EMBEDDING RIEMANNIAN MANIFOLDS BY THE HEAT KERNEL OF THE CONNECTION LAPLACIAN

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Abstract. Given a class of closed Riemannian manifolds with prescribed geometric conditions, we introduce an embedding of the manifolds into ℓ^2 based on the heat kernel of the Connection Laplacian associated with the Levi-Civita connection on the tangent bundle. As a result, we can construct a distance in this class which leads to a pre-compactness theorem on the class under consideration.

1. Introduction

In [2], the following class of closed Riemannian manifolds $\mathcal{M}_{d,k,D}$ with prescribed geometric constrains are considered:

$$\mathcal{M}_{d,k,D} = \{(M,g)|\,\dim(M) = d,\, \mathrm{Ric}(g) \geq (d-1)kg,\, \mathrm{diam}(M) \leq D\},$$

where Ric is the Ricci curvature and diam is the diameter. The authors embed $M \in \mathcal{M}_{d,k,D}$ into the space ℓ^2 of real-valued, square integrable series by considering the heat kernel of the Laplace-Beltrami operator of M. A distance on $\mathcal{M}_{d,k,D}$, referred to as the spectral distance, is then introduced based on the embedding so that the class under consideration is precompact.

Over the past decades many works in the manifold learning field benefit from this embedding scheme, for example, the diffusion map [3] and the manifold parameterizations [6]. Recently, a new mathematical framework, referred to as the *vector diffusion maps* (VDM), for organizing and analyzing massive high dimensional data sets, images and shapes was introduced in [7]. In brief, VDM is a mathematical and algorithmic generalization of diffusion maps and other non-linear dimensionality reduction methods. While diffusion maps are based on the heat kernel of the Laplace-Beltrami operator over the manifold, VDM is based on the heat kernel of the connection Laplacian associated with the Levi-Civita connection on the tangent bundle of the manifold. The introduction of VDM was motivated by the problem of finding an efficient way to organize complex data sets, embed them in a low dimensional space, and interpolate and regress vector fields over the data. In particular, it equips the data with a metric, which we refer to as the *vector diffusion distance*. The application of VDM to the cyro-electron microscopy problem, which is aimed to reconstruct the three dimensional geometric structure of the macromolecule, provides a better organization of the given noisy projection images, and hence a better reconstruction result [5, 9]. Furthermore, the VDM can be slightly modified to determine the orientability of a manifold and obtain its orientable double covering if the manifold is non-orientable [8].

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In this paper, we consider the same class of closed Riemannian manifolds $\mathcal{M}_{d,k,D}$ and focus on the connection Laplacian associated with the Levi-Civita connection on the tangent bundle. We analyze how the VDM embeds the manifold $M \in \mathcal{M}_{d,k,D}$ into ℓ^2 based on the heat kernel of the connection Laplacian of the tangent bundle. Based on the vector diffusion distance, we introduce a new spectral distance referred to as *vector spectral distance* on $\mathcal{M}_{d,k,D}$, which leads to the pre-compactness result.

The paper is organized in the following way. We start from providing the background material in Section 2, and then define the vector diffusion maps in Section 3 and discuss its embedding property. In Section 4 we define a new metric in the manifold set $\mathcal{M}_{d,k,D}$, referred to as *the vector spectral distance*. The key ingredients in this section are the generalized Kato's type inequality comparing the trace of the heat kernel of the Laplace-Beltrami operator and the trace of the heat kernel of the connection Laplacian and a nice isoperimetric inequality for heat kernel comparisons. With these key ingredients we show that the vector spectral distance is a distance between isometry classes of Riemannian manifolds in $\mathcal{M}_{d,k,D}$. With the vector spectral distance, in Section 5 the pre-compactness of the manifold set $\mathcal{M}_{d,k,D}$ is derived from the Rellich's Theorem and the following Lemma:

Lemma 1.1. [2, Lemma 15] *Let (E, δ) be a metric space. Let $\mathcal{F}(E)$ denote the set of non-empty closed subsets of E, equipped with the Hausdorff distance h_δ associated with δ. If the metric space (E, δ) is precompact, so is the metric space $(\mathcal{F}(E), h_\delta)$.*

In fact, we view the vector diffusion maps of a given manifold in $\mathcal{M}_{d,k,D}$ as a point of a set consisting of all embedded manifolds in $\mathcal{M}_{d,k,D}$, and then apply Lemma 1.1 to show the pre-compactness of $\mathcal{M}_{d,k,D}$.

2. Background material

Let (M, g) be a closed Riemannian manifold and TM the tangent bundle. Denote $C^\infty(TM)$ the smooth vector fields and $L^2(TM)$ the vector fields satisfying

$$\int_M \langle X, X\rangle(x) \mathrm{d}V(x) \leq \infty,$$

where $\mathrm{d}V$ is the volume form associated with g and $\langle X, X\rangle(x) := g(X(x), X(x))$. Denote ∇ the Levi-Civita connection of $\mathcal{M}$ and $P_{x,y}$ the parallel transport from y to x via the geodesic linking them. Denote ∇^2 the connection Laplacian associated ∇ on the tangent bundle TM [4]. The connection Laplacian ∇^2 is a self-adjoint, second order elliptic operator [4]. From the classical elliptic theory [4] we know that the heat semigroup, $e^{t\nabla^2}$, $t > 0$, with the infinitesimal generator ∇^2 is a family of self-adjoint operators with the heat kernel $k_{TM}(t, x, y)$ so that

$$e^{t\nabla^2} X(x) = \int_M k_{TM}(t, x, y) X(y) \mathrm{d}V(y).$$

The heat kernel $k_{TM}(t, x, y)$ is smooth in x and y and analytic in t [4].

It is well known [4] that the spectrum of ∇^2 is discrete inside $\mathbb{R}^-$, the non-positive real numbers, and the only possible accumulation point is $-\infty$. We will denote the spectrum of ∇^2 as $\{-\lambda_k\}_{k=1}^\infty$, where $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \ldots$, and its eigen-vector fields as $\{X_k\}_{k=1}^\infty$. Notice that λ_0 may not exist due to the topological obstruction. For example, we can not find a nowhere non-vanishing vector field on S^2. In other words, $\nabla^2 X_k = -\lambda_k X_k$ for all $k = 1, 2, \ldots$. It is also well known [4] that $\{X_k\}_{k=1}^\infty$ form an orthonormal basis for $L^2(TM)$. Denote the heat kernel of ∇^2 by $k_{TM}(t,x,y)$, which can be expressed as [4]:

$$k_{TM}(t,x,y)=\sum_{n=1}^{\infty}e^{-\lambda_n t}X_n(x)\otimes\overline{X_n(y)}.$$

A calculation of the Hilbert-Schmidt norm of the heat kernel at (t,x,y) gives

$$\begin{aligned}\|k_{TM}(t,x,y)\|_{HS}^2 &= \mathrm{Tr}\left[k_{TM}(t,x,y)\overline{k_{TM}(t,x,y)}\right]\\ &= \sum_{n,m=1}^{\infty}e^{-(\lambda_n+\lambda_m)t}\langle X_n(x),X_m(x)\rangle\overline{\langle X_n(y),X_m(y)\rangle}.\end{aligned}\tag{1}$$

On the other hand, the classical elliptic theory [4] allows us to decompose $L^2(TM)$ as $L^2(TM)=\oplus_{k=1}^\infty E_k$, where E_k is the eigenspace of ∇^2 corresponding to increasing eigenvalues, denoted as ν_k. Denote by $m(\nu_k)$ the multiplicity of ν_k. It is also well known that $m(\nu_k)$ is finite. Denote $\mathcal{B}(E_k)$ the set of bases of E_k, which is identical to the orthogonal group $O(m(\nu_k))$. Denote the set of the corresponding orthonormal bases of $L^2(TM)$ by

$$\mathcal{B}(M,g)=\Pi_{k=1}^\infty\mathcal{B}(E_k).$$

By Tychonoff's theorem, we know $\mathcal{B}(M,g)$ is compact since $O(m(\nu_k))$ is compact for all $k\in\mathbb{N}$. Also note that the dot products $\langle X_n(x),X_m(x)\rangle$, where $n,m\in\mathbb{N}$, are invariant to the choice of basis for T_xM.

