d+1} + O(t^{d+2})] dt d\theta. \tag{B.17}
\end{aligned}$$

Due to the fact that K and K' decay exponentially, by the same argument as that of Lemma B1, we can replace the integrals $\int_{S^{d-1}} \int_0^{h^\gamma}$ by $\int_{S^{d-1}} \int_0^\infty$ by paying the price of error of order h^2 which depends on $\|X^{(\ell)}\|_{L^\infty}$, where $\ell = 0, 1, \dots, 4$. Thus, after rearrangement we have

$$\begin{aligned}
A &= \mathbf{p}^{1-\alpha}(x)X(x) \int_{S^{d-1}} \int_0^\infty \left\{ K\left(\frac{t}{\sqrt{h}}\right) [1 + \text{Ric}(\theta, \theta)t^2] + K'\left(\frac{t}{\sqrt{h}}\right) \frac{\|\Pi(\theta, \theta)\| t^3}{24\sqrt{h}} \right\} t^{d-1} dt d\theta \\
&\quad + \mathbf{p}^{1-\alpha}(x) \int_{S^{d-1}} \int_0^\infty K\left(\frac{t}{\sqrt{h}}\right) \nabla_{\theta, \theta}^2 X(x) \frac{t^{d+1}}{2} dt d\theta \\
&\quad + X(x) \int_{S^{d-1}} \int_0^\infty K\left(\frac{t}{\sqrt{h}}\right) \nabla_{\theta, \theta}^2(\mathbf{p}^{1-\alpha})(x) \frac{t^{d+1}}{2} dt d\theta \\
&\quad + \int_{S^{d-1}} \int_0^\infty K\left(\frac{t}{\sqrt{h}}\right) \nabla_\theta X(x) \nabla_\theta(\mathbf{p}^{1-\alpha})(x) t^{d+1} dt d\theta + O(h^{d/2+2}), \tag{B.18}
\end{aligned}$$

where the implied constant in $O(h^{d/2+2})$ depends on $\|X^{(\ell)}\|_{L^\infty}$, $\ell = 0, 1, \dots, 4$. Following the same argument as that in [33], we have

$$\int_{S^{d-1}} \nabla_{\theta, \theta}^2 X(x) d\theta = \frac{|S^{d-1}|}{d} \nabla^2 X(x) \quad \text{and} \quad \int_{S^{d-1}} \text{Ric}(\theta, \theta) d\theta = \frac{|S^{d-1}|}{d} s(x). \tag{B.19}$$

Therefore,

$$\begin{aligned}
A &= h^{d/2} \mathbf{p}^{1-\alpha}(x) \left\{ \left(1 + \frac{h\mu_{1,2}^{(0)}}{d} \frac{\Delta(\mathbf{p}^{1-\alpha})(x)}{2\mathbf{p}^{1-\alpha}(x)} + \frac{h\mu_{1,2}^{(0)}}{d} w(x) \right) X(x) + \frac{h\mu_{1,2}^{(0)}}{2d} \nabla^2 X(x) \right\} \\
&\quad + h^{d/2+1} \frac{\mu_{1,2}^{(0)}}{d} \nabla X(x) \cdot \nabla(\mathbf{p}^{1-\alpha})(x) + O(h^{d/2+2}), \tag{B.20}
\end{aligned}$$

where the implied constant in $O(h^{d/2+2})$ depends on $\|X^{(\ell)}\|_{L^\infty}$, $\ell = 0, 1, \dots, 4$.

To evaluate B , denote $\underline{Q}(y) := \mathbf{p}^{1-\alpha}(y) \left(w(y) + \frac{\Delta \mathbf{p}(y)}{2\mathbf{p}(y)} \right) \in C^2(\mathbf{M})$ to simplify notation. We have

$$\begin{aligned} B &= \int_{B_{h^{1/\gamma}}(x)} K_h(x, y) \mathbb{I}_y^x X(y) \underline{Q}(y) \, dV(y) \\ &= \int_{S^{d-1}} \int_0^{h^\gamma} \left[K\left(\frac{t}{\sqrt{h}}\right) + O\left(\frac{t^3}{\sqrt{h}}\right) \right] [X(x) + \nabla_\theta X(x)t + O(t^2)] \\ &\quad \times [Q(x) + \nabla_\theta Q(x)t + O(t^2)] [t^{d-1} + O(t^{d+1})] \, dt \, d\theta \\ &= h^{d/2} X(x) \underline{Q}(x) + O(h^{d/2+1}), \end{aligned} \tag{B.21}$$

where the implied constant in $O(h^{d/2+1})$ depends on $\|X\|_{L^\infty}$, $\|X^{(1)}\|_{L^\infty}$ and $\|X^{(2)}\|_{L^\infty}$. In conclusion, the numerator of $T_{h,\alpha}X(x)$ becomes

$$\begin{aligned} &h^{d/2} \frac{\mathbf{p}^{1-\alpha}(x)}{\mathbf{p}_h^\alpha(x)} \left\{ 1 + h \frac{\mu_{1,2}^{(0)}}{d} \left[\frac{\Delta(\mathbf{p}^{1-\alpha})(x)}{2\mathbf{p}^{1-\alpha}(x)} - \alpha \frac{\Delta \mathbf{p}(x)}{2\mathbf{p}(x)} \right] \right\} X(x) \\ &+ h^{d/2+1} \frac{\mu_{1,2}^{(0)} \mathbf{p}^{1-\alpha}(x)}{d \mathbf{p}_h^\alpha(x)} \left\{ \frac{\nabla^2 X(x)}{2} + \frac{\nabla X(x) \cdot \nabla(\mathbf{p}^{1-\alpha})(x)}{\mathbf{p}^{1-\alpha}(x)} \right\} + O(h^{d/2+2}), \end{aligned} \tag{B.22}$$

where the implied constant in $O(h^{d/2+2})$ depends on $\|X^{(\ell)}\|_{L^\infty}$, $\ell = 0, 1, \dots, 4$. Similar calculation of the denominator of the $T_{h,\alpha}X(x)$ gives

$$h^{d/2} \frac{\mathbf{p}^{1-\alpha}(x)}{\mathbf{p}_h^\alpha(x)} \left\{ 1 + h \frac{\mu_{1,2}^{(0)}}{d} \left(\frac{\Delta(\mathbf{p}^{1-\alpha})(x)}{2\mathbf{p}^{1-\alpha}(x)} - \alpha \frac{\Delta \mathbf{p}(x)}{2\mathbf{p}(x)} \right) \right\} + O(h^{d/2+2}). \tag{B.23}$$

Putting all the above together, we then have $x \in \mathbf{M} \setminus \mathbf{M}_{h^\gamma}$,

$$T_{h,\alpha}X(x) = X(x) + h \frac{\mu_{1,2}^{(0)}}{2d} \left(\nabla^2 X(x) + \frac{2\nabla X(x) \cdot \nabla(\mathbf{p}^{1-\alpha})(x)}{\mathbf{p}^{1-\alpha}(x)} \right) + O(h^2), \tag{B.24}$$

where the implied constant in $O(h^2)$ depends on $\|X^{(\ell)}\|_{L^\infty}$, $\ell = 0, 1, \dots, 4$.

Next we consider the case when $x \in \mathbf{M}_{h^\gamma}$. By Lemma B3, we get

$$\mathbf{p}_h(y) = m_{h,0} \mathbf{p}(y) + \sqrt{h} m_{h,1} \partial_d \mathbf{p}(x) + O(h^{2\gamma}), \tag{B.25}$$

which leads to

$$\frac{\mathbf{p}(y)}{\mathbf{p}_h^\alpha(y)} = \frac{\mathbf{p}^{1-\alpha}(y)}{m_{h,0}^\alpha} \left[1 - \sqrt{h} \frac{\alpha m_{h,1}}{m_{h,0}} \frac{\partial_d \mathbf{p}(y)}{\mathbf{p}(y)} + O(h^{2\gamma}) \right]. \tag{B.26}$$

By Taylor's expansion and Lemma B2, the numerator of $T_{h,\alpha}X$ becomes

$$\begin{aligned}
& \int_{B_{h^\gamma}(x)} K_{h,\alpha}(x,y) //_y^x X(y) \mathbf{p}(y) \, dV(y) \\
&= \frac{p_h^{-\alpha}(x)}{m_{h,0}^\alpha} \int_{S_\eta} \int_{-h^\gamma}^{h^\gamma} K \left(\frac{\sqrt{\|\mathbf{u}\|^2 + \eta^2}}{\sqrt{h}} \right) \left(X(x) + \sum_{i=1}^{d-1} u_i \nabla_{\partial_i} X(x) + \eta \nabla_{\partial_d} X(x) + O(h^2) \right) \\
&\quad \times \left(\mathbf{p}^{1-\alpha}(x) + \sum_{i=1}^{d-1} u_i \nabla_{\partial_i} \mathbf{p}^{1-\alpha}(x) + \eta \nabla_{\partial_d} \mathbf{p}^{1-\alpha}(x) + O(h^2) \right) \\
&\quad \times \left[1 - \sqrt{h} \frac{\alpha m_{h,1}}{m_{h,0}} \frac{\partial_d \mathbf{p}(y)}{\mathbf{p}(y)} \right] d\eta \, d\mathbf{u} + O(h^{d/2+2\gamma}) \\
&= \frac{p_h^{-\alpha}(x)}{m_{h,0}^\alpha} \int_{\tilde{S}_\eta} \int_{-h^\gamma}^{h^\gamma} K \left(\frac{\sqrt{\|\mathbf{u}\|^2 + \eta^2}}{\sqrt{h}} \right) \left(X(x) + \sum_{i=1}^{d-1} u_i \nabla_{\partial_i} X(x) + \eta \nabla_{\partial_d} X(x) + O(h^2) \right) \\
&\quad \times \left(\mathbf{p}^{1-\alpha}(x) + \sum_{i=1}^{d-1} u_i \nabla_{\partial_i} \mathbf{p}^{1-\alpha}(x) + \eta \nabla_{\partial_d} \mathbf{p}^{1-\alpha}(x) + O(h^2) \right) \\
&\quad \times \left[1 - \sqrt{h} \frac{\alpha m_{h,1}}{m_{h,0}} \frac{\partial_d \mathbf{p}(x)}{\mathbf{p}(x)} \right] d\eta \, d\mathbf{u} + O(h^{d/2+2\gamma}), \tag{B.27}
\end{aligned}$$

