EMBEDDING RIEMANNIAN MANIFOLDS BY THE HEAT KERNEL OF THE CONNECTION LAPLACIAN

HAU-TIENG WU

Abstract. Given a class of closed Riemannian manifolds with prescribed geometric conditions, we introduce an embedding of the manifolds into $\ell^2$ 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:

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

where Ric is the Ricci curvature and diam is the diameter. The authors embed $M \in \mathcal{M}_{d,k,D}$ into the space $\ell^2$ 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].

Department of Mathematics, Stanford University, Stanford CA 94305 USA, email: hauwu@stanford.edu.
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 $\ell^2$ 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 $(E, \delta)$ be a metric space. Let $\mathcal{F}(E)$ denote the set of non-empty closed subsets of $E$, equipped with the Hausdorff distance $h_\delta$ associated with $\delta$. If the metric space $(E, \delta)$ 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

$$\int_M \langle X, X \rangle(x) dV(x) \leq \infty,$$

where $dV$ is the volume form associated with $g$ and $\langle X, X \rangle(x) := g(X(x), X(x))$. Denote $\nabla$ the Levi-Civita connection of $M$ and $P_{x,y}$ the parallel transport from $y$ to $x$ via the geodesic linking them. Denote $\nabla^2$ the connection Laplacian associated $\nabla$ on the tangent bundle $TM$ [4]. The connection Laplacian $\nabla^2$ 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 $\nabla^2$ is a family of self-adjoint operators with the heat kernel $k_{TM}(t, x, y)$ so that

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

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 $\nabla^2$ is discrete inside $\mathbb{R}^-$, the non-positive real numbers, and the only possible accumulation point is $-\infty$. We will denote the spectrum of $\nabla^2$ 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 $\lambda_0$ 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 \( \nabla^2 \) 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

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

On the other hand, the classical elliptic theory \(^{4}\) allows us to decompose \( L^2(TM) \) as \( L^2(TM) = \bigoplus_{k=1}^{\infty} E_k \), where \( E_k \) is the eigenspace of \( \nabla^2 \) corresponding to increasing eigenvalues, denoted as \( \nu_k \). Denote by \( m(\nu_k) \) the multiplicity of \( \nu_k \). It is also well known that \( m(\nu_k) \) is finite. Denote \( B(E_k) \) 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

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

By Tychonoff’s theorem, we know \( B(M,g) \) 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 \( T_x M \).

### 3. Vector Diffusion Mappings

Based on these observations, given \( a \in B(M,g) \) and \( t > 0 \), the authors in \(^{7}\) define the vector diffusion mappings \( V^a_t \) which maps \( x \in M \) to the Hilbert space \( \ell^2 \) by:

\[
V^a_t : x \mapsto \text{Vol}(M) \left( e^{-\langle \lambda_n + \lambda_m \rangle t / 2} \langle X_n(x), X_m(x) \rangle \right)_{n,m=1}^{\infty}.
\]

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

\[
\|k_{TM}(t,x,y)\|_{HS}^2 = \frac{1}{\text{Vol}(M)^2} (V^a_t(x), V^a_t(y))_{\ell^2}.
\]

Fix \( a \in B(M,g) \). For all \( t > 0 \), the following Theorem states that the vector diffusion mapping \( V^a_t \) is an embedding of the compact Riemannian manifold \( M \) into \( \ell^2 \). 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 \( \nabla^2 \), then for any \( t > 0 \), the vector diffusion map \( V^a_t \) is a diffeomorphic embedding of \( M \) into \( \ell^2 \).

It is Theorem 3.1 that allows the authors to define the vector diffusion distance between \( x,y \in M \), denoted as \( d_{VDM,1}(x,y) \), in \(^{7}\):

\[
d_{VDM,1}(x,y) := \|V^a_t(x) - V^a_t(y)\|_{\ell^2},
\]

\(^{1}\)Note that the basis \( a \) and the volume of \( M \) are not taken into consideration in the definition of the vector diffusion map in \(^{2}\). To prove the precompactness theorem, we need to take them into consideration.
Theorem 4.1. Then recall the following result: 

\begin{align}
\mu \text{ that isometry classes in } M - \text{and eigenfunctions by } Z(\phi) \text{ which are related by the following generalized Kato's type inequality } \text{[1, p. 135]}: \\
\exp(x) \text{ is clearly a distance function over } M. \text{ Define }
\end{align}

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

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

4. Vector Spectral Distances

In this section and the next, we show that based on the vector diffusion map \(V_t\), we can define a family of vector spectral distance \(d_t\), \(t > 0\), on the space of the isometry classes in \(M_{d,k,D}\) so that for any \(t > 0\) the space of the isometry classes in \(M_{d,k,D}\) is \(d_t\)-precompact.