3. Vector Diffusion Mappings

Based on these observations, given $a\in\mathcal{B}(M,g)$ and $t>0$, the authors in [7] define the *vector diffusion mappings* V_t^a which maps $x\in M$ to the Hilbert space ℓ^2 by[1]:

$$V_t^a : x\mapsto \mathrm{Vol}(M)\left(e^{-(\lambda_n+\lambda_m)t/2}\langle X_n(x),X_m(x)\rangle\right)_{n,m=1}^{\infty},\tag{2}$$

where $a=\{X_n\}_{n=1}^\infty$. A direct calculation shows that

$$\|k_{TM}(t,x,y)\|_{HS}^2=\frac{1}{\mathrm{Vol}(M)^2}\langle V_t^a(x),V_t^a(y)\rangle_{\ell^2}.\tag{3}$$

Fix $a\in\mathcal{B}(M,g)$. For all $t>0$, the following Theorem states that the vector diffusion mapping V_t^a is an embedding of the compact Riemannian manifold M into ℓ^2. The proof of the theorem is given in [7, Theorem 8.1].

Theorem 3.1. *Given a d-dim closed Riemannian manifold (M,g) and an orthonormal basis $a=\{X_k\}_{k=1}^\infty$ of $L^2(TM)$ composed of the eigenvector-fields of the connection Laplace ∇^2, then for any $t>0$, the vector diffusion map V_t^a is a diffeomorphic embedding of M into ℓ^2.*

It is Theorem 3.1 that allows the authors to define the *vector diffusion distance* between $x,y\in M$, denoted as $d_{\mathrm{VDM},t}(x,y)$, in [7]:

$$d_{\mathrm{VDM},t}(x,y):=\|V_t^a(x)-V_t^a(y)\|_{\ell^2},\tag{4}$$

[1]Note that the basis a and the volume of M are not taken into consideration in the definition of the vector diffusion map in [7]. To prove the precompactness theorem, we need to take them into consideration.

which is clearly a distance function over M. We mention that by the following expansion

$$
\begin{aligned}
& d^2_{\mathrm{VDM},t}(x,y) = \|V^a_t(x) - V^a_t(y)\|^2_{\ell^2} \\
= & \operatorname{Vol}(M)^2 \sum_{n,m=1}^{\infty} e^{-(\lambda_n+\lambda_m)t}(\langle X_n(x), X_m(x)\rangle - \langle X_n(y), X_m(y)\rangle)^2 \\
= & \operatorname{Vol}(M)^2 \big[\operatorname{Tr}(k_{TM}(t,x,x)k_{TM}(t,x,x)^*) + \\
& \operatorname{Tr}(k_{TM}(t,y,y)k_{TM}(t,y,y)^*) - 2\operatorname{Tr}(k_{TM}(t,x,y)k_{TM}(t,x,y)^*)\big],
\end{aligned} \tag{5}
$$

the defined vector diffusion distance $d_{\mathrm{VDM},t}$ does not depend on the choice of the basis a. The following theorem shows that in this asymptotic limit the vector diffusion distance behaves like the geodesic distance. The proof of the theorem is given in [7, Theorem 8.2].

Theorem 3.2. *Let (M,g) be a smooth d-dim closed Riemannian manifold. Suppose $x, y \in M$ so that $x = \exp_y v$, where $v \in T_yM$. For any $t > 0$, when $\|v\|^2 \ll t \ll 1$ we have the following asymptotic expansion of the vector diffusion distance:*

$$d^2_{\mathrm{VDM},t}(x,y) = d\operatorname{Vol}(M)^2(4\pi)^{-d}\frac{\|v\|^2}{t^{d+1}} + O(t^{-d}\|v\|^2)$$

4. Vector Spectral Distances

In this section and the next, we show that based on the vector diffusion map V^a_t, we can define a family of *vector spectral distance* d_t, $t > 0$, on the space of the isometry classes in $\mathcal{M}_{d,k,D}$ so that for any $t > 0$ the space of the isometry classes in $\mathcal{M}_{d,k,D}$ is d_t-precompact.

Denote the Laplace-Beltrami operator over (M,g) by Δ_M and its eigenvalues and eigenfunctions by $-\mu_k$ and ϕ_k, where $k \in \{0\} \cup \mathbb{N}$, that is, $\Delta_M \phi_k = -\mu_k \phi_k$, so that $\mu_0 = 0 < \mu_1 \le \mu_2 \ldots$. Define the following partition functions

$$Z_{TM}(t) := \sum_{j=1}^{\infty} e^{-\lambda_j t}$$

and

$$Z_M(t) := \sum_{j=0}^{\infty} e^{-\mu_j t},$$

which are related by the following generalized Kato's type inequality [1, p. 135]:

$$Z_{TM}(t) \le dZ_M(t) \text{ for all } t > 0. \tag{6}$$

Then recall the following result:

Theorem 4.1. [1, p.108 C.26] *Let (M,g) be an d-dimensional closed Riemannian manifold. Define*

$$r_{min}(M) = \inf\{\operatorname{Ric}(v,v) : \|v\| = 1\}$$

and the diameter of M by $D(M)$. If (M,g) satisfies $r_{min}(M)D(M)^2 \ge (d-1)\epsilon\alpha^2$ for $\epsilon \in \{-1,0,1\}$ and $\alpha > 0$, then

$$\operatorname{Vol}(M)k_M(t,x,x) \le \operatorname{Vol}(S^d(R))k_{S^d}(t,y,y) = Z_{S^d(R)}(t) = Z_{S^d(1)}(t/R^2), \tag{7}$$

where $y \in S^d(R)$, $R = D(M)/a(d,\epsilon,\alpha)$ *and*

$$a(d,\epsilon,\alpha) = \begin{cases} \alpha\omega_d^{1/d}\left(2\int_0^{\alpha/2}\cos^{d-1}(t)\mathrm{d}t\right)^{-1/d} & \text{if} \quad \epsilon = 1 \\ (1+d\omega_d)^{1/d} - 1 & \text{if} \quad \epsilon = 0 \\ \alpha c(\alpha) & \text{if} \quad \epsilon = -1, \end{cases}$$

where $\omega_d = \mathrm{Vol}(S^d)/\mathrm{Vol}(S^{d-1})$ *and* $c(\alpha)$ *is the unique positive root* $z > 0$ *of the equation*

$$z\int_0^\alpha (\cosh(t) + z\sinh(t))^{d-1}\mathrm{d}t = \omega_d.$$

With inequalities (6) and (7), we prove the following lemmas, which is essential in showing the pre-compactness result. We omit the dependence on M to simplify the statement of the lemmas and the proof.

Lemma 4.2. *With the above notations, there exist positive constants* $A(d,k,D)$, $B(d,k,D)$ *and* $E(d,k,D)$ *that depend only on* d,k *and* D *such that for any* $(M,g) \in \mathcal{M}_{d,k,D}$*:*
(a) $\lambda_j \geq A(d,k,D)j^{2/d}$*;*
(b) $N(\lambda) := \#\{j \mid j \geq 0,\ \lambda_j \leq \lambda\} \leq ed + B(d,k,D)\lambda^{d/2}$*;*
(c) *for all* $x \in M$ *and* $\alpha \geq 0$*, we have*

$$\sum_{n,m\geq 1}(\lambda_n+\lambda_m)^\alpha e^{-t(\lambda_n+\lambda_m)}\langle X_n(x), X_m(x)\rangle^2 \leq \frac{E(d,k,D)}{\mathrm{Vol}(M)^2}F(\alpha,d)t^{-\alpha-d}, \tag{8}$$

where

$$F(\alpha,d) = \int_0^\infty\int_0^\infty (x+y)^\alpha x^d y^d e^{-(x+y)}\mathrm{d}x\mathrm{d}y. \tag{9}$$