where the implied constant in $O(h^{d/2+2\gamma})$ depends on $\|X^{(\ell)}\|_{L^\infty}$, $\ell = 0, 1, 2$, and the last equality holds due to Lemma B2. The symmetry of the kernel implies that for $i = 1, \dots, d-1$,

$$\int_{\tilde{S}_\eta} K \left(\frac{\sqrt{\|\mathbf{u}\|^2 + \eta^2}}{\sqrt{h}} \right) u_i \, d\mathbf{u} = 0, \tag{B.28}$$

and hence the numerator of $T_{h,\alpha}X(x)$ becomes

$$\begin{aligned}
& h^{d/2} \frac{m_{h,0}^{1-\alpha}}{p_h^\alpha(x)} \left[X(x) \mathbf{p}^{1-\alpha}(x) + \sqrt{h} \frac{m_{h,1}}{m_{h,0}} \left(X(x) \partial_d \mathbf{p}^{1-\alpha}(x) + \mathbf{p}^{1-\alpha}(x) \nabla_{\partial_d} X(x) + \frac{\alpha X(x) \partial_d \mathbf{p}(x)}{m_{h,0} \mathbf{p}(x)} \right) \right] \\
& \quad + O(h^{d/2+2\gamma}), \tag{B.29}
\end{aligned}$$

where the implied constant in $O(h^{d/2+2\gamma})$ depends on $\|X\|_{L^\infty}$, $\|X^{(1)}\|_{L^\infty}$ and $\|X^{(2)}\|_{L^\infty}$ and $m_{h,0}$ and $m_{h,1}$ are defined in (B.12). Similarly, the denominator of $T_{h,\alpha}X$ can be expanded as:

$$\begin{aligned}
& \int_{B_{h^\gamma}(x)} K_{h,\alpha}(x,y) \mathbf{p}(y) \, dV(y) \\
&= h^{d/2} \frac{m_{h,0}^{1-\alpha}}{p_h^\alpha(x)} \left[\mathbf{p}^{1-\alpha}(x) + \sqrt{h} \frac{m_{h,1}}{m_{h,0}} \left(\partial_d \mathbf{p}^{1-\alpha}(x) + \frac{\alpha \partial_d \mathbf{p}(x)}{m_{h,0} \mathbf{p}(x)} \right) \right] + O(h^{d/2+2\gamma}). \tag{B.30}
\end{aligned}$$

Moreover, by (B.7), we have

$$//_x^{x_0} \partial_l(x) = \partial_l(x_0) + O(h^{2\gamma}), \tag{B.31}$$

for all $l = 1, \dots, d$. Thus, together with the expansion of the numerator and denominator of $T_{h,\alpha}X$, we have the following asymptotic expansion:

$$T_{h,\alpha}X(x) = X(x) + \sqrt{h} \frac{m_{h,1}}{m_{h,0}} \Big\|_{x_0}^x \nabla_{\partial_d} X(x_0) + O(h^{2\gamma}), \quad (\text{B.32})$$

where the implied constant in $O(h^{2\gamma})$ depends on $\|X^{(\ell)}\|_{L^\infty}$, $\ell = 0, 1, 2$, which finish the proof. \square

Appendix C. Proof of Theorem 5.3

The proof is a generalization of that of [33, Theorem B.3] to the principal bundle structure. Note that in [33, Theorem B.3] only the uniform sampling p.d.f. case was discussed. The main ingredient in the stochastic fluctuation analysis of the GCL when n is finite is the large deviation analysis. Note that the term in which we have interest, the connection Laplacian (or Laplace–Beltrami operator when we consider GL), is the second order term, that is, it is of order h , which is much smaller than the 0th order term. Thus, by applying the Bernstein’s inequality with the large deviation to control the error to be much smaller than h , we are able to achieve this rate. Here, for the sake of self-containment and clarifying some possible confusions in [31], we provide a detailed proof for this large deviation bound.

LEMMA C1 Assume Assumptions 4.1–4.3 hold. We have the following two statements.

(A) Suppose $h = h(n)$ so that $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+s}} \rightarrow 0$ and $h \rightarrow 0$ as $n \rightarrow \infty$, where $s \geq 0$. With probability higher than $1 - 1/n^2$, the following kernel density estimation holds for all $i = 1, \dots, n$

$$\widehat{\mathbf{p}}_{h,n}(x_i) = \mathbf{p}_h(x_i) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right). \quad (\text{C.1})$$

(B) Take $f \in C^4(\mathbf{M})$ and $1/4 < \gamma < 1/2$. For the points away from the boundary, suppose $h = h(n)$ so that $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2}} \rightarrow 0$ and $h \rightarrow 0$ as $n \rightarrow \infty$. Then, with probability higher than $1 - 1/n^2$, the following holds for all $x_i \notin \mathbf{M}_{h^\gamma}$:

$$\frac{\sum_{j=1}^n K_h(x_i, x_j)(f(x_j) - f(x_i))}{\sum_{j=1}^n K_h(x_i, x_j)} = (T_{h,0}f - f)(x_i) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/2}}\right), \quad (\text{C.2})$$

and the following holds for all $x_i \in \mathbf{M}_{h^\gamma}$:

$$\frac{\sum_{j=1}^n K_h(x_i, x_j)(f(x_j) - f(x_i))}{\sum_{j=1}^n K_h(x_i, x_j)} = (T_{h,0}f - f)(x_i) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/4}}\right). \quad (\text{C.3})$$

REMARK C1 In this lemma, (A) means that when we have enough points, the kernel density estimation of the p.d.f. converges faster than h ; that is, when $s > 0$, $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}/h^s \rightarrow 0$ as $h \rightarrow 0$. This is important for the convergence of the normalized GCL.

Proof. We will prove (B). The proof of (A) is the same by applying the Hoeffding’s inequality, and will be shown when we prove (B). Fix x_i . Note that $\frac{\sum_{j=1}^n K_h(x_i, x_j)(f(x_j) - f(x_i))}{\sum_{j=1}^n K_h(x_i, x_j)}$ is actually the un-normalized GL.

Denote $F_j := h^{-d/2}K_h(x_i, x_j)(f(x_j) - f(x_i))$ and $G_j := h^{-d/2}K_h(x_i, x_j)$, then the un-normalized GL could be rewritten as

$$\frac{\sum_{j=1}^n K_h(x_i, x_j)(f(x_j) - f(x_i))}{\sum_{j=1}^n K_h(x_i, x_j)} = \frac{\frac{1}{n} \sum_{j=1}^n F_j}{\frac{1}{n} \sum_{j=1}^n G_j}. \quad (\text{C.4})$$

Define two random variables

$$F := h^{-d/2}K_h(x_i, Y)(f(Y) - f(x_i)) \quad \text{and} \quad G := h^{-d/2}K_h(x_i, Y). \quad (\text{C.5})$$

Clearly, F_j (respectively G_j), when $j \neq i$, can be viewed as randomly sampled i.i.d. from F (respectively G). Note that the un-normalized GL is a ratio of two dependent random variables, therefore the variance cannot be simply computed.

$$\frac{\frac{1}{n} \sum_{j=1}^n F_j}{\frac{1}{n} \sum_{j=1}^n G_j} \approx \frac{\mathbb{E}[F]}{\mathbb{E}[G]} \quad (\text{C.6})$$

and to control the size of the fluctuation as a function of n and h by the Bernstein type inequality. Note that we have

$$\frac{1}{n} \sum_{j=1}^n F_j = \frac{n-1}{n} \left[\frac{1}{n-1} \sum_{j=1, j \neq i}^n F_j \right] \quad (\text{C.7})$$

since $K_h(x_i, x_j)(f(x_j) - f(x_i)) = 0$ when $x_j = x_i$. Also, since $\frac{n-1}{n} \rightarrow 1$ as $n \rightarrow \infty$, we can simply focus on analyzing $\frac{1}{n-1} \sum_{j=1, j \neq i}^n F_j$. A similar argument holds for $\frac{1}{n} \sum_{j=1}^n G_j$ —clearly, $K_h(x_i, x_i) = K(0) > 0$, so this term will contribute to the error term of order $\frac{1}{n}$. Thus, we have

$$\frac{\frac{1}{n} \sum_{j=1}^n F_j}{\frac{1}{n} \sum_{j=1}^n G_j} = \frac{\frac{1}{n-1} \sum_{j=1, j \neq i}^n F_j}{\frac{1}{n-1} \sum_{j=1, j \neq i}^n G_j} + O\left(\frac{1}{n}\right). \quad (\text{C.8})$$

As we will see shortly, the $O(1/n)$ term will be dominated, and can thus be ignored.