Denote the Laplace-Beltrami operator over \((M, g)\) by \(\Delta_M\) and its eigenvalues and eigenfunctions by \(-\mu_k\) and \(\phi_k\), where \(k \in \{0\} \cup \mathbb{N}\), that is, \(\Delta_M \phi_k = -\mu_k \phi_k\), so that \(\mu_0 = 0 < \mu_1 \leq \mu_2 \ldots\). 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\text{ p. 135}]: \]

\[Z_{TM}(t) \leq dZ_{M}(t) \text{ for all } t > 0.\]

Then recall the following result:

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

\[r_{\min}(M) = \inf \{\text{Ric}(v, v) : \|v\| = 1\}\]

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

\[\text{Vol}(M)k_M(t, x, x) \leq \text{Vol}(S^d(R))k_{S^d}(t, y, y) = Z_{S^d(R)}(t) = Z_{S^d(1)}/R^2,\]
where \( y \in S^d(R) \), \( R = D(M)/a(d, \epsilon, \alpha) \) and

\[
a(d, \epsilon, \alpha) = \begin{cases} 
\alpha \omega^1_d \left( \frac{2}{d} \int_0^{\epsilon/2} \cos^{d-1}(t) dt \right)^{-1/d} & \text{if } \epsilon = 1 \\
(1 + d \omega_d)^{1/d} - 1 & \text{if } \epsilon = 0 \\
\alpha c(\alpha) & \text{if } \epsilon = -1,
\end{cases}
\]

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

\[
z \int_0^z (\cosh(t) + z \sinh(t))^{d-1} dt = \omega_d.
\]

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

\[
\sum_{n,m \geq 1} (\lambda_n + \lambda_m)^{\alpha} e^{-(\lambda_n + \lambda_m)} (X_n(x), X_m(x))^2 \leq \frac{E(d, k, D)}{\text{Vol}(M)^2} F(\alpha, d) t^{-\alpha - d},
\]

where

\[
F(\alpha, d) = \int_0^\infty \int_0^\infty (x+y)^\alpha x^y e^{-(x+y)} dx dy.
\]

**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 \( k \geq 0, r_{\min} D^2 > 0 \) and if \( k < 0, r_{\min} D^2 \geq (d - 1)kD \). Thus we can apply Theorem 4.1 with \( \epsilon \) and \( \alpha \) depending only on \( k \) and \( D \). Thus,

\[
Z_{TM}(t) \leq dZ_{TM}(t) = d \int_M k_M(t, x, x) dx \leq d\text{Vol}(M) \sup_{x \in M} k_M(t, x, x)
\]

\[
\leq d\text{Vol}(S^d(R)) k_{S^d(R)}(t, y, y) = dZ_{S^d(R)}(t) = dZ_{S^d(1)}(t/R^2),
\]

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

\[
j \leq N(\lambda_j) \leq e \sum_{0 \leq \lambda_i \leq \lambda_j} e^{-\lambda_i/\lambda_j} \leq eZ_{TM}(1/\lambda_j)
\]

\[
\leq edZ_{S^d(1)} \left( \frac{1}{\lambda_j R^2} \right) \leq ed + edb(d) R^d \lambda_j^{d/2}
\]

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 $\mu_x$ on $\mathbb{R} \times \mathbb{R}_+$ by

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

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

$$\langle X_n(x), X_m(x) \rangle^2 \leq \langle X_n(x), X_n(x) \rangle \langle X_m(x), X_m(x) \rangle,$$

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

$$\sum_{n,m \geq 1} (\lambda_n + \lambda_m)^\alpha e^{-t(\lambda_n + \lambda_m)} \langle X_n(x), X_m(x) \rangle^2$$

$$= \int_{\mathbb{R}} \int_{\mathbb{R}} (\lambda + \nu)^\alpha e^{-t(\lambda + \nu)} \langle X_n(x), X_m(x) \rangle^2 d\mu_x$$

$$\leq \int_{\mathbb{R}} \int_{\mathbb{R}} (\lambda + \nu)^\alpha e^{-t(\lambda + \nu)} \langle X_n(x), X_n(x) \rangle \langle X_m(x), X_m(x) \rangle d\mu_x$$