Proof. The proofs for (a) and (b) are almost the same as the proofs of Theorem 3 in [2] except that we apply (6). We provide the proofs here for completion. If $k \geq 0$, $r_{min}D^2 \geq 0$ and if $k < 0$, $r_{min}D^2 \geq (d-1)kD$. Thus we can apply Theorem 4.1 with ϵ and α depending only on k and D. Thus,

$$\begin{aligned} Z_{TM}(t) &\leq dZ_M(t) = d\int_M k_M(t,x,x)\mathrm{d}x \leq d\mathrm{Vol}(M)\sup_{x\in M}k_M(t,x,x) \\ &\leq d\mathrm{Vol}(S^d(R))k_{S^d(R)}(t,y,y) = dZ_{S^d(R)}(t) = dZ_{S^d(1)}(t/R^2), \end{aligned}$$

where $y \in S^d(R)$. The trace of the heat kernel Z_{TM} is thus uniformly bounded on the set $\mathcal{M}_{d,k,D}$. Note that there exists a constant $b(d)$, depending on d only, such that for any $t > 0$,

$$Z_{S^d(1)}(t) - 1 \leq b(d)t^{-d/2}.$$

Also not that $j \leq N(\lambda_j)$, $j \in \mathbb{N}\cup\{0\}$, in general, and $j = N(\lambda_j)$ when all eigenvalues are simple. As a consequence, we have

$$\begin{aligned} j \leq N(\lambda_j) &\leq e\sum_{0\leq\lambda_i\leq\lambda_j} e^{-\lambda_i/\lambda_j} \leq eZ_{TM}(1/\lambda_j) \\ &\leq edZ_{S^d(1)}\left(\frac{1}{\lambda_j R^2}\right) \leq ed + edb(d)R^d\lambda_j^{d/2} \end{aligned}$$

and hence

$$\lambda_j \geq \left(\frac{j-ed}{edb(d)R^d}\right)^{2/d} \geq (edb(d)R^d)^{-2/d}j^{2/d}.$$

Since $R = a(d,\epsilon,\alpha)D(M) \leq a(d,\epsilon,\alpha)D$ and $a(d,\epsilon,\alpha)$ only depends on d, k and D, this proves (1) and (2).

Next we prove (c). Define the positive measure μ_x on $\mathbb{R}_+ \times \mathbb{R}_+$ by

$$\mathrm{d}\mu_x = \sum_{n,m\geq 1} \langle X_n(x), X_m(x)\rangle^2 \delta_{\lambda_n} \times \delta_{\lambda_m}$$

where δ_{λ_n} is the Dirac measure at $\lambda_n \in \mathbb{R}_+$. By the Cauchy-Schwartz inequality:

$$\langle X_n(x), X_m(x)\rangle^2 \leq \langle X_n(x), X_n(x)\rangle \langle X_m(x), X_m(x)\rangle, \tag{10}$$

Thus, the left hand side of (8) can be bounded by:

$$\begin{aligned}
&\sum_{n,m\geq 1} (\lambda_n+\lambda_m)^\alpha e^{-t(\lambda_n+\lambda_m)} \langle X_n(x), X_m(x)\rangle^2 \\
=\ & \int_{\mathbb{R}}\int_{\mathbb{R}} (\lambda+\nu)^\alpha e^{-t(\lambda+\nu)} \langle X_n(x), X_m(x)\rangle^2 \mathrm{d}\mu_x \\
\leq\ & \int_{\mathbb{R}}\int_{\mathbb{R}} (\lambda+\nu)^\alpha e^{-t(\lambda+\nu)} \langle X_n(x), X_n(x)\rangle \langle X_n(x), X_n(x)\rangle \mathrm{d}\mu_x
\end{aligned} \tag{11}$$

Define a $L^1_{loc}(\mathbb{R})$ function:

$$\mu(\lambda) := \sum_{n:\ 0\leq\lambda_n\leq\lambda} \langle X_n(x), X_n(x)\rangle.$$

Since $t > 0$, $(\lambda+\nu)e^{-t(\lambda+\nu)}$ decays fast enough. So by the definition of the derivative of a given distribution, (11) becomes

$$\begin{aligned}
&\int_{\mathbb{R}}\int_{\mathbb{R}} (\lambda+\nu)^\alpha e^{-t(\lambda+\nu)} \langle X_n(x), X_n(x)\rangle \langle X_n(x), X_n(x)\rangle \mathrm{d}\mu_x \\
=\ & \int_{\mathbb{R}}\int_{\mathbb{R}} (\lambda+\nu)^{\alpha-1} e^{-t(\lambda+\nu)} ((\lambda+\nu)t-\alpha)\mu(\lambda)\mathrm{d}\lambda \frac{\mathrm{d}\mu(\nu)}{\mathrm{d}\nu} \\
=\ & \int_0^\infty\int_0^\infty \left[t^2(\lambda+\nu)^2 - 2\alpha t(\lambda+\nu) + \alpha(\alpha-1)\right] \times \\
& \qquad (\lambda+\nu)^{\alpha-2} e^{-t(\lambda+\nu)} \mu(\lambda)\mu(\nu)\mathrm{d}\lambda\mathrm{d}\nu.
\end{aligned}$$

To finish the proof, we claim that:

$$\sum_{k=1}^\infty e^{-\lambda_k t} \langle X_k(x), X_k(x)\rangle \leq k_M(t,x,x). \tag{12}$$

Indeed, by Cauchy-Schwartz inequality and the positivity of the metric, for $t > 0$ we have

$$\begin{aligned}
&\Big(\sum_{k=1}^\infty e^{-\lambda_k t} \langle X_k(x), X_k(x)\rangle\Big)^2 \\
=& \sum_{k,l=1}^\infty e^{-(\lambda_k+\lambda_l)t} \langle X_k(x), X_k(x)\rangle \langle X_l(x), X_l(x)\rangle \\
=& \|k_{TM}(t,x,x)\|^2_{HS} \leq k^2_M(t,x,x),
\end{aligned}$$

where the last quality holds due to the fact that $\|k_{TM}(t,x,x)\|_{HS} \leq k_M(t,x,x)$ [2, p137] for all $t > 0$ and $x \in M$.

Now we bound $\mu(\lambda)$ when $\lambda > 0$. By (7) and (12) we have

$$\begin{aligned}
\mu(\lambda) &= \sum_{n:\ 0\le\lambda_n\le\lambda} \langle X_n(x), X_n(x)\rangle \le e \sum_{n:\ 0\le\lambda_n\le\lambda} e^{-\lambda_n/\lambda}\langle X_n(x), X_n(x)\rangle \\
&\le e\sum_{n=1}^{\infty} e^{-\lambda_n/\lambda}\langle X_n(x), X_n(x)\rangle \le e k_M(1/\lambda, x, x) \\
&\le \frac{e}{\mathrm{Vol}(M)} Z_{S^n}(1/\lambda R^2) \le \frac{C(d,k,D)}{\mathrm{Vol}(M)}\lambda^{d/2}, \qquad (13)
\end{aligned}$$

where R is defined in Theorem 4.1 and $C(d, k, D)$ is an universal constant depending on d, k and D. Thus we conclude

$$\begin{aligned}
&\sum_{n,m\ge 1} (\lambda_n+\lambda_m)^{\alpha} e^{-t(\lambda_n+\lambda_m)} \langle X_n(x), X_m(x)\rangle^2 \\
\le\ & \frac{C(d,k,D)^2}{\mathrm{Vol}(M)^2} \int_0^\infty \int_0^\infty \left[t^2(\lambda+\nu)^2 - 2\alpha t(\lambda+\nu) + \alpha(\alpha-1)\right] \times \\
& \qquad (\lambda+\nu)^{\alpha-2} e^{-t(\lambda+\nu)} \lambda^d \nu^d \mathrm{d}\lambda \mathrm{d}\nu \\
\le\ & \frac{E(d,k,D)}{\mathrm{Vol}(M)^2} F(\alpha, d) t^{-\alpha-d},
\end{aligned}$$

where $E(d, k, D)$ is an universal positive constant that depends only on d, k and D, and F is defined in (9). □

Recall that the vector diffusion map V_t^a depends on the choice of an orthonormal basis a of eigen-vector fields. Given a finite dimensional Euclidean space E, we can define the distance between $R_1, R_2 \in O(\mathrm{dim}E)$ by

$$d_E(R_1, R_2) = \|R_1^{-1}R_2 - I\|_{HS}.$$

It is clear that $d_E(R_1, R_2) \le 2\sqrt{\mathrm{dim}E}$. As we discussed above, $\mathcal{B}(M, g)$ is a compact set with respect to the product topology. This topology can be described by the distance $d_{\mathcal{B}(M,g)}$ between $a, b \in \mathcal{B}(M, g)$ defined as

$$d_{\mathcal{B}(M,g)}(a,b)^2 = \sum_{i=1}^{\infty} \nu_i^{-N} d_{E_i}(a|_{E_i}, b|_{E_i})^2, \qquad (14)$$

where the series on the right hand side converges when $N > d/2$ due to Lemma 4.2(a).