First of all, we consider $x_i \notin \mathbf{M}_{h^\gamma}$, By Theorem 5.2, we have

$$\begin{aligned} \mathbb{E}[F] &= \int_{\mathbf{M}} h^{-d/2} K_h(x_i, y)(f(y) - f(x_i)) \mathbf{p}(y) \, dV(y) = h \frac{\mu_{1,2}^{(0)}}{2} \Delta((f(y) - f(x_i)) \mathbf{p}(y))|_{y=x_i} + O(h^2) \\ \mathbb{E}[G] &= \int_{\mathbf{M}} h^{-d/2} K_h(x_i - y) \mathbf{p}(y) \, dV(y) = \mathbf{p}(x_i) + O(h) \end{aligned} \quad (\text{C.9})$$

and

$$\begin{aligned} \mathbb{E}[F^2] &= \int_{\mathbf{M}} h^{-d} K_h^2(x_i - y)(f(x_i) - f(y))^2 \mathbf{p}(y) \, dV(y) \\ &= \frac{1}{h^{d/2-1}} \frac{\mu_{2,2}^{(0)}}{2} \Delta((f(x_i) - f(y))^2 \mathbf{p}(y))|_{y=x_i} + O\left(\frac{1}{h^{d/2-2}}\right) \end{aligned}$$

$$\mathbb{E}[G^2] = \int_{\mathbb{M}} h^{-d} K_h^2(x_i - y) \mathbf{p}(y) \, dV(y) = \frac{1}{h^{d/2}} \mu_{2,0}^{(0)} \mathbf{p}(x_i) + O\left(\frac{1}{h^{d/2-1}}\right) \quad (\text{C.10})$$

Thus, we conclude that⁷

$$\begin{aligned} \text{Var}(F) &= \frac{1}{h^{d/2-1}} \frac{\mu_{2,2}^{(0)}}{2} \Delta((f(y) - f(x_i))^2 \mathbf{p}(y))|_{y=x_i} + O\left(\frac{1}{h^{d/2-2}}\right) \\ \text{Var}(G) &= \frac{1}{h^{d/2}} \mu_{2,0}^{(0)} \mathbf{p}(x_i) + O\left(1, \frac{1}{h^{d/2-1}}\right). \end{aligned} \quad (\text{C.11})$$

With the above bounds, we could apply the large deviation theory. First, note that the random variable F is uniformly bounded by

$$c = 2\|f\|_{L^\infty} \|K\|_{L^\infty} h^{-d/2} \quad (\text{C.12})$$

and its variance, denoted as σ^2 , is shown in (C.11). Here, to simplify the discussion, we assume that $\frac{\mu_{2,2}^{(0)}}{2} \Delta((f(y) - f(x_i))^2 \mathbf{p}(y))|_{y=x_i} \neq 0$ so that $\sigma^2 = O(h^{-d/2+1})$ when h is small enough. In the case that $\frac{\mu_{2,2}^{(0)}}{2} \Delta((f(y) - f(x_i))^2 \mathbf{p}(y))|_{y=x_i} = 0$, the variance is of higher order $h^{-d/2+2}$, and the proof is the same. We see that

$$\sigma^2/c \rightarrow 0 \text{ as } h \rightarrow 0, \quad (\text{C.13})$$

so Bernstein's inequality could in principle provide a tighter large deviation bound than that provided by Hoeffding's inequality. Recall Bernstein's inequality

$$\Pr \left\{ \frac{1}{n-1} \sum_{j=1, j \neq i}^n (F_j - \mathbb{E}[F]) > \beta \right\} \leq e^{-\frac{n\alpha^2}{2\sigma^2 + \frac{2}{3}c\alpha}}, \quad (\text{C.14})$$

where $\beta > 0$. Since our goal is to estimate a quantity of order h (the prefactor of the Laplacian), we need to take $\beta = \beta(h)$ much smaller than h in the sense that $\beta/h \rightarrow 0$ as $h \rightarrow 0$. In this case, $c\beta$ is much smaller than $2\|f\|_{L^\infty} \|K\|_{L^\infty} h^{-d/2+1}$, where the right-hand side is of the same order of σ^2 . Hence,

⁷ Note that since

$$\begin{aligned} \mathbb{E}[FG] &= \int_{\mathbb{M}} K_h^2(x_i - y) (f(x_i) - f(y)) \mathbf{p}(y) \, dV(y) = \frac{1}{h^{d/2-1}} \frac{\mu_{2,2}^{(0)}}{2} \Delta((f(x_i) - f(y)) \mathbf{p}(y))|_{y=x_i} + O\left(\frac{1}{h^{d/2-2}}\right) \\ \text{Cov}(F, G) &= \mathbb{E}[FG] - \mathbb{E}[F]\mathbb{E}[G] = \frac{1}{h^{d/2-1}} \frac{\mu_{2,2}^{(0)}}{2} \Delta((f(y) - f(x_i)) \mathbf{p}(y))|_{y=x_i} + O\left(h, \frac{1}{h^{d/2-2}}\right), \end{aligned}$$

the correlation between F and G is

$$\rho(F, G) = \frac{\text{Cov}(F, G)}{\sqrt{\text{Var}(F)}\sqrt{\text{Var}(G)}} = O\left(\frac{\sqrt{h^{d/2+d/2-1}}}{h^{d/2-1}}\right) = O(\sqrt{h}).$$

$2\sigma^2 + \frac{2}{3}c\beta \leq 3\sigma^2$ when h is smaller enough. Thus, the exponent in Bernstein's inequality is bounded from below by

$$\frac{n\beta^2}{2\sigma^2 + \frac{2}{3}c\beta} \geq \frac{n\beta^2}{3\sigma^2} \geq \frac{n\beta^2 h^{d/2-1}}{3\mu_{2,2}^{(0)} \Delta((f(y) - f(x_i))^2 \mathbf{p}(y))|_{y=x_i}}. \quad (\text{C.15})$$

Suppose n is chosen large enough so that

$$\frac{n\beta^2 h^{d/2-1}}{3\mu_{2,2}^{(0)} \Delta((f(y) - f(x_i))^2 \mathbf{p}(y))|_{y=x_i}} = 3 \log(n); \quad (\text{C.16})$$

that is, the deviation from the mean is set to

$$\beta = \frac{3\sqrt{\log(n)} \sqrt{\mu_{2,2}^{(0)} \Delta((f(y) - f(x_i))^2 \mathbf{p}(y))|_{y=x_i}}}{n^{1/2} h^{d/4-1/2}} = O\left(\frac{\sqrt{\log(n)}}{n^{1/2} h^{d/4-1/2}}\right), \quad (\text{C.17})$$

where the implied constant in $O\left(\frac{\sqrt{\log(n)}}{n^{1/2} h^{d/4-1/2}}\right)$ is $3\sqrt{\mu_{2,2}^{(0)} \|\Delta((f(y) - f(x))^2 \mathbf{p}(y))|_{y=x}\|_{L^\infty}}$, where Δ acts on y and $\|\cdot\|_{L^\infty}$ acts on x . Note that by the assumption that $h = h(n)$ so that $\frac{\sqrt{\log(n)}}{n^{1/2} h^{d/4+1/2}} \rightarrow 0$ as $h \rightarrow 0$, we know that $\beta/h = \frac{\sqrt{\log(n)}}{n^{1/2} h^{d/4+1/2}} \rightarrow 0$. It implies that the deviation happens with probability less than $1/n^3$.

To get the result for the numerator, note that when $\frac{\mu_{2,2}^{(0)}}{2} \Delta((f(y) - f(x_i))^2 \mathbf{p}(y))|_{y=x_i} = 0$, the variance is smaller than the case when $\frac{\mu_{2,2}^{(0)}}{2} \Delta((f(y) - f(x_i))^2 \mathbf{p}(y))|_{y=x_i} \neq 0$, and hence the deviation is smaller. Thus, by a simple union bound, we have

$$\Pr \left\{ \frac{1}{n-1} \sum_{j=1, j \neq i}^n (F_j - \mathbb{E}[F]) > \beta; i = 1, \dots, n \right\} \leq n e^{-\frac{n\alpha^2}{2\sigma^2 + \frac{2}{3}c\alpha}}, \quad (\text{C.18})$$

which implies that for all $i = 1, \dots, n$, the deviation happens with probability less than $1/n^2$.

To control the denominator, note that the variance of G , shown in (C.11), is of the same order as the bound of G . Thus, by the same large deviation argument with the simple bound by Hoeffding's inequality, we have the deviation bound for the denominator; that is, with probability higher than $1 - 1/n^2$, for all $i = 1, \dots, n$, we have

$$\left| \frac{1}{n-1} \sum_{j=1, j \neq i}^n (G_j - \mathbb{E}[G]) \right| = O\left(\frac{\sqrt{\log(n)}}{n^{1/2} h^{d/4}}\right), \quad (\text{C.19})$$

where we note that $\frac{\sqrt{\log(n)}}{n^{1/2} h^{d/4}}/h^{1/2} \rightarrow 0$ as $h \rightarrow 0$ under the assumption of the relationship between n and h . Note that the same argument holds for (A); that is, the assumption that $\frac{\sqrt{\log(n)}}{n^{1/2} h^{d/4+s}} \rightarrow 0$ leads to $\beta/h^s = \beta(h)/h^s \rightarrow 0$ as $h \rightarrow 0$ for all $i = 1, \dots, n$, with probability higher than $1 - 1/n^2$.

To finish proof of the first part of (B), note that by the assumption that \mathbf{p} is uniformly bounded from below, when h is small enough, $\mathbb{E}[G]$ is bounded from below by $\min_{x \in \mathbf{M}} \mathbf{p}(x)/2$. Altogether, with probability higher than $1 - 1/n^2$, for all $i = 1, \dots, n$, we have

$$\begin{aligned} \frac{\frac{1}{n-1} \sum_{j=1, j \neq i}^n F_j}{\frac{1}{n-1} \sum_{j=1, j \neq i}^n G_j} &= \frac{\mathbb{E}[F] + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/2}}\right)}{\mathbb{E}[G] + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right)} = h \left[\frac{h^{-1}\mathbb{E}[F] + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/2}}\right)}{\mathbb{E}[G] + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right)} \right] \\ &= \frac{\mathbb{E}[F]}{\mathbb{E}[G]} + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/2}}\right), \end{aligned} \quad (\text{C.20})$$

where the last equality holds since $\mathbb{E}[G] \geq \min_{x \in \mathbf{M}} \mathbf{p}(x)/2$. Therefore, since $\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/2}}$ dominates $\frac{1}{n}$ when $h = h(n)$ and n is large enough, we obtain the conclusion for all $x_i \notin \mathbf{M}_{h^\gamma}$.