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

$$\int_{\mathbb{R}} \int_{\mathbb{R}} (\lambda + \nu)^\alpha e^{-t(\lambda + \nu)} \langle X_n(x), X_n(x) \rangle \langle X_m(x), X_m(x) \rangle d\mu_x$$

$$= \int_{\mathbb{R}} \int_{\mathbb{R}} (\lambda + \nu)^{-\alpha-1} e^{-t(\lambda + \nu)} ((\lambda + \nu)t - \alpha) \mu(\lambda) d\lambda \frac{d\mu(\nu)}{d\nu}$$

$$= \int_0^{\infty} \int_0^{\infty} \left[ t^2(\lambda + \nu)^2 - 2\alpha t(\lambda + \nu) + \alpha(\alpha - 1) \right] \times$$

$$(\lambda + \nu)^{-\alpha-2} e^{-t(\lambda + \nu)} \mu(\lambda) \mu(\nu) d\lambda d\nu.$$

To finish the proof, we claim that:

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

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

$$\sum_{k=1}^{\infty} e^{-\lambda_k t} \langle X_k(x), X_k(x) \rangle^2$$

$$= \sum_{k,l=1}^{\infty} e^{-(\lambda_k + \lambda_l)t} \langle X_k(x), X_k(x) \rangle \langle X_l(x), X_l(x) \rangle$$

$$= \|k_{TM}(t, x, x)\|_{HS}^2 \leq k_M^2(t, x, x),$$

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
\[
\mu(\lambda) = \sum_{n: 0 \leq \lambda_n \leq \lambda} \langle X_n(x), X_n(x) \rangle \leq e \sum_{n: 0 \leq \lambda_n \leq \lambda} e^{-\lambda_n/\lambda} \langle X_n(x), X_n(x) \rangle
\]
\[
\leq e \sum_{n=1}^{\infty} e^{-\lambda_n/\lambda} \langle X_n(x), X_n(x) \rangle \leq ek_M(1/\lambda, x, x)
\]
(13)
\[
\leq \frac{e}{\text{Vol}(M)} Z_{S^N}(1/\lambda R^2) \leq \frac{C(d, k, D)}{\text{Vol}(M)} \lambda^{d/2},
\]
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
\[
\sum_{n, m \geq 1} (\lambda_n + \lambda_m)^\alpha e^{-t(\lambda_n + \lambda_m)} \langle X_n(x), X_m(x) \rangle^2
\]
\[
\leq \frac{C(d, k, D)^2}{\text{Vol}(M)^2} \int_0^\infty \int_0^\infty \left[ t^2 (\lambda + \nu)^2 - 2\alpha t (\lambda + \nu) + \alpha(\alpha - 1) \right] \times
\]
\[
(\lambda + \nu)^{\alpha - 2} e^{-t(\lambda + \nu)} \lambda^d \nu^d d\lambda d\nu
\]
\[
\leq \frac{E(d, k, D)}{\text{Vol}(M)^2} F(\alpha, d) t^{-\alpha - d},
\]
where \(E(d, k, D)\) is an universal positive constant that depends only on \(d, k\) and \(D\), and \(F\) is defined in [11].

Recall that the vector diffusion map \(V^n_a\) 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 \(R_1, R_2 \in \mathcal{O}(\dim E)\) by
\[
d_E(R_1, R_2) = \| R_1^{-1} R_2 - I \|_{HS}.
\]
It is clear that \(d_E(R_1, R_2) \leq 2\sqrt{\dim E}\). 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
\[
d_{\mathcal{B}(M, g)}(a, b)^2 = \sum_{i=1}^{\infty} \nu_i^{-N} d_{E_i}(a|_{E_i}, b|_{E_i})^2,
\]
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 \(V(t, a, x) := V^n_a(x)\) is continuous and satisfies:
\[
\|V^n_a(x) - V^n_b(y)\|_2^2 \leq \text{Vol}(M)^2 \left\{ \|k_{TM}(t, x, x)\|_{HS} + \|k_{TM}(s, y, y)\|_{HS} \right\}
\]
(15)
\[
-2 \left\| k_{TM} \left( \frac{t + s}{2}, x, y \right) \right\|_{HS} + 2d_{\mathcal{B}(M, g)}(a, b) k_{TM}^{(N)}(t, x, x)^{1/2} k_{TM}^{(N)}(s, y, y)^{1/2}
\]
where \(t > 0, a, b \in \mathcal{B}(M, g), x, y \in M,\) and
\[
k_{TM}^{(N)}(t, x, x) = \sum_{n,m=1}^{\infty} (\lambda_n^{N/2} + \lambda_m^{N/2}) e^{-t(\lambda_n + \lambda_m)} \langle X_n^a(x), X_m^a(x) \rangle^2.
\]
Proof. We denote the basis \( a \in \mathcal{B}(M, g) \) by \( \{X^a_n\}_{n=1}^\infty \). First we have