Lemma 4.3. *Let (M, g) be a smooth d-dim closed Riemannian manifold. The map $V : \mathbb{R}_+ \times \mathcal{B}(M, g) \times M \to \ell^2$ defined by $V(t, a, x) := V_t^a(x)$ is continuous and satisfies:*

$$\begin{aligned}
&\|V_t^a(x) - V_s^b(y)\|_{\ell^2}^2 \le \mathrm{Vol}(M)^2 \Big\{ \|k_{TM}(t,x,x)\|_{HS} + \|k_{TM}(s,y,y)\|_{HS} \\
&-2\left\|k_{TM}\left(\frac{t+s}{2}, x, y\right)\right\|_{HS} + 2d_{\mathcal{B}(M,g)}(a,b) k_{TM}^{(N)}(t,x,x)^{1/2} k_{TM}^{(N)}(s,y,y)^{1/2}\Big\} \qquad (15)
\end{aligned}$$

where $t > 0$, $a, b \in \mathcal{B}(M, g)$, $x, y \in M$, and

$$k_{TM}^{(N)}(t,x,x) = \sum_{n,m=1}^{\infty} (\lambda_n^{N/2} + \lambda_m^{N/2}) e^{-t(\lambda_n+\lambda_m)} \langle X_n^a(x), X_m^a(x)\rangle^2. \qquad (16)$$

Proof. We denote the basis $a \in \mathcal{B}(M,g)$ by $\{X_n^a\}_{n=1}^\infty$. First we have

$$
\begin{aligned}
&\|V_t^a(x) - V_s^b(y)\|_{\ell^2}^2\\
=&\mathrm{Vol}(M)^2 \sum_{n,m=1}^\infty \Big(e^{-t(\lambda_n+\lambda_m)/2}\langle X_n^a(x), X_m^a(x)\rangle - e^{-s(\lambda_n+\lambda_m)/2}\langle X_n^b(y), X_m^b(y)\rangle\Big)^2\\
=&\mathrm{Vol}(M)^2\Big\{\|k_{TM}(t,x,x)\|_{HS} + \|k_{TM}(s,y,y)\|_{HS}\\
&-2\sum_{n,m=1}^\infty e^{-(t+s)(\lambda_n+\lambda_m)/2}\langle X_n^a(x), X_m^a(x)\rangle\langle X_n^b(y), X_m^b(y)\rangle\Big\}\\
=&\mathrm{Vol}(M)^2\Big\{\|k_{TM}(t,x,x)\|_{HS} + \|k_{TM}(s,y,y)\|_{HS} - \left\|k_{TM}\left(\frac{t+s}{2},x,y\right)\right\|_{HS}\\
&-2\sum_{n,m=1}^\infty e^{-(t+s)(\lambda_n+\lambda_m)/2}\langle X_n^a(x), X_m^a(x)\rangle\Big(\langle X_n^b(y), X_m^b(y)\rangle - \langle X_n^a(y), X_m^a(y)\rangle\Big)\Big\},
\end{aligned}
$$

where we denote the last summation on the right hand side as A. Denote the eigenvector fields inside the eigenspace E_n by $X^b_{n(j)}(y)$, where $j = 1, ..., m(\nu_n)$, when the basis of $L^2(TM)$ is chosen to be $b \in \mathcal{B}(M,g)$. By definition, we have the following relationship:

$$
X^b_{n(j)}(y) = \sum_{k=1}^{m(\nu_n)} \alpha_{j,k}(b,a) X^a_{n(k)}(y)
$$

where the matrix $[\alpha_{j,k}(b,a)]_{k,j=1}^{m(\nu_j)} \in O(m(\nu_n))$. Thus we can rewrite A as

$$
\begin{aligned}
A =& \sum_{n,m=1}^\infty e^{-(t+s)(\nu_n+\nu_m)/2} \sum_{k=1}^{m(\nu_n)}\sum_{l=1}^{m(\nu_m)} \langle X^a_{n(k)}(x), X^a_{m(l)}(x)\rangle \times\\
&\left(\langle X^a_{n(k)}(y), X^a_{m(l)}(y)\rangle - \sum_{i=1}^{m(\nu_n)}\sum_{j=1}^{m(\nu_m)} \alpha_{k,i}(b,a)\alpha_{l,l}(b,a)\langle X^a_{n(i)}(y), X^a_{n(j)}(y)\rangle\right)\\
=& \sum_{n,m=1}^\infty e^{-(t+s)(\nu_n+\nu_m)/2} \sum_{i,k=1}^{m(\nu_n)}\sum_{j,l=1}^{m(\nu_m)} \langle X^a_{n(k)}(x), X^a_{m(l)}(x)\rangle \times\\
&\langle X^a_{n(i)}(y), X^a_{m(j)}(y)\rangle\Big(\delta_{k,i}\delta_{l,j} - \alpha_{k,i}(b,a)\alpha_{l,j}(b,a)\Big),
\end{aligned}
$$

where $[\delta_{k,l}]_{k,l=1}^{m(\nu_j)}$ is an $m(\nu_j) \times m(\nu_j)$ identity matrix. Note that

$$
(\delta_{k,i}\delta_{l,j} - \alpha_{k,i}(b,a)\alpha_{l,j}(b,a)) = \delta_{k,i}(\delta_{l,j} - \alpha_{l,j}(b,a)) + \alpha_{l,j}(b,a)(\delta_{k,i} - \alpha_{k,i}(b,a))
$$

which is bounded by $d_{E_n}(a|_{E_n}, b|_{E_n}) + d_{E_m}(a|_{E_m}, b|_{E_m})$. Hence, by the Cauchy-Schwartz inequality, A is bounded by

$$|A| \leq \sum_{n,m=1}^{\infty} e^{-(t+s)(\nu_n+\nu_m)/2} \left(\sum_{k=1}^{m(\nu_n)} \sum_{l=1}^{m(\nu_m)} \langle X^a_{n(k)}(x), X^a_{m(l)}(x) \rangle^2 \right)^{1/2} \times$$

$$\left(\sum_{i=1}^{m(\nu_n)} \sum_{j=1}^{m(\nu_m)} \langle X^a_{n(i)}(y), X^a_{m(j)}(y) \rangle^2 \right)^{1/2} \Big(d_{E_n}(a|_{E_n}, b|_{E_n}) + d_{E_m}(a|_{E_m}, b|_{E_m}) \Big)$$

$$\leq 2 d_{\mathcal{B}(M,g)}(a,b) \sum_{n,m=1}^{\infty} (\nu_n^{N/2} + \nu_m^{N/2}) e^{-(t+s)(\nu_n+\nu_m)/2} \times$$

$$\left(\sum_{k=1}^{m(\nu_n)} \sum_{l=1}^{m(\nu_m)} \langle X^a_{n(k)}(x), X^a_{m(l)}(x) \rangle^2 \right)^{1/2} \left(\sum_{i=1}^{m(\nu_n)} \sum_{j=1}^{m(\nu_m)} \langle X^a_{n(i)}(y), X^a_{m(j)}(y) \rangle^2 \right)^{1/2}$$

$$\leq 2 d_{\mathcal{B}(M,g)}(a,b) \left(\sum_{n,m=1}^{\infty} (\lambda_n^{N/2} + \lambda_m^{N/2}) e^{-t(\lambda_n+\lambda_m)} \langle X^a_n(x), X^a_m(x) \rangle^2 \right)^{1/2} \times$$

$$\left(\sum_{n,m=1}^{\infty} (\lambda_n^{N/2} + \lambda_m^{N/2}) e^{-s(\lambda_n+\lambda_m)} \langle X^a_n(y), X^a_m(y) \rangle^2 \right)^{1/2}$$

$$= 2 d_{\mathcal{B}(M,g)}(a,b) k^{(N)}_{TM}(t,x,x)^{1/2} k^{(N)}_{TM}(s,y,y)^{1/2},$$

where $k^{(N)}_{TM}(t,x,x)$ is defined in (16). Due to Lemma 4.2(c), $k^{(N)}_{TM}(t,x,x)$ is bounded, and thus the proof is finished. □