For $x_i \in \mathbf{M}_{h^\gamma}$, a similar argument holds and we provide key steps in the proof for the completion. Again, the random variable F is uniformly bounded by

$$c = 2\|f\|_{L^\infty} \|K\|_{L^\infty} h^{-d/2} \quad (\text{C.21})$$

and by (5.3), its variance is

$$\sigma^2 = h^{-d/2+1/2} \frac{m'_{h,1}}{m'_{h,0}} \nabla_{\partial_d} f(x_0) + O(h^{-d/2+2\gamma}), \quad (\text{C.22})$$

where $x_0 = \operatorname{argmin}_{y \in \partial \mathbf{M}} d(x_i, y)$, ∂_d is the outer normal direction to the boundary at x_0 , and

$$\begin{cases} m'_{h,0} := \int_{\tilde{S}_\eta} \int_{-h^\gamma}^{h^\gamma} h^{-d/2} K^2 \left(\frac{\sqrt{\|u\|^2 + \eta^2}}{\sqrt{h}} \right) d\eta dx \\ m'_{h,1} := \int_{\tilde{S}_\eta} \int_{-h^\gamma}^{h^\gamma} h^{-d/2-1/2} K^2 \left(\frac{\sqrt{\|u\|^2 + \eta^2}}{\sqrt{h}} \right) \eta d\eta dx. \end{cases} \quad (\text{C.23})$$

Note that the first order term cannot be canceled when x_i is near the boundary, so the variance is of order $h^{-(d/2-1/2)}$ instead of order $h^{-(d/2-1)}$. Thus, under the assumption that $\beta/h^{1/2} \rightarrow 0$ as $h \rightarrow \infty$, the Bernstein's inequality leads to the large deviation bound of the numerator, and similarly for the denominator. As a result, with probability higher than $1 - 1/n^2$, for all $i = 1, \dots, n$, we obtain

$$\begin{aligned} \frac{\frac{1}{n-1} \sum_{j=1, j \neq i}^n F_j}{\frac{1}{n-1} \sum_{j=1, j \neq i}^n G_j} &= \frac{\mathbb{E}[F] + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/4}}\right)}{\mathbb{E}[G] + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right)} = h^{1/2} \left[\frac{h^{-1/2}\mathbb{E}[F] + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4+1/4}}\right)}{\mathbb{E}[G] + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right)} \right] \\ &= \frac{\mathbb{E}[F]}{\mathbb{E}[G]} + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4-1/4}}\right), \end{aligned} \quad (\text{C.24})$$

where the last term holds since $\mathbb{E}[G] \geq \min_{x \in \mathbf{M}} \mathbf{p}(x)/2$. \square

Proof of Theorem 5.3. The proof is essentially the same as that of Lemma (C1), so we will just show the key steps without showing all details. Fix i and $0 < \alpha \leq 1$. By definition we have

$$\begin{aligned} (\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X} - \mathbf{X})[i] &= \frac{\frac{1}{n} \sum_{j=1}^n \frac{K_h(x_i, x_j)}{\widehat{\rho}_{h,n}^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i])}{\frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\widehat{\rho}_{h,n}^\alpha(x_l)}} \\ &= \frac{\frac{1}{n} \sum_{j=1}^n \frac{K_h(x_i, x_j)}{\widehat{\rho}_h^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i])}{\frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\widehat{\rho}_h^\alpha(x_l)}} \end{aligned} \quad (\text{C.25})$$

$$+ \frac{\frac{1}{n} \sum_{j=1}^n \left(\frac{1}{\widehat{\rho}_{h,n}^\alpha(x_j)} - \frac{1}{\widehat{\rho}_h^\alpha(x_j)} \right) K_h(x_i, x_j) (g_{ij} \mathbf{X}[j] - \mathbf{X}[i])}{\frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\widehat{\rho}_h^\alpha(x_l)}} \quad (\text{C.26})$$

$$+ \frac{1}{n} \sum_{j=1}^n \frac{K_h(x_i, x_j)}{\widehat{\rho}_{h,n}^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i]) \left(\frac{1}{\frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\widehat{\rho}_{h,n}^\alpha(x_l)}} - \frac{1}{\frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\widehat{\rho}_h^\alpha(x_l)}} \right). \quad (\text{C.27})$$

We will thus control the deviation by analyzing three terms, (C.25), (C.26) and (C.27).

Note that when $j = i$, $\frac{K_h(x_i, x_j)}{\widehat{\rho}_h^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i]) = 0$, thus we have the following re-formulation

$$\frac{1}{n} \sum_{j=1}^n \frac{K_h(x_i, x_j)}{\widehat{\rho}_h^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i]) = \frac{n-1}{n} \left(\frac{1}{n-1} \sum_{j=1, j \neq i}^n \frac{K_h(x_i, x_j)}{\widehat{\rho}_h^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i]) \right). \quad (\text{C.28})$$

Note that $\frac{n-1}{n}$ will converge to 1. Thus, we can focus on analyzing the stochastic fluctuation of $\frac{1}{n-1} \sum_{j=1, j \neq i}^n \frac{K_h(x_i, x_j)}{\widehat{\rho}_h^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i])$. The same comment applies to the other terms. Clearly, $F_j := \frac{K_h(x_i, x_j)}{\widehat{\rho}_h^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i])$, $j \neq i$, are i.i.d. sampled from a q -dimension/dimensional random vector F , and $G_j := \frac{K_h(x_i, x_j)}{\widehat{\rho}_h^\alpha(x_j)}$ are i.i.d. sampled from a random variable G . Thus, the analysis of the random vector $\frac{\frac{1}{n-1} \sum_{j=1, j \neq i}^n F_j}{\frac{1}{n-1} \sum_{j=1, j \neq i}^n G_j}$ can be viewed as an analysis of q random variables. To apply Lemma C1, we have to clarify the regularity issue of $g_{ij} \mathbf{X}[j] - \mathbf{X}[i]$. Note that by definition, $g_{ij} \mathbf{X}[j] := u_i^{-1} \mathbb{I}_j^i X(x_j)$, thus we can view $g_{ij} \mathbf{X}[j]$ as the value of the vector-valued function $u_i^{-1} \mathbb{I}_y^i X(y)$ at $y = x_j$. Clearly, $u_i^{-1} \mathbb{I}_y^i X(\cdot) \in C^4(\mathcal{M} \setminus C_{x_i}) \cap L^\infty(\mathcal{M})$. Thus, the same argument as that in Lemma C1 (B) can be directly applied. Indeed, we view $\frac{g_{ij} \mathbf{X}[j] - \mathbf{X}[i]}{\widehat{\rho}_h^\alpha(x_j)}$ (respectively $\frac{1}{\widehat{\rho}_h^\alpha(x_j)}$) in the numerator (respectively denominator) as a discretization of the function $\frac{u_i^{-1} \mathbb{I}_y^i X(y) - X(x_i)}{\widehat{\rho}_h^\alpha(y)}$ (respectively $\frac{1}{\widehat{\rho}_h^\alpha(y)}$). As a result, for all $x_i \notin \mathcal{M}_{h^\gamma}$, with probability higher than $1 - 1/2n^2$

$$\frac{\frac{1}{n-1} \sum_{j=1, j \neq i}^n \frac{K_h(x_i, x_j)}{\widehat{\rho}_h^\alpha(x_j)} (g_{ij} \mathbf{X}[j] - \mathbf{X}[i])}{\frac{1}{n-1} \sum_{l=1, l \neq i}^n \frac{K_h(x_i, x_l)}{\widehat{\rho}_h^\alpha(x_l)}} = u_i^{-1} (T_{h,\alpha} \mathbf{X} - \mathbf{X})(x_i) + \mathcal{O} \left(\frac{\sqrt{\log(n)}}{n^{1/2} h^{d/4-1/2}} \right). \quad (\text{C.29})$$

Denote Ω_1 to be the event space that (C.29) holds.

Similarly, by Lemma C1, with probability higher than $1 - 1/2n^2$,

$$|\widehat{\mathbf{p}}_{h,n}(x_j) - \mathbf{p}_h(x_j)| = O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right) \quad (\text{C.30})$$

for all $j = 1, \dots, n$. Thus, by Assumption 4.3, when h is small enough, we have for all $x_i \in \mathcal{X}$

$$p_m/2 \leq |\mathbf{p}_h(x_i)| \leq p_M, \quad p_m/4 \leq |\widehat{\mathbf{p}}_{h,n}(x_i)| \leq 2p_M. \quad (\text{C.31})$$

Denote Ω_2 to be the event space that (C.30) (and hence (C.31)) holds. Thus, when conditional on Ω_2 , by Taylor's expansion and (C.31) we have

$$|\widehat{\mathbf{p}}_{h,n}^{-\alpha}(x_i) - \mathbf{p}_h(x_i)^{-\alpha}| \leq \frac{\alpha}{(p_m/4)^{1+\alpha}} |\widehat{\mathbf{p}}_{h,n}(x_i) - \mathbf{p}_h(x_i)| = O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right). \quad (\text{C.32})$$

With these bounds, when conditional on Ω_2 , (C.26) becomes $O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right)$, where the implied constant depends on $\|X\|_{L^\infty}$. Similarly, when conditional on Ω_2 , we have the following bound for the difference term in (C.27):

$$\left| \frac{1}{\frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\widehat{\mathbf{p}}_{h,n}^\alpha(x_l)}} - \frac{1}{\frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\mathbf{p}_h^\alpha(x_l)}} \right| = \left| \frac{\frac{1}{n} \sum_{l=1}^n K_h(x_i, x_l) \left(\frac{1}{\widehat{\mathbf{p}}_h^\alpha(x_l)} - \frac{1}{\mathbf{p}_h^\alpha(x_l)} \right)}{\frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\widehat{\mathbf{p}}_{h,n}^\alpha(x_l)} \frac{1}{n} \sum_{l=1}^n \frac{K_h(x_i, x_l)}{\mathbf{p}_h^\alpha(x_l)}} \right| = O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right).$$

Hence, (C.27) becomes $O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right)$, where the implied constant depends on $\|X\|_{L^\infty}$.

Putting the above together, when conditional on $\Omega_1 \cap \Omega_2$, we have

$$(\mathbf{D}_{h,\alpha,n}^{-1} \mathbf{S}_{h,\alpha,n} \mathbf{X} - \mathbf{X})[i] = u_i^{-1}(T_{h,\alpha} \mathbf{X} - \mathbf{X})(x_i) + O\left(\frac{\sqrt{\log(n)}}{n^{1/2}h^{d/4}}\right), \quad (\text{C.33})$$

for all $i = 1, \dots, n$. Note that the measure of $\Omega_1 \cap \Omega_2$ is greater than $1 - 1/n^2$, so we finish the proof when $0 < \alpha \leq 1$.

When $\alpha = 0$, clearly (C.26) and (C.27) disappear, and we only have (C.25). Since the convergence behavior of (C.25) has been shown in (C.29), we thus finish the proof when $\alpha = 0$. A similar argument holds for $x_i \in \mathbf{M}_{h^\gamma}$, and we skip the details. \square

Appendix D. Symmetric isometric embedding

Suppose we have a closed, connected and smooth d -dimension/dimensional Riemannian manifold (\mathbf{M}, g) with free isometric $\mathbb{Z}_2 := \{1, z\}$ action on it. Note that \mathbf{M} can be viewed as a principal bundle $P(\mathbf{M}/\mathbb{Z}_2, \mathbb{Z}_2)$ with the group \mathbb{Z}_2 as the fiber. Without loss of generality, we assume the diameter of \mathbf{M} is less than 1. The eigenfunctions $\{\phi_j\}_{j \geq 0}$ of the Laplace–Beltrami operator $\Delta_{\mathbf{M}}$ are known to form an orthonormal basis of $L^2(\mathbf{M})$, where $\Delta_{\mathbf{M}} \phi_j = -\lambda_j \phi_j$ with $\lambda_j \geq 0$. Denote E_λ the eigenspace of $\Delta_{\mathbf{M}}$ with eigenvalue

λ . Since \mathbb{Z}_2 commutes with Δ_M , E_λ is a representation of \mathbb{Z}_2 , where the action of z on ϕ_j is defined by $z \circ \phi_j(x) := \phi_j(z \circ x)$.

We claim that all the eigenfunctions of Δ_M are either even or odd. Indeed, since \mathbb{Z}_2 is an abelian group and all the irreducible representations of \mathbb{Z}_2 are real, we know $z \circ \phi_i = \pm \phi_i$ for all $i \geq 0$. We can thus distinguish two different types of eigenfunctions:

$$\phi_i^e(z \circ x) = \phi_i^e(x) \quad \text{and} \quad \phi_i^o(z \circ x) = -\phi_i^o(x), \quad (\text{D.1})$$

where the superscript e (resp. o) means even (resp. odd) eigenfunctions.

It is well known that the heat kernel $k(x, y, t)$ of Δ_M is a smooth function over x and y and analytic over $t > 0$, and can be written as

$$k(x, y, t) = \sum_i e^{-\lambda_i t} \phi_i(x) \phi_i(y). \quad (\text{D.2})$$

We also know that for all $t > 0$ and $x \in M$, $\sum_j e^{-\lambda_j t} \phi_j(x) \phi_j(x) < \infty$. Thus we can define a family of maps by exceptionally taking odd eigenfunctions into consideration:

$$\begin{aligned} \Psi_t^o : M &\rightarrow \ell^2 && \text{for } t > 0, \\ x &\mapsto \{e^{-\lambda_j t/2} \phi_j^o(x)\}_{j \geq 1} \end{aligned} \quad (\text{D.3})$$

LEMMA D1 For $t > 0$, the map Ψ_t^o is an embedding of M into ℓ^2 .

Proof. If $x_n \rightarrow x$, we have by definition

$$\begin{aligned} \|\Psi_t^o(x_n) - \Psi_t^o(x)\|_{\ell^2}^2 &= \sum_j |e^{-\lambda_j t/2} \phi_j^o(x_n) - e^{-\lambda_j t/2} \phi_j^o(x)|^2 \\ &\leq \sum_j |e^{-\lambda_j t/2} \phi_j^o(x_n) - e^{-\lambda_j t/2} \phi_j^o(x)|^2 + \sum_j |e^{-\lambda_j t/2} \phi_j^e(x_n) - e^{-\lambda_j t/2} \phi_j^e(x)|^2 \\ &= k(x_n, x_n, t) + k(x, x, t) - 2k(x_n, x, t), \end{aligned} \quad (\text{D.4})$$

which goes to 0 as $n \rightarrow \infty$ due to the smoothness of the heat kernel. Thus Ψ_t^o is continuous.

Since the eigenfunctions $\{\phi_j\}_{j \geq 0}$ of the Laplace–Beltrami operator form an orthonormal basis of $L^2(M)$, it follows that they separate points. We now show that odd eigenfunctions are enough to separate points. Given $x \neq y$ two distinct points on M , we can find a small enough neighborhood N_x of x that separates it from y . Take a characteristic odd function f such that $f(x) = 1$ on N_x , $f(z \circ x) = -1$ on $z \circ N_x$ and 0 otherwise. Clearly we know $f(x) \neq f(y)$. Since f is odd, it can be expanded by the odd eigenfunctions:

$$f = \sum_j a_j \phi_j^o. \quad (\text{D.5})$$

Hence $f(x) \neq f(y)$ implies that there exists α such that $\phi_\alpha^o(x) \neq \phi_\alpha^o(y)$.

Suppose we have $\Psi_t^o(x) = \Psi_t^o(y)$, then $\phi_i^o(x) = \phi_i^o(y)$ for all i . By the above argument, we conclude that $x = y$, that is, Ψ_t^o is a 1–1 map. To show that Ψ_t^o is an immersion, consider a neighborhood N_x

so that $N_x \cap z \circ N_x = \emptyset$. Suppose there exists $x \in \mathbf{M}$ so that $d\Psi_t^o(X) = 0$ for $X \in T_x\mathbf{M}$, which implies $d\phi_i^o(X) = 0$ for all i . Thus by the same argument as above, we know $df(X) = 0$ for all $f \in C_c^\infty(N_x)$, which implies $X = 0$. In conclusion, Ψ_t^o is continuous and 1–1 immersion from \mathbf{M} , which is compact, onto $\Psi_t^o(\mathbf{M})$, so it is an embedding. \square

Note that $\Psi_t^o(\mathbf{M})$ is symmetric with respect to 0, that is, $\Psi_t^o(z \circ x) = -\Psi_t^o(x)$. However, it is not an isometric embedding and the embedded space is of infinite dimension. Now we construct an isometric symmetric embedding of \mathbf{M} to a finite dimensional space by extending the Nash embedding theorem [26,27]. We start from considering an open covering of \mathbf{M} in the following way. Since Ψ_t^o , $t > 0$ is an embedding of \mathbf{M} into ℓ^2 , for each given $p \in \mathbf{M}$, there exists d odd eigenfunctions $\{\phi_j^o\}_{j=1}^d$ so that

$$\begin{aligned} v_p : x \in \mathbf{M} &\mapsto (\phi_1^o(x), \dots, \phi_d^o(x)) \in \mathbb{R}^d \\ v_{z \circ p} : z \circ x \in \mathbf{M} &\mapsto -(\phi_1^o(x), \dots, \phi_d^o(x)) \in \mathbb{R}^d \end{aligned} \quad (\text{D.6})$$

are of full rank at p and $z \circ p$. We choose a small enough neighborhood N_p of p so that $N_p \cap z \circ N_p = \emptyset$ and v_p and $v_{z \circ p}$ are embedding of N_p and $z \circ N_p$. It is clear that $\{N_p, z \circ N_p\}_{p \in \mathbf{M}}$ is an open covering of \mathbf{M} .