With the above preparation, we are ready to introduce the vector spectral distance. Recall the following definitions. Suppose (X, δ) is s metric space, where δ is the metric, and $A, B \subset X$. The distance between A and B is defined as:

$$h(A,B) := \inf\{\delta(a,b) : a \in A, b \in B\}.$$

Denote the generalized ball of radius $\epsilon > 0$ around A:

$$\mathcal{N}(A,\epsilon) := \{x \in X : h(x,A) < \epsilon\}.$$

Given two subsets $A, B \subset X$, we can define the Hausdorff distance, denoted as HD, associated with δ by

$$\mathrm{HD}(A,B) = \inf\{\epsilon : A \subset \mathcal{N}(B,\epsilon),\ B \subset \mathcal{N}(A,\epsilon)\},$$

or equivalently

$$\mathrm{HD}(A,B) = \max\Big\{ \sup_{x\in A} \inf_{y \in B} \delta(x,y),\ \sup_{y \in B} \inf_{x\in A} \delta(x,y) \Big\}. \tag{17}$$

In the following, we focus on the metric space $(\ell^2, \|\cdot\|_{\ell^2})$. Let HD denote the Hausdorff distance between compact subsets of ℓ^2 associated with $\|\cdot\|_{\ell^2}$. Given two Riemannian manifolds M and M' and $t > 0$, we define a family of functions

$d_t : \mathcal{M}_{d,k,D} \times \mathcal{M}_{d,k,D} \mapsto \mathbb{R}$ by

$$d_t(M,M') := \max\left\{ \sup_{a\in\mathcal{B}(M,g)} \inf_{a'\in\mathcal{B}(M',g')} \mathrm{HD}(V_t^a(M), V_t^{a'}(M')), \right. \tag{18}$$
$$\left. \sup_{a'\in\mathcal{B}(M',g')} \inf_{a\in\mathcal{B}(M,g)} \mathrm{HD}(V_t^{a'}(M'), V_t^a(M')) \right\}.$$

We justify that d_t, $t>0$, is a distance of the space of the isometry classes in $\mathcal{M}_{d,k,D}$, and call it *vector spectral distance*. The following lemmas are needed for the justification.

Lemma 4.4. *Let (M,g) be a smooth d-dim closed Riemannian manifold and $\{X_n\}_{n\in\mathbb{N}}$ is an orthonormal basis of $L^2(TM)$ constituted of the eigen-vector fields of the connection Laplacian. Then*

$$\mathtt{span}\{\langle X_n, X_m\rangle :\ n,m\in\mathbb{N},\, n\neq m\} = L^2(M)\backslash\{\mathbb{R}\},$$

that is, all L^2 functions over M without the constant functions.

Proof. Fix $f\in L^2(M)$. If $\int_M \langle X_n, X_m\rangle(x) f(x)\mathrm{d}x = \int_M \langle fX_n, X_m\rangle(x)\mathrm{d}x = 0$ for all $n\neq m$, we show that f is constant. Since $\{X_n\}_{n\in\mathbb{N}}$ is an orthonormal basis of $L^2(TM)$, we can rewrite $fX_n = \sum_{k\in\mathbb{N}} \alpha_{n,k} X_k$, and hence we have

$$0 = \int_M \langle X_n, X_m\rangle f\mathrm{d}x = \sum_{k\in\mathbb{N}} \alpha_{n,k}\int_M \langle X_k, X_m\rangle \mathrm{d}x = \alpha_{n,m}.$$

As a result, we know $fX_n = \alpha_{n,n}X_n$, which implies that f is constant. □

Lemma 4.5. *Let (M,g) be a smooth d-dim closed Riemannian manifold and $\{X_n\}_{n\in\mathbb{N}}$ is an orthonormal basis of $L^2(TM)$ constituted of the eigen-vector fields of the connection Laplacian. For any $x_0\in M$, there exist d pairs of $\{(n_i,m_i)\}_{i=1}^d$, where $n_i, m_i\in\mathbb{N}$, so that the gradient vectors $\nabla\langle X_{n_i}, X_{m_i}\rangle(x_0)$ span $T_{x_0}M$.*

Proof. If not, there is a vector $v\in T_{x_0}M$ perpendicular to $\mathrm{span}\{\nabla\langle X_n,X_m\rangle(x_0)\}_{n,m\in\mathbb{N}}$. It is well known that any function $u\in C^\infty(M)$ can be expanded by the eigenfunctions of the Laplace Beltrami operator, $\{\phi_i\}_{i=0}^\infty$, that is, $u = \sum_{j=0}^{K-1}\phi_j + \sum_{i=K}^\infty u_i\phi_i$, where K is the number of connected components, $\Delta_M\phi_j = 0$ for all $j = 0,1,\ldots,K-1$, and $u_i = \int_{\mathcal{M}} u\phi_i\mathrm{d}x$ for all $i = K, K+1,\ldots$. It follows that $\nabla u(x_0) = \sum_{i=K}^\infty u_i\nabla\phi_i(x_0)$. Since any vector $v\in T_{x_0}M$ can be written as $\nabla u(x_0)$ for some smooth function u, we know

$$v = \sum_{i=K}^\infty v_i\nabla\phi_i(x_0)$$

for some constants v_i. On the other hand, by Lemma 4.4, ϕ_i, $i = K, K+1,\ldots$, can be expanded by $\{\langle X_n, X_m\rangle\}_{n,m\in\mathbb{N},n\neq m}$, which leads to

$$v = \sum_{i=K}^\infty v_i \sum_{n,m=1}^\infty w_{i,n,m}\nabla\langle X_n,X_m\rangle(x_0) = \sum_{n,m=1}^\infty\left(\sum_{i=K}^\infty v_i w_{i,n,m}\right)\nabla\langle X_n,X_m\rangle(x_0)$$

for some constants $w_{i,n,m}$, which is absurd. Since $\dim T_{x_0}M$ is finite, we finish the proof. □

Theorem 4.6. *For any fixed $t > 0$, d_t is a distance between isometry classes of Riemannian manifolds in $\mathcal{M}_{d,k,D}$. In particular, two Riemannian manifolds $(M, g), (M', g') \in \mathcal{M}_{d,k,D}$ satisfy $d_t(M, M') = 0$ if and only if M and M' are isometric.*

Proof. By definition, it is clear that $d_t(M, M') \geq 0$, $d_t(M, M') = d_t(M', M)$ and the triangular inequality holds. To finish the proof that d_t is a distance we need to show that $d_t(M, M') = 0$ if and only if M is isometric to M'. If M and M' are isometric, then it is trivial to see that $d_t(M, M') = 0$. Now we consider the opposite direction. Fix $t > 0$. If $d_t(M, M') = 0$, we claim that M is isometric to M'. By the definition of d_t, we know

$$\inf_{a \in \mathcal{B}(M,g)} \mathrm{HD}(V_t^a(M), V_t^{a'}(M')) = 0$$

for a given $a' \in \mathcal{B}(M', g')$. Thus there exists a sequence $a_n \in \mathcal{B}(M, g)$, $n = 1, 2, \ldots$, so that

$$\lim_{n\to\infty} \mathrm{HD}(V_t^{a_n}(M), V_t^{a'}(M')) = 0.$$

By the compactness of $\mathcal{B}(M, g)$, a subsequence $\{a_{n_j}\}_{j=1}^{\infty}$ converges to $a_0 \in \mathcal{B}(M, g)$, that is,

$$\lim_{j\to\infty} d_{\mathcal{B}(M,g)}(a_{n_j}, a_0) = 0,$$

and it follows that $\mathrm{HD}(V_t^{a_0}(M), V_t^{a'}(M')) = 0$.