With the open covering $\{N_p, z \circ N_p\}_{p \in \mathbf{M}}$, it is a well-known fact [35] that there exists an atlas of \mathbf{M}

$$\mathcal{A} = \{(V_j, h_j), (z \circ V_j, h_j^z)\}_{j=1}^L, \quad (\text{D.7})$$

where $V_j \subset \mathbf{M}$, $z \circ V_j \subset \mathbf{M}$, $h_j : \mathbf{M} \rightarrow \mathbb{R}^d$, $h_j^z : \mathbf{M} \rightarrow \mathbb{R}^d$, so that the following holds and the symmetry is taken into account:

- (a) \mathcal{A} is a locally finite refinement of $\{N_p, z \circ N_p\}_{p \in \mathbf{M}}$, that is, for every V_i (resp. $z \circ V_i$), there exists a $p_i \in \mathbf{M}$ (resp. $z \circ p_i \in \mathbf{M}$) so that $V_i \subset N_{p_i}$ (resp. $z \circ V_i \subset z \circ N_{p_i}$),
- (b) $h_j(V_j) = B_2$, $h_j^z(z \circ V_j) = B_2$, and $h_j(x) = h_j^z(z \circ x)$ for all $x \in V_j$,
- (c) for the p_i chosen in (a), there exists $\phi_{p_i}^o$ so that $\phi_{p_i}^o(x) \neq \phi_{p_i}^o(z \circ x)$ for all $x \in V_i$,
- (d) $\mathbf{M} = \cup_j (h_j^{-1}(B_1) \cup (h_j^z)^{-1}(B_1))$. Denote $O_j = h_j^{-1}(B_1)$,

where $B_r = \{x \in \mathbb{R}^d : \|x\| < r\}$. We fix the point $p_i \in \mathbf{M}$ when we determine \mathcal{A} , that is, if $V_i \in \mathcal{A}$, we have a unique $p_i \in \mathbf{M}$ so that $V_i \subset N_{p_i}$. Note that (c) holds since Ψ_t^o , $t > 0$ is an embedding of \mathbf{M} into ℓ^2 and the eigenfunctions of $\Delta_{\mathbf{M}}$ are smooth. We will fix a partition of unity $\{\eta_i \in C_c^\infty(V_i), \eta_i^z \in C_c^\infty(z \circ V_i)\}$ subordinate to $\{V_j, z \circ V_j\}_{j=1}^L$. Due to symmetry, we have $\eta_i(x) = \eta_i^z(z \circ x)$ for all $x \in V_i$. To ease notation, we define

$$\psi_i(x) = \begin{cases} \eta_i(x) & \text{when } x \in V_i \\ \eta_i^z(x) & \text{when } x \in z \circ V_i \end{cases} \quad (\text{D.8})$$

so that $\{\psi_i\}_{i=1}^L$ is a partition of unit subordinate to $\{V_i \cup z \circ V_i\}_{i=1}^L$.

LEMMA D2 There exists a symmetric embedding $\tilde{u} : \mathbf{M}^d \hookrightarrow \mathbb{R}^N$ for some $N \in \mathbb{N}$.

Proof. Fix V_i and hence $p_i \in \mathbf{M}$. Define

$$u_i : x \in \mathbf{M} \mapsto (\phi_{ip_i}^o(x), v_{p_i}(x)) \in \mathbb{R}^{d+1}, \quad (\text{D.9})$$

where v_{p_i} is defined in (D.6). Note that u_i is of full rank at p_i . Due to symmetry, the assumption (c) and the fact that $V_i \cap z \circ V_i = \emptyset$, we can find a rotation $R_i \in SO(d+1)$ and modify the definition of u_i :

$$u_i : x \mapsto R_i(\phi_{ip_i}^o(x), v_{p_i}(x)), \quad (\text{D.10})$$

which is an embedding of $V_i \cup z \circ V_i$ onto \mathbb{R}^{d+1} so that $u_i(V_i \cup z \circ V_i)$ does not meet all the axes of \mathbb{R}^{d+1} . Note that since $v_{z \circ p}(z \circ x) = -v_p(x)$ and $\phi_{ip_i}^o(z \circ x) = -\phi_{ip_i}^o(x)$, we have $u_i(z \circ x) = -u_i(x)$. Define

$$\bar{u} : x \mapsto (u_1(x), \dots, u_L(x)). \quad (\text{D.11})$$

Since locally $d\bar{u}$ is of full rank and

$$\bar{u}(z \circ x) = (u_1(z \circ x), \dots, u_L(z \circ x)) = -(u_1(x), \dots, u_L(x)) = -\bar{u}(x), \quad (\text{D.12})$$

\bar{u} is clearly a symmetric immersion from \mathbf{M} to $\mathbb{R}^{L(d+1)}$. Denote

$$\epsilon = \min_{i=1, \dots, L} \min_{x \in V_i \cup z \circ V_i} \min_{k=1, \dots, d+1} \langle u_i(x), e_k \rangle, \quad (\text{D.13})$$

where $\{e_k\}_{k=1, \dots, d+1}$ is the canonical basis of \mathbb{R}^{d+1} . By the construction of u_i , $\epsilon > 0$.

By the construction of the covering $\{O_i \cup g \circ O_i\}_{i=1}^L$, we know $L \geq 2$. We claim that by properly perturbing \bar{u} , we can generate a symmetric 1–1 immersion from \mathbf{M} to $\mathbb{R}^{L(d+1)}$.

Suppose \bar{u} is 1–1 in $W \subset \mathbf{M}$, which is invariant under \mathbb{Z}_2 action by the construction of \bar{u} . Consider a symmetric closed subset $K \subset W$. Let $O_i^1 = W \cap (O_i \cup g \circ O_i)$ and $O_i^2 = (\mathbf{M} \setminus K) \cap (O_i \cup g \circ O_i)$. Clearly $\{O_i^1, O_i^2\}_{i=1}^L$ is a covering of \mathbf{M} . Consider a partition of unity $\mathcal{P} = \{\theta_\alpha\}$ subordinate to this covering so that $\theta_\alpha(z \circ x) = \theta_\alpha(x)$ for all α . Index \mathcal{P} by integer numbers so that for all $i > 0$, we have $\text{supp}\theta_i \subset O_i^2$.

We will inductively define a sequence \tilde{u}_k of immersions by properly choosing constants $b_i \in \mathbb{R}^{L(d+1)}$:

$$\tilde{u}_k = \bar{u} + \sum_{i=1}^k b_i s_i \theta_i, \quad (\text{D.14})$$

where $s_i \in C_c^\infty(\mathbf{M})$ so that $\text{supp}(s_i) \subset N_i \cup z \circ N_i$ and

$$s_i(x) = \begin{cases} 1 & \text{when } x \in V_i \\ -1 & \text{when } x \in z \circ V_i \end{cases}. \quad (\text{D.15})$$

Note that u_k by definition will be symmetric. Suppose u_k is properly defined to become an immersion and $\|\tilde{u}_j - \tilde{u}_{j-1}\|_{C^\infty} < 2^{-j-2}\epsilon$ for all $j \leq k$.

Denote

$$D_{k+1} = \{(x, y) \in \mathbf{M} \times \mathbf{M} : s_{k+1}(x)\theta_{k+1}(x) \neq s_{k+1}(y)\theta_{k+1}(y)\}, \quad (\text{D.16})$$

which is of dimension $2d$. Define $G_{k+1} : D_{k+1} \rightarrow \mathbb{R}^{L(d+1)}$ as

$$G_{k+1}(x, y) = \frac{\tilde{u}_k(x) - \tilde{u}_k(y)}{s_{k+1}(x)\theta_{k+1}(x) - s_{k+1}(y)\theta_{k+1}(y)}. \quad (\text{D.17})$$

Since G_{k+1} is differentiable and $L \geq 2$, by Sard's Theorem $G_{k+1}(D_{k+1})$ is of measure zero. By choosing $b_{k+1} \notin G_{k+1}(D_{k+1})$ small enough, \tilde{u}_{k+1} can be made an immersion and $\|\tilde{u}_{k+1} - \tilde{u}_k\| < 2^{-k-3}\epsilon$. In this case $\tilde{u}_{k+1}(y_1) = \tilde{u}_{k+1}(y_2)$ implies

$$b_{k+1}(s_{k+1}(x)\theta_{k+1}(x) - s_{k+1}(y)\theta_{k+1}(y)) = \tilde{u}_k(x) - \tilde{u}_k(y). \quad (\text{D.18})$$

Since $b_{k+1} \notin G_{k+1}(D_{k+1})$, this can happen only if $s_{k+1}(x)\theta_{k+1}(x) = s_{k+1}(y)\theta_{k+1}(y)$ and $\tilde{u}_k(x) = \tilde{u}_k(y)$.

Define

$$\tilde{u} = \tilde{u}_L. \quad (\text{D.19})$$

By definition \tilde{u} is a symmetric immersion and differs from \bar{u} by $\epsilon/2$ in C^∞ .

Now we claim that \tilde{u} is 1-1. Suppose $\tilde{u}(x) = \tilde{u}(y)$. Note that by the construction of b_j this implies $s_L(x)\theta_L(x) = s_L(y)\theta_L(y)$ and $u_{L-1}(x) = u_{L-1}(y)$. Inductively we have $\bar{u}(x) = \bar{u}(y)$ and $s_j(x)\theta_j(x) = s_j(y)\theta_j(y)$ for all $j > 0$. Suppose $x \in W$ but $y \notin W$, then $s_j(y)\theta_j(y) = s_j(x)\theta_j(x) = 0$ for all $j > 0$, which is impossible. Suppose both x and y are outside W , then there are two cases to discuss. First, if x and y are both inside V_i for some i , then $s_j(x)\theta_j(x) = s_j(y)\theta_j(y)$ for all $j > 0$ and $\bar{u}(x) = \bar{u}(y)$ imply $x = y$ since \bar{u} embeds V_i . Secondly, if $x \in V_i \setminus V_j$ and $y \in V_j \setminus V_i$ where $i \neq j$, then $s_j(x)\theta_j(x) = s_j(y)\theta_j(y)$ for all $j > 0$ is impossible. In conclusion, \tilde{u} is 1-1.

Since \mathbf{M} is compact and \tilde{u} is continuous, we conclude that \tilde{u} is a symmetric embedding of \mathbf{M} into $\mathbb{R}^{L(d+1)}$. \square

The above Lemma shows that we can always find a symmetric embedding of \mathbf{M} into $\mathbb{R}^{L(d+1)}$ for some $L > 0$. The next Lemma helps us to show that we can further find a symmetric embedding of \mathbf{M} into \mathbb{R}^p for some $p > 0$, which is isometric. We define $s_p := \frac{p(p+1)}{2}$ in the following discussion.