Let $a_0 = \{X_n\}_{n\in\mathbb{N}}$ and $a' = \{X'_n\}_{n\in\mathbb{N}}$. From the definition of Hausdorff distance and the compactness of $V_t^{a_0}(M)$ and $V_t^{a'}(M')$, we have

$$\begin{aligned} &\text{for all } x \in M, \text{ there exists } y'_t \in M' \text{ s.t. for all } n, m \geq 1 \\ &\mathrm{Vol}(M) e^{-(\lambda_n+\lambda_m)t/2} \langle X_n(x), X_m(x)\rangle = \mathrm{Vol}(M') e^{-(\lambda'_n+\lambda'_m)t/2} \langle X'_n(y'_t), X'_m(y'_t)\rangle \\ &\text{for all } y' \in M', \text{ there exists } x_t \in M \text{ s.t. for all } n, m \geq 1 \\ &\mathrm{Vol}(M) e^{-(\lambda_n+\lambda_m)t/2} \langle X_n(x_t), X_m(x_t)\rangle = \mathrm{Vol}(M') e^{-(\lambda'_n+\lambda'_m)t/2} \langle X'_n(y'), X'_m(y')\rangle \end{aligned} \tag{19}$$

Because $\{\langle X_n(x), X_m(x)\rangle\}_{n,m=1}^{\infty}$ (resp. $\{\langle X_n(y'), X_m(y')\rangle\}_{n,m=1}^{\infty}$) separate the points in the manifold by Theorem 3.1, the point y'_t (resp. x_t) is uniquely defined and hence the corresponding map $f_t : x \to y'_t$ (resp. $h_t : y' \to x_t$) is well-defined, and it is clear that f_t and h_t are inverse to each other. It is also clear that f_t and h_t are continuous. Indeed, by Lemma 3.2, the geodesic distances between $x, \bar{x}$ and $y'_t = f_t(x), \bar{y}'_t = f_t(\bar{x})$ are related by:

$$\begin{aligned} d_g(x, \bar{x}) &= \frac{(4\pi)^{d/2}}{d^{1/2}\mathrm{Vol}(M)} t^{\frac{d+1}{2}} d_{\mathrm{VDM},t}(x, \bar{x})(1 + O(t)) \\ &= \frac{(4\pi)^{d/2}}{d^{1/2}\mathrm{Vol}(M')} t^{\frac{d+1}{2}} d_{\mathrm{VDM},t}(y'_t, \bar{y}'_t)(1 + O(t)) = d_{g'}(y'_t, \bar{y}'_t)(1 + O(t)), \end{aligned}$$

which implies the continuity of f_t. Similarly we get the continuity of h_t. Then, we show that f_t and h_t are C^∞ diffeomorphism. Define a map $F : M \times M' \to \mathbb{R}^d$ by

$$F(x, y') = (\langle X_{n_i}(x), X_{m_i}(x)\rangle - c_{n_i,m_i}(t)\langle X'_{n_i}(y'), X'_{m_i}(y')\rangle)_{i=1}^d,$$

where

$$c_{n_i,m_i}(t) = \frac{\mathrm{Vol}(M')}{\mathrm{Vol}(M)} e^{(\lambda_{n_i}+\lambda_{m_i}-\lambda'_{n_i}-\lambda'_{m_i})t/2}.$$

Note that $F(h_t(y'), y') = 0$. Let $y'_0 = f_t(x_0)$. From Lemma 4.5, it follows that the partial differentiation of F with related to the first variable at (x_0, y_0) is an isomorphism and hence h_t is locally smooth at y'_0 by the implicit function theorem. It follows that h_t is smooth. The same proof shows that f_t is smooth, too.

Next, we show that $\text{Vol}(M) = \text{Vol}(M')$. Denote the induced volume form $(f_t)_*\text{d}V_M$ by $a_t\text{d}V_{M'}$, where a_t is smooth. Integrating the relation (19), we obtain for $n \neq m$, $n, m \in \mathbb{N}$:

$$\begin{aligned}
0 &= \text{Vol}(M)e^{-(\lambda_n+\lambda_m)t/2}\int_M \langle X_n(x), X_m(x)\rangle \text{d}V_M(x)\\
&= \text{Vol}(M')e^{-(\lambda'_n+\lambda'_m)t/2}\int_M \langle X'_n(f_t(x)), X'_m(f_t(x))\rangle \text{d}V_M(x)\\
&= \text{Vol}(M')e^{-(\lambda'_n+\lambda'_m)t/2}\int_{M'} \langle X'_n(y), X'_m(y)\rangle a_t(y)\text{d}V_{M'}(y),
\end{aligned}$$

and similarly for $n = m$, $n \in \mathbb{N}$:

$$\begin{aligned}
1 &= \text{Vol}(M)e^{-\lambda_n t}\int_M \langle X_n(x), X_n(x)\rangle \text{d}V_M(x)\\
&= \text{Vol}(M')e^{-\lambda'_n t}\int_M \langle X'_n(f_t(x)), X'_n(f_t(x))\rangle \text{d}V_M(x)\\
&= \text{Vol}(M')e^{-\lambda'_n t}\int_{M'} \langle X'_n(y), X'_n(y)\rangle a_t(y)\text{d}V_{M'}(y).
\end{aligned}$$

In other words, we have when $n \neq m$,

$$\int_{M'} \langle X'_n(y), X'_m(y)\rangle a_t(y)\text{d}V_{M'}(y) = 0, \tag{20}$$

and when $n = m$,

$$\int_{M'} \langle X'_n(y), X'_n(y)\rangle a_t(y)\text{d}V_{M'}(y) = 1. \tag{21}$$

We claim that from (20) and (21), $a_t = 1$. Indeed, since a_t is smooth and $\{X_k\}_{k=1}^{\infty}$ form an orthonormal basis of $L^2(TM)$, by Lemma 4.4 and (20) we conclude that $a_t(y)$ is constant from (20). From (21), we know $a_t(y) = 1$. Hence,

$$\text{Vol}(M) = \int_M \text{d}V_M(x) = \int_{M'} (f_t)_*\text{d}V_{M'}(y) = \text{Vol}(M'). \tag{22}$$

Plug $\text{Vol}(M) = \text{Vol}(M')$ into (19). Integrating (19) gives $e^{-(\lambda_n+\lambda_m)t/2} = e^{-(\lambda'_n+\lambda'_m)t/2}$, which implies $e^{-\lambda_n t} = e^{-\lambda'_n t}$ for all $n \geq 1$ and hence $\lambda_n = \lambda'_n$ for all $n \geq 1$.

So far, (19) becomes: for all $n, m = 1, 2, \ldots$, $\lambda_n = \lambda'_n$ and

$$\langle X_n(x), X_m(x)\rangle = \langle X'_n(f_t(x)), X'_m(f_t(x))\rangle. \tag{23}$$

We now show that f_t is an isometry. Fix $p \in M$. Note that since f_t is a diffeomorphism, we can find an orthonormal frame $\{E_i\}_{i=1}^d$ around p and $\{E'_i\}_{i=1}^d$ around $f_t(p)$ so that $\text{d}f_t|_p E_i = a_i(p)E'_i(f_t(p))$, where $a_i(p) > 0$. To finish the proof, we have to show that $a_i(p) = 1$ for all $i = 1, \ldots, d$. Choose a vector field $Z \in C^\infty(TM)$

so that

$$
\begin{cases}
Z = \sum_{n=1}^{\infty} \alpha_n X_n, \\
Z(p) = 0,\ \nabla Z(p) = 0,\ \nabla^2 Z(p) = 0, \\
\nabla^2_{E_1,E_1} Z(p) \neq 0, \\
\nabla^2_{E_1,E_1} Z(p) + \nabla^2_{E_2,E_2} Z(p) = 0, \\
\nabla^2_{E_l,E_l} Z(p) = 0 \text{ for all } l = 3, \ldots, d
\end{cases} \tag{24}
$$

Construct $Z' \in C^\infty(TM')$ by $Z' = \sum_{n=1}^{\infty} \alpha_n X'_n$. Denote the Levi-Civita connection of M' as ∇'. We claim that

$$
\begin{cases}
Z' = \sum_{n=1}^{\infty} \alpha_n X'_n, \\
Z'(f_t(p)) = 0,\ \nabla' Z'(f_t(p)) = 0,\ {\nabla'}^2 Z'(f_t(p)) = 0, \\
{\nabla'}^2_{E'_1,E'_1} Z'(f_t(p)) \neq 0, \\
{\nabla'}^2_{E'_1,E'_1} Z'(f_t(p)) + {\nabla'}^2_{E'_2,E'_2} Z'(f_t(p)) = 0, \\
{\nabla'}^2_{E'_l,E'_l} Z'(f_t(p)) = 0 \text{ for all } l = 3, \ldots, d
\end{cases} \tag{25}
$$

By (23), we know

$$
\begin{aligned}
&\langle Z'(f_t(p)), Z'(f_t(p)) \rangle = \sum_{k,l=1}^{\infty} \alpha_k \alpha_l \langle X'_k(f_t(p)), X'_l(f_t(p)) \rangle \\
= &\sum_{k,l=1}^{\infty} \alpha_k \alpha_l \langle X_k(p), X_l(p) \rangle = \langle Z(p), Z(p) \rangle = 0
\end{aligned}
$$

and

$$
\begin{aligned}
&\langle {\nabla'}^2 Z'(f_t(p)), {\nabla'}^2 Z'(f_t(p)) \rangle = \sum_{k,l=1}^{\infty} \alpha_k \lambda'_k \alpha_l \lambda'_l \langle X'_k(f_t(p)), X'_l(f_t(p)) \rangle \\
= &\sum_{k,l=1}^{\infty} \alpha_k \lambda_k \alpha_l \lambda_l \langle X_k(p), X_l(p) \rangle = \langle \nabla^2 Z(p), \nabla^2 Z(p) \rangle = 0,
\end{aligned}
$$

which implies $Z'(f_t(p)) = 0$ and ${\nabla'}^2 Z'(f_t(p)) = 0$. Take $v \in T_pM$ and a curve $\gamma : [0, \epsilon) \to M$ so that $\gamma(0) = p$ and $\gamma'(0) = v$. By extending v to $V \in \Gamma(TM)$ so that $V(\gamma(t)) = \gamma'(t)$, we have

$$
\begin{aligned}
&\frac{\mathrm{d}^2}{\mathrm{d}t^2}\Big|_{t=0} \langle Z, Z \rangle(\gamma(t)) = 2 \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \langle \nabla_V Z, Z \rangle(\gamma(t)) \\
= \;& 2\big(\langle \nabla_V \nabla_V Z, Z \rangle(p) + \langle \nabla_V Z, \nabla_V Z \rangle(p) \big) = 2 \langle \nabla_V Z, \nabla_V Z \rangle(p),
\end{aligned}
$$

where the last equality holds since $Z(p) = 0$. On the other hand, by (23) we have

$$
\begin{aligned}
&\frac{\mathrm{d}^2}{\mathrm{d}t^2}\Big|_{t=0} \langle Z, Z \rangle(\gamma(t)) \\
= \;& \frac{\mathrm{d}^2}{\mathrm{d}t^2}\Big|_{t=0} \langle Z', Z' \rangle(f_t \circ \gamma(t)) \\
= \;& 2 \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \langle \nabla'_{f_{t*}V} Z', Z' \rangle(f_t \circ \gamma(t)) \\
= \;& 2\big(\langle \nabla'_{f_{t*}V} \nabla'_{f_{t*}V} Z', Z' \rangle(f_t(p)) + \langle \nabla'_{f_{t*}V} Z', \nabla'_{f_{t*}V} Z' \rangle(f_t(p)) \big) \\
= \;& 2 \langle \nabla'_{f_{t*}V} Z', \nabla'_{f_{t*}V} Z' \rangle(f_t(p)),
\end{aligned}
$$

where the last equality comes from the fact that $Z'(f_t(p)) = 0$. Thus, we have

$$\langle \nabla'_{f_{t*}V} Z', \nabla'_{f_{t*}V} Z' \rangle (f_t(p)) = \langle \nabla_V Z, \nabla_V Z \rangle (p) = 0,$$

which implies $\nabla'_{f_{t*}v} Z'(f_t(p)) = 0$. Since f_t is diffeomorphic and v is arbitrary, we conclude that $\nabla' Z'(f_t(p)) = 0$.

Next choose the same curve γ and take the fourth order derivative:

$$\begin{aligned}
&\frac{\mathrm{d}^4}{\mathrm{d}t^4}|_{t=0} \langle Z, Z \rangle (\gamma(t)) \\
= \;& 2\langle \nabla_V \nabla_V \nabla_V \nabla_V Z,\, Z \rangle (p) \\
&+8\langle \nabla_V \nabla_V \nabla_V Z,\, \nabla_V Z \rangle (p) \\
&+6\langle \nabla_V \nabla_V Z,\, \nabla_V \nabla_V Z \rangle (p) \\
= \;& 6\langle \nabla_V \nabla_V Z,\, \nabla_V \nabla_V Z \rangle (p) \\
= \;& 6\langle {\nabla^2}_{V,V} Z + \nabla_{\nabla_V V} Z,\, {\nabla^2}_{V,V} Z + \nabla_{\nabla_V V} Z \rangle (p) \\
= \;& 6\langle {\nabla^2}_{V,V} Z,\, {\nabla^2}_{V,V} Z \rangle (p)
\end{aligned}$$

where the second and the fourth equalities come from the fact that $Z(p) = 0$ and $\nabla Z(p) = 0$. Similarly, by the fact that $Z'(f_t(p)) = 0$ and $\nabla' Z'(f_t(p)) = 0$ we have

$$\begin{aligned}
&\frac{\mathrm{d}^4}{\mathrm{d}t^4}|_{t=0} \langle Z, Z \rangle (\gamma(t)) \\
= \;& \frac{\mathrm{d}^4}{\mathrm{d}t^4}|_{t=0} \langle Z', Z' \rangle (f_t \circ \gamma(t)) \\
= \;& 2\langle {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} Z',\, Z' \rangle (f_t(p)) \\
&+8\langle {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} Z',\, {\nabla'}_{f_{t*}V} Z' \rangle (f_t(p)) \\
&+6\langle {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} Z',\, {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} Z' \rangle (f_t(p)) \\
= \;& 6\langle {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} Z',\, {\nabla'}_{f_{t*}V} {\nabla'}_{f_{t*}V} Z' \rangle (f_t(p)) \\
= \;& 6\langle {\nabla'}^2_{f_{t*}V,\; f_{t*}V} Z' + {\nabla'}_{\nabla'_{f_{t*}V} f_{t*}V} Z',\, {\nabla'}^2_{f_{t*}V, f_{t*}V} Z' + {\nabla'}_{\nabla_{f_{t*}V} f_{t*}V} Z' \rangle (f_t(p)) \\
= \;& 6\langle {\nabla'}^2_{f_{t*}V, f_{t*}V} Z',\, {\nabla'}^2_{f_{t*}V, f_{t*}V} Z' \rangle (f_t(p)).
\end{aligned}$$

Since v is arbitrary, we have

$$\langle \nabla^2_{E_i,E_i} Z,\; \nabla^2_{E_i,E_i} Z \rangle (p) = \langle {\nabla'}^2_{f_{t*}E_i, f_{t*}E_i} Z',\; {\nabla'}^2_{f_{t*}E_i, f_{t*}E_i} Z' \rangle (f_t(p)).$$

Thus, we have shown the claim (25).

Next we claim that $a_1(p) = a_2(p)$. Take another smooth vector field $Y \in C^\infty(TM)$ so that $Y = \sum_{n=1}^\infty \gamma_n X_n$ and $Y(p) \neq 0$ and construct $Y' \in C^\infty(TM)$ so that $Y' = \sum_{n=1}^\infty \gamma_n X'_n$. Then by taking the curve γ so that $\gamma'(0) = E_i$, where $i = 1, \ldots, d$, we have

$$\begin{aligned}
&\frac{\mathrm{d}^2}{\mathrm{d}t^2}|_{t=0} \langle Z, Y \rangle (\gamma(t)) \\
= \;& \langle \nabla_{E_i} \nabla_{E_i} Z, Y \rangle (p) + 2\langle \nabla_{E_i} Z, \nabla_{E_i} Y \rangle (p) + \langle Z, \nabla_{E_i} \nabla_{E_i} Y \rangle (p) \\
= \;& \langle \nabla^2_{E_i,E_i} Z + \nabla_{\nabla_{E_i} E_i} Z, Y \rangle (p) \\
= \;& \langle \nabla^2_{E_i,E_i} Z,\, Y \rangle (p) \qquad (26)
\end{aligned}$$

since $Z(p) = 0$ and $\nabla Z(p) = 0$. On the other hand, by the same arguments as those for (26), the construction of Z' and E'_i, we have

$$\begin{aligned} & \frac{\mathrm{d}^2}{\mathrm{d}t^2}|_{t=0}\langle Z, Y\rangle(\gamma(t)) \\ = & \frac{d^2}{\mathrm{d}t^2}|_{t=0}\langle Z', Y'\rangle(f\circ\gamma(t)) \\ = & \langle {\nabla'}^2_{f_{t*}E_i, f_{t*}E_i} Z', Y'\rangle(f_t(p)) \\ = & a_i(p)^2\langle {\nabla'}^2_{E'_i,E'_i} Z', Y'\rangle(f_t(p)) \end{aligned} \tag{27}$$

From (26) and (27), we have

$$\langle \nabla^2_{E_i,E_i} Z, Y\rangle(p) = a_i(p)^2\langle {\nabla'}^2_{E'_i,E'_i} Z', Y'\rangle(f_t(p)).$$

Hence, by the assumption of Z we have

$$\begin{aligned} 0 &= \langle \nabla^2 Z, Y\rangle(p) = \langle \nabla^2_{E_1,E_1} Z + \nabla^2_{E_2,E_2} Z, Y\rangle(p) \\ &= a_1(p)^2\langle {\nabla'}^2_{E'_1,E'_1} Z', Y'\rangle(f_t(p)) + a_2(p)^2\langle {\nabla'}^2_{E'_2,E'_2} Z', Y'\rangle(f_t(p)) \end{aligned}$$

Since $Y'(f_t(p))$ is arbitrary, we know

$$a_1(p)^2{\nabla'}^2_{E'_1,E'_1} Z'(f_t(p)) + a_2(p)^2{\nabla'}^2_{E'_2,E'_2} Z'(f_t(p)) = 0. \tag{28}$$

Combining with the fact that

$${\nabla'}^2_{E'_1,E'_1} Z'(f_t(p)) + {\nabla'}^2_{E'_2,E'_2} Z'(f_t(p)) = 0$$

in (25), we know $a_1(p) = a_2(p)$.