LEMMA D3 There exists a symmetric smooth map Φ from \mathbb{R}^p to \mathbb{R}^{s_p+p} so that $\partial_i \Phi(x)$ and $\partial_{ij} \Phi(x)$, $i, j = 1, \dots, p$, are linearly independent as vectors in \mathbb{R}^{s_p+p} for all $x \neq 0$.

Proof. Denote $x = (x_1, \dots, x_p) \in \mathbb{R}^p$. We define the map Φ from \mathbb{R}^p to \mathbb{R}^{s_p+p} by

$$\Phi : x \mapsto \left(x_1, \dots, x_p, x_1 \frac{e^{x_1} + e^{-x_1}}{2}, x_1 \frac{e^{x_2} + e^{-x_2}}{2}, \dots, x_p \frac{e^{x_p} + e^{-x_p}}{2} \right), \quad (\text{D.20})$$

where $i, j = 1, \dots, p$ and $i \neq j$. It is clear that Φ is a symmetric smooth map, that is, $\Phi(-x) = -\Phi(x)$. Note that

$$\partial_{ij} \left(x_k \frac{e^{x_\ell} + e^{-x_\ell}}{2} \right) = \delta_{jk} \frac{e^{x_i} - e^{-x_i}}{2} + \delta_{ik} \frac{e^{x_j} - e^{-x_j}}{2} + x_k \delta_{j\ell} \frac{e^{x_i} + e^{-x_i}}{2}. \quad (\text{D.21})$$

Thus when $x \neq 0$, for all $i = 1, \dots, p$, $\partial_i \Phi(x)$ and $\partial_{ij} \Phi(x)$, $i, j = 1, \dots, p$, are linearly independent as vectors in \mathbb{R}^{s_p+p} . \square

Combining Lemmas D2 and D3, we know there exists a symmetric embedding $u: \mathbb{M}^d \hookrightarrow \mathbb{R}^{sL(d+1)+L(d+1)}$ so that $\partial_i u(x)$ and $\partial_{ij} u(x)$, $i, j = 1, \dots, d$, are linearly independent as vectors in $\mathbb{R}^{sL(d+1)+L(d+1)}$ for all $x \in \mathbb{M}$. Indeed, we define

$$u = \Phi \circ \tilde{u}. \quad (\text{D.22})$$

Clearly u is a symmetric embedding of \mathbb{M} into $\mathbb{R}^{sL(d+1)+L(d+1)}$. Note that $\tilde{u}(x) \neq 0$, otherwise \tilde{u} is not an embedding. Moreover, by the construction of \tilde{u} , we know $u_i(V_i \cup z \circ V_i)$ is away from the axes of $\mathbb{R}^{L(d+1)}$ by $\epsilon/2$, so the result.

Next we control the metric on $u(\mathbb{M})$ induced by the embedding. By properly scaling u , we have $g - du^2 > 0$. We will assume properly scaled u in the following.

LEMMA D4 Given the atlas \mathcal{A} defined in (D.7), there exists $\xi_i \in C^\infty(V_i, \mathbb{R}^{s_d+d})$ and $\xi_i^z \in C^\infty(z \circ V_i, \mathbb{R}^{s_d+d})$ so that $\xi_i^z - \xi_i > cI_{s_d+d}$ for some $c > 0$ and

$$g - du^2 = \sum_{j=1}^m \eta_j^2 d\xi_j^2 + \sum_{j=1}^m (\eta_j^z)^2 (d\xi_j^z)^2. \quad (\text{D.23})$$

Proof. Fix V_i . By applying the local isometric embedding theorem [35], we have smooth maps $x_i: h_i(V_i) \hookrightarrow \mathbb{R}^{s_d+d}$ and $x_i^z: h_i^z(z \circ V_i) \hookrightarrow \mathbb{R}^{s_d+d}$ so that

$$(h_i^{-1})^* g = dx_i^2 \quad \text{and} \quad ((h_i^z)^{-1})^* g = (dx_i^z)^2, \quad (\text{D.24})$$

where dx_i^2 (resp. $(dx_i^z)^2$) means the induced metric on $h_i(V_i)$ (resp. $h_i^z(z \circ V_i)$) from \mathbb{R}^{s_d+d} . Note that the above relationship is invariant under affine transformation of x_i and x_i^z . By assumption (b) of \mathcal{A} we have $h_i(x) = h_i^z(z \circ x)$ for all $x \in V_i$, so we modify x_i and x_i^z , so that

$$x_i^z = x_i + c_i I_{s_d+d}, \quad (\text{D.25})$$

where $c_i > 0$, $I_{s_d+d} = (1, \dots, 1)^T \in \mathbb{R}^{s_d+d}$ and $x_i(B_1) \cap x_i^z(B_1) = \emptyset$. Denote $c = \max_{i=1}^L \{c_i\}$ and further set

$$x_i^z = x_i + cI_{s_d+d} \quad (\text{D.26})$$

for all i . By choosing x_i and x_i^z in this way, we have embedded V_i and $z \circ V_i$ simultaneously into the same Euclidean space. Note that

$$g = h_i^*(h_i^{-1})^* g = d(x_i \circ h_i)^2 \quad (\text{D.27})$$

on V_i and

$$g = (h_i^z)^*((h_i^z)^{-1})^* g = d(x_i^z \circ h_i^z)^2 \quad (\text{D.28})$$

on $z \circ V_i$. Thus, by defining $\xi_i = x_i \circ h_i$ and $\xi_i^z = x_i^z \circ h_i^z$, and applying the partition of unity with (D.8), we have the results. \square

THEOREM D1 Any smooth, closed manifold (\mathbf{M}, g) with free isometric \mathbb{Z}_2 action admits a smooth symmetric, isometric embedding in \mathbb{R}^p for some $p \in \mathbb{N}$.

Proof. By the remark following Lemma D2 and D3, we have a smooth embedding $u : \mathbf{M} \hookrightarrow \mathbb{R}^N$ so that $g - du^2 > 0$, where $N = s_{L(d+1)} + L(d+1)$. By Lemma D4, with atlas \mathcal{A} fixed, we have

$$g - du^2 = \sum_j \eta_j^2 d\xi_j^2 + \sum_j (\eta_j^z)^2 (d\xi_j^z)^2, \quad (\text{D.29})$$

where $\xi_i^z - \xi_i = cI_{s_d+d}$. Denote $c = \frac{(2\ell+1)\pi}{\lambda}$, where λ and ℓ will be determined later. To ease the notion, we define

$$\gamma_i(x) = \begin{cases} \xi_i(x) & \text{when } x \in N_i \\ \xi_i^z(x) & \text{when } x \in g \circ N_i \end{cases}. \quad (\text{D.30})$$

Then by the definition (D.8), we have

$$g - du^2 = \sum_{j=1}^L \psi_j^2 d\gamma_j^2. \quad (\text{D.31})$$

Given $\lambda > 0$, we can define the following map $u_\lambda : \mathbf{M} \rightarrow \mathbb{R}^{2L}$:

$$u_\lambda = \left(\frac{1}{\lambda} \psi_i \cos(\lambda \gamma_i), \frac{1}{\lambda} \psi_i \sin(\lambda \gamma_i) \right)_{i=1}^L, \quad (\text{D.32})$$

where $\cos(\lambda \gamma_i)$ means taking cosine on each entry of $\lambda \gamma_i$. Set ℓ so that $\frac{(2\ell+1)\pi}{\lambda} > 1$ and we claim that u_λ is a symmetric map. Indeed,

$$\psi_i(z \circ x) \cos(\lambda \gamma_i(z \circ x)) = \psi_i(x) \cos\left(\lambda \left(\gamma_i(x) + \frac{(2\ell+1)\pi}{\lambda}\right)\right) = -\psi_i(x) \cos(\lambda \gamma_i(x)) \quad (\text{D.33})$$

and

$$\psi_i(z \circ x) \sin(\lambda \gamma_i(z \circ x)) = \psi_i(x) \sin\left(\lambda \left(\gamma_i(x) + \frac{(2\ell+1)\pi}{\lambda}\right)\right) = -\psi_i(x) \sin(\lambda \gamma_i(x)). \quad (\text{D.34})$$

Direct calculation gives us

$$g - du^2 = du_\lambda^2 - \frac{1}{\lambda^2} \sum_{j=1}^L d\psi_j^2. \quad (\text{D.35})$$

We show that when λ is big enough, there exists a smooth symmetric embedding w so that

$$dw^2 = du^2 - \frac{1}{\lambda^2} \sum_i^L d\psi_i^2. \quad (\text{D.36})$$

Since for all $\lambda > 0$ we can find an ℓ so that u_λ is a symmetric map without touching ψ_i , we can thus choosing λ as large as possible so that (D.36) is solvable. The solution w provides us with a symmetric isometric embedding $(w, u_\lambda) : \mathbf{M} \hookrightarrow \mathbb{R}^{N+2L}$ so that we have

$$g = du_\lambda^2 + dw^2. \quad (\text{D.37})$$

Now we solve (D.36). Fix V_i and its relative $p \in V_i$. Suppose $w = u + a^2v$ is the solution where $a \in C_c^\infty(V_i)$ with $a = 1$ on $\text{supp}\eta$. We claim if $\epsilon := \lambda^{-1}$ is small enough, we can find a smooth map $v : N_i \rightarrow \mathbb{R}^N$ so that Equation D.36 is solved on V_i .