By repeating the arguments from (24) to (28), we conclude that $a_1(p) = a_2(p) = \ldots = a_d(p)$. Denote the $a(p) = a_1(p)$. To finish the proof, we choose $W \in C^\infty(TM)$ so that $W = \sum_{l=1}^\infty \beta_l X_l$, $W(p) = 0$, $\nabla W(p) = 0$ and $\nabla^2 W(p) \neq 0$. Construct $W' = \sum_{l=1}^\infty \beta_l X'_l$. By the same argument, we know $W'(f_t(p)) = 0$ and $\nabla' W'(f_t(p)) = 0$. The same arguments for (26) and (27) hold for W, that is, when $\gamma(t)$ is a curve on M so that $\gamma(0) = p$ and $\gamma'(0) = E_i(p)$ we have

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}|_{t=0}\langle W, Y\rangle(\gamma(t)) = \langle \nabla^2_{E_i,E_i} W, Y\rangle(p)$$

and

$$\begin{aligned} & \frac{\mathrm{d}^2}{\mathrm{d}t^2}|_{t=0}\langle W, Y\rangle(\gamma(t)) = \frac{\mathrm{d}^2}{\mathrm{d}t^2}|_{t=0}\langle W', Y'\rangle(f\circ\gamma(t)) \\ = & \langle {\nabla'}^2_{f_{t*}E_i, f_{t*}E_i} W', Y'\rangle(f_t(p)) = a(p)^2\langle {\nabla'}^2_{E'_i,E'_i} W', Y'\rangle(f_t(p)). \end{aligned}$$

Thus we have

$$a(p)^2\langle {\nabla'}^2 W', Y'\rangle = a(p)^2\langle \sum_{i=1}^d {\nabla'}^2_{E'_i,E'_i} W', Y'\rangle = \langle \sum_{i=1}^d \nabla^2_{E_i,E_i} W, Y\rangle = \langle \nabla^2 W, Y\rangle.$$

On the other hand, the following equality holds due to the definition of W' and Y':

$$\begin{aligned} \langle {\nabla'}^2 W', Y'\rangle &= \langle \sum_{l=1}^\infty \beta_l \lambda'_l X'_l, \sum_{k=1}^\infty \gamma_k X'_k\rangle = \sum_{l,k=1}^\infty \beta_l \lambda'_l \gamma_k \langle X'_l, X'_k\rangle \\ &= \sum_{l,k=1}^\infty \beta_l \lambda_l \gamma_k \langle X_l, X_k\rangle = \langle \nabla^2 W, Y\rangle, \end{aligned}$$

which gives us $a(p) = 1$ and hence f_t is isometric. We have thus finished the proof. □

5. Precompactness of $\mathcal{M}_{d,k,D}$

By Theorem 4.6, we have a distance, referred to as the vector spectral distance, in the space of the isometry classes in $\mathcal{M}_{d,k,D}$. We finally can state the precompactness theorem. We need Lemma 1.1 to finish the proof.

Theorem 5.1. *For any $t > 0$, the space of the isometry classes in $\mathcal{M}_{d,k,D}$ is d_t-precompact.*

Proof. Fix $t > 0$. For any $M \in \mathcal{M}_{d,k,D}$, $a \in \mathcal{B}(M, g)$ and $x \in M$, we have

$$\begin{aligned}
\|V_t^a(x)\|_{h^1}^2 &:= \mathrm{Vol}(M)^2 \sum_{i,j\geq 1} (1 + i^{2/d} + j^{2/d}) e^{-(\lambda_i+\lambda_j)t} \langle X_i(x), X_j(x)\rangle^2 \\
&\leq A(d, k, D)\mathrm{Vol}(M)^2 \sum_{i,j\geq 1} (1 + \lambda_i + \lambda_j) e^{-(\lambda_i+\lambda_j)t} \langle X_i(x), X_j(x)\rangle^2 \\
&\leq A(d, k, D)E(d, k, D)t^{-d}(F(0, d) + t^{-1}F(1, d)),
\end{aligned}$$

where the first inequality follows from Lemma 4.2(1) and the second inequality follows from Lemma 4.2(3). Since $A(d, k, D)$, $E(d, k, D)$, $F(0, d)$ and $F(1, d)$ are universal constants, we know that the set

$$K_0 := \{V_t^a(x)\}_{x\in M, M\in\mathcal{M}_{d,k,D}, a\in\mathcal{B}(M,g)} \subset h^{1/d}$$

is bounded in $h^1 \subset \ell^2$, which is hence relative compact inside ℓ^2 by Rellich's Theorem. Denote the closure of K_0 in ℓ^2 by K. Denote the set of all non-empty closed subsets of K by $\mathcal{F}(K)$, equipped with the Hausdorff distance HD associated with the canonical metric on ℓ^2. By Lemma 1.1, the metric space $(\mathcal{F}(K), \mathrm{HD})$ is precompact.

By Theorem 3.1, since M is compact, $V_t^a(M)$ is compact inside ℓ^2 for any $a \in \mathcal{B}(M, g)$ and $M \in \mathcal{M}_{d,k,D}$, and hence $V_t^a(M) \in \mathcal{F}(K)$. Consider a subset E of $\mathcal{F}(K)$ consisting of $V_t^a(M)$, where $M \in \mathcal{M}_{d,k,D}, a \in \mathcal{B}(M, g)$, that is,

$$E = \{V_t^a(M)\}_{M\in\mathcal{M}_{d,k,D}, a\in\mathcal{B}(M,g)} \subset \mathcal{F}(K).$$

Note that E is precompact with related to the distance HD since closed subsets of a compact set are compact. Given $M \in \mathcal{M}_{d,k,D}$, define a subset $V_t(M)$ of E consisting of $V_t^a(M)$ for all $a \in \mathcal{B}(M, g)$, that is,

$$V_t(M) := \{V_t^a(M)\}_{a\in\mathcal{B}(M,g)} \subset E. \tag{29}$$

Here we view $V_t^a(M)$ as a point in the set E. By Lemma 4.3, $V_t(M)$ is a closed subset of E with related to the Hausdorff distance HD. Indeed, by the closeness of $\mathcal{B}(M, g)$ and Lemma 4.3 we have

$$\mathrm{HD}(V_t^a(M), V_t^b(M)) \leq 2\mathrm{Vol}(M)^2 d_{\mathcal{B}(M,g)}(a, b) \sup_{x\in M} |K_{TM}^{(N)}(t, x, x)|,$$

which implies the closeness of $V_t(M)$. Then, consider $\mathcal{F}(E)$ the set of non-empty closed subsets of E, equipped with the Hausdorff distance h_{HD} associated with the distance HD. By Lemma 1.1 again, we conclude that $\mathcal{F}(E)$ is precompact with related to the distance h_{HD}. Finally, the set $\{V_t(M)\}_{M\in\mathcal{M}_{d,k,D}}$, which is a subset of $\mathcal{F}(E)$, is precompact with related to the Hausdorff distance h_{HD}.

Notice that by the definition of the Hausdorff distance in (17) and Theorem 4.6, (18) is nothing but the Hausdorff distance h_{HD}, that is,

$$d_t(M, M') = d_{\mathrm{HD}}(V_t(M), V_t(M')),$$

and we conclude the proof.

□

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