Equation D.36 can be written as

$$d(u + a^2v)^2 = du^2 - \frac{1}{\lambda^2} \sum_i^L d\psi_i^2, \quad (\text{D.38})$$

which after expansion is

$$\begin{aligned} & \partial_j(a^2\partial_i u \cdot v) + \partial_i(a^2\partial_j u \cdot v) - 2a^2\partial_{ij}u \cdot v + a^4\partial_{iv} \cdot \partial_jv + \partial_i(a^3\partial_j a|v|^2) + \partial_j(a^3\partial_i a|v|^2) \\ & = -\frac{1}{\lambda^2} d\psi_i^2 + 2a^2(\partial_i a\partial_j a + a\partial_{ij}a)|v|^2. \end{aligned} \quad (\text{D.39})$$

To simplify this equation we will solve the following Dirichlet problem:

$$\begin{cases} \Delta(a\partial_{iv} \cdot \partial_jv) = \partial_i(a\Delta v \cdot \partial_jv) + \partial_j(a\Delta v \cdot \partial_iv) + r_{ij}(v, a) \\ a\partial_{iv} \cdot \partial_jv|_{\partial V_i} = 0, \end{cases} \quad (\text{D.40})$$

where

$$r_{ij} = \Delta a\partial_{iv} \cdot \partial_jv - \partial_j a\Delta v \cdot \partial_iv - \partial_j a\partial_{iv}\Delta v + 2\partial_\ell a\partial_\ell(\partial_{iv} \cdot \partial_jv) + 2a(\partial_{i\ell}v \cdot \partial_{j\ell}v - \Delta v \cdot \partial_{ij}v). \quad (\text{D.41})$$

By solving this equation and multiplying it by a^3 , we have

$$\begin{aligned} a^4\partial_{iv} \cdot \partial_jv &= \partial_i(a^3\Delta^{-1}(a\Delta v \cdot \partial_jv)) + \partial_j(a^3\Delta^{-1}(a\Delta v \cdot \partial_iv)) - 3a^2\partial_i a\Delta^{-1}(a\Delta v \cdot \partial_jv) \\ &\quad - 3a^2\partial_j a\Delta^{-1}(a\Delta v \cdot \partial_iv) + a^3\Delta^{-1}r_{ij}(v, a). \end{aligned} \quad (\text{D.42})$$

Plug Equation (D.42) into Equation (D.39), we have

$$\partial_j(a^2\partial_i u \cdot v - a^2N_i(v, a)) + \partial_i(a^2\partial_j u \cdot v - a^2N_j(v, a)) - 2a^2\partial_{ij}u \cdot v = -\frac{1}{\lambda^2} d\psi_i^2 - 2a^2M_{ij}(v, a), \quad (\text{D.43})$$

where for $i, j = 1, \dots, d$

$$\begin{cases} N_i(v, a) = -a\Delta^{-1}(a\Delta v \cdot \partial_iv) - a\partial_i a|v|^2 \\ M_{ij}(v, a) = \frac{1}{2}a\Delta^{-1}r_{ij}(v, a) - (a\partial_{ij}a + \partial_i a\partial_j a)|v|^2 - \frac{3}{2}(\partial_i a\Delta^{-1}(a\Delta v \cdot \partial_jv)) + \partial_j a\Delta^{-1}(a\Delta v \cdot \partial_iv). \end{cases} \quad (\text{D.44})$$

Note that by definition and the regularity theory of elliptic operator, we know both $N_i(\cdot, a)$ and $M_{ij}(\cdot, a)$ are maps in $C^\infty(V_i)$. We will solve Equation (D.43) through solving the following differential system:

$$\begin{cases} \partial_i u \cdot v &= N_i(v, a) \\ \partial_{ij} u \cdot v &= -\frac{1}{\lambda^2} d\psi_i^2 - M_{ij}(v, a). \end{cases} \quad (\text{D.45})$$

Since by construction we know u has linearly independent $\partial_i u$ and $\partial_{ij} u$, $i, j = 1, \dots, d$, we can solve the under-determined linear system (D.45) by

$$v = E(u)F(v, h), \quad (\text{D.46})$$

where

$$E(u) = \left[\begin{pmatrix} \partial_i u \\ \partial_{ij} u \end{pmatrix}^T \begin{pmatrix} \partial_i u \\ \partial_{ij} u \end{pmatrix} \right]^{-1} \begin{pmatrix} \partial_i u \\ \partial_{ij} u \end{pmatrix}^T \quad (\text{D.47})$$

and

$$F(v, \epsilon) = \left(N_i(v, a), -\frac{1}{\lambda^2} d\psi_i^2 - M_{ij}(v, a) \right)^T = \left(N_i(v, a), -\epsilon^2 d\psi_i^2 - M_{ij}(v, a) \right)^T. \quad (\text{D.48})$$

Next we will apply contraction principle to show the existence of the solution v . Substitute $v = \mu v'$ for some $\mu \in \mathbb{R}$ to be determined later. By the fact that $N_i(0, a) = 0$ and $M_{ij}(0, a) = 0$, we can rewrite Equation (D.46) as

$$w = \mu E(u)F(v', 0) + \frac{1}{\mu} E(u)F(0, \epsilon). \quad (\text{D.49})$$

Set

$$\Sigma = \{w \in C^{2,\alpha}(V_i, \mathbb{R}^N); \|w\|_{2,\alpha} \leq 1\} \quad (\text{D.50})$$

and

$$Tw = \mu E(u)F(v', 0) + \frac{1}{\mu} E(u)F(0, \epsilon). \quad (\text{D.51})$$

By taking

$$\mu = \left(\frac{\|E(u)F(0, \epsilon)\|_{2,\alpha}}{\|E(u)\|_{2,\alpha}} \right)^{1/2}, \quad (\text{D.52})$$

we have

$$\|Tw\|_{2,\alpha} \leq \mu \|E(u)\|_{2,\alpha} \|F(v', 0)\|_{2,\alpha} + \frac{1}{\mu} \|E(u)F(0, \epsilon)\|_{2,\alpha} = C_1 (\|E(u)\|_{2,\alpha} \|E(u)F(0, \epsilon)\|_{2,\alpha})^{1/2}, \quad (\text{D.53})$$

where C_1 depends only on $\|a\|_{4,\alpha}$. Thus T maps Σ into Σ if $\|E(u)\|_{2,\alpha} \|E(u)F(0, \epsilon)\|_{2,\alpha} \leq 1/C_1^2$. This can be achieved by taking ϵ small enough, that is, by taking λ big enough.

Similarly we have

$$\begin{aligned} \|Tw_1 - Tw_2\|_{2,\alpha} &\leq \mu \|E(u)\|_{2,\alpha} \|F(w_1, 0) - F(w_2, 0)\|_{2,\alpha} \\ &\leq C_2 \|w_1 - w_2\|_{2,\alpha} (\|E(u)\|_{2,\alpha} \|E(u)F(0, \epsilon)\|_{2,\alpha})^{1/2}. \end{aligned} \quad (\text{D.54})$$

Then if $\|E(u)\|_{2,\alpha} \|E(u)F(0, \epsilon)\|_{2,\alpha} \leq \frac{1}{C_1^2 + C_2^2}$ we show that T is a contraction map. By the contraction mapping principle, we have a solution $v \in \Sigma$.

Further, since we have

$$v = \mu^2 E(u)F(w, 0) + E(u)F(0, \epsilon), \quad (\text{D.55})$$

by definition of μ , we have

$$\|v\|_{2,\alpha} \leq C \|E(u)F(0, \epsilon)\|_{2,\alpha}, \quad (\text{D.56})$$

where C is independent of u and v . Thus by taking ϵ small enough, we can not only make $w = u + a^2v$ satisfy Equation (D.36), but also make w an embedding. Thus we are done with the patch V_i .

Now we take care V_i 's companion $z \circ V_i$. Fix charts around $x \in V_i$ and $z \circ x \in z \circ V_i$ so that $y \in V_i$ and $g \circ y \in z \circ V_i$ have the same coordinates for all $y \in V_i$. Working on these charts, we have

$$\partial_j u = \partial_j(\Phi \circ \tilde{u}) = \partial_\ell \Phi \partial_j \tilde{u}^\ell \quad (\text{D.57})$$

and

$$\partial_{ij} u = \partial_{ij}(\Phi \circ \tilde{u}) = \partial_{k\ell} \Phi \partial_i \tilde{u}^k \partial_j \tilde{u}^\ell + \partial_\ell \Phi \partial_{ij} \tilde{u}^\ell. \quad (\text{D.58})$$

Note that, since the first derivative of Φ is an even function while the second derivative of Φ is an odd function and $\tilde{u}(g \circ y) = -\tilde{u}(y)$ for all $y \in N_i$, we have

$$E(u)(z \circ x) = -E(u)(x). \quad (\text{D.59})$$

Moreover, we have $N_i(v, a) = N_i(-v, a)$ and $M_{ij}(v, a) = M_{ij}(-v, a)$ for all $i, j = 1, \dots, d$. Thus in $g \circ N_i$, we have $-v$ as the solution to Equation (D.45) and $w - a^2v$ as the modified embedding. After finishing the perturbation of V_i and $z \circ V_i$, the modified embedding is again symmetric.

Inductively, we can perturb the embedding of V_i for all $i = 1, \dots, L$. Since there are only finitely many patches, by choosing ϵ small enough, we finish the proof. \square

Note that we do not show the optimal dimension p of the embedded Euclidean space, but simply show the existence of the symmetric isometric embedding. How to take the symmetry into account in the optimal isometric embedding will be reported in the future work.

COROLLARY D1 Any smooth, closed non-orientable manifold (M, g) has an orientable double covering embedded symmetrically inside \mathbb{R}^p for some $p \in \mathbb{N}$.

Proof. It is well known that the orientable double covering of M has isometric free \mathbb{Z}_2 action. By applying [Theorem D1](#) we get the result. \square