\[
\|V^a_t(x) - V^b_t(y)\|^2_c \\
= \text{Vol}(M)^2 \sum_{n, m=1}^\infty \left( e^{-t(\lambda_n + \lambda_m)/2} \langle X^a_n(x), X^a_m(x) \rangle - e^{-s(\lambda_n + \lambda_m)/2} \langle X^b_n(y), X^b_m(y) \rangle \right)^2 \\
= \text{Vol}(M)^2 \left\{ \|k_{TM}(t, x, x)\|_{HS} + \|k_{TM}(s, y, y)\|_{HS} - 2 \sum_{n, m=1}^\infty \left[ e^{-t(\lambda_n + \lambda_m)/2} \langle X^a_n(x), X^a_m(x) \rangle \langle X^b_n(y), X^b_m(y) \rangle \right] \right\}
\]

where we denote the last summation on the right hand side as \( A \). Denote the eigenvector fields inside the eigenspace \( E_\nu \) 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 \( \{\alpha_{j,k}(b, a)\}_{k,j=1}^{m(\nu_n) m(\nu_n)} \in O(m(\nu_n)) \). Thus we can rewrite \( A \) as

\[
A = \sum_{n, m=1}^\infty e^{-t(\nu_n + \nu_m)/2} \sum_{k=1}^{m(\nu_n)} \sum_{l=1}^{m(\nu_m)} \left[ X^a_n(k)(x), X^a_m(l)(x) \times \langle X^a_n(k)(y), X^a_m(l)(y) \rangle - \sum_{j=1}^{m(\nu_m)} \sum_{i=1}^{m(\nu_n)} \alpha_{k,i}(b, a) \alpha_{l,j}(b, a) \langle X^a_n(i)(y), X^a_m(j)(y) \rangle \right]
\]

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

\[
\langle \delta_{k,i}, \delta_{l,j} - \alpha_{k,i}(b, a) \alpha_{l,j}(b, a) \rangle = \delta_{k,i} (\delta_{l,j} - \alpha_{l,j}(b, a)) + \alpha_{l,j}(b, a) (\delta_{k,i} - \alpha_{k,i}(b, a))
\]
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

\[
|A| \leq \sum_{n,m=1}^{\infty} e^{-(t+s)(\nu_n + \nu_m)/2} \left( \sum_{k=1}^{m(\nu_n)} \sum_{l=1}^{m(\nu_m)} (X_n^a(k)(x), X_m^a(l)(x))^2 \right)^{1/2} \times \\
\left( \sum_{i=1}^{m(\nu_n)} \sum_{j=1}^{m(\nu_m)} (X_n^a(i)(y), X_m^a(j)(y))^2 \right)^{1/2} \left( d_{E_n}(a|E_n, b|E_n) + d_{E_m}(a|E_m, b|E_m) \right)
\]

\[
\leq 2d_{B(M,g)}(a, b) \sum_{n,m=1}^{\infty} (\nu_n^{N/2} + \nu_m^{N/2}) e^{-(t+s)(\nu_n + \nu_m)/2} \times \\
\left( \sum_{k=1}^{m(\nu_n)} \sum_{l=1}^{m(\nu_m)} (X_n^a(k)(x), X_m^a(l)(x))^2 \right)^{1/2} \left( \sum_{i=1}^{m(\nu_n)} \sum_{j=1}^{m(\nu_m)} (X_n^a(i)(y), X_m^a(j)(y))^2 \right)^{1/2}
\]

\[
\leq 2d_{B(M,g)}(a, b) \left( \sum_{n,m=1}^{\infty} (\lambda_n^{N/2} + \lambda_m^{N/2}) e^{-(t+n+\lambda_m)} (X_n^a(x), X_m^a(x))^2 \right)^{1/2} \times \\
\left( \sum_{n,m=1}^{\infty} (\lambda_n^{N/2} + \lambda_m^{N/2}) e^{-(t+n+\lambda_m)} (X_n^a(y), X_m^a(y))^2 \right)^{1/2} = 2d_{B(M,g)}(a, b) k_{TM}^{(N)}(t, x, x)^{1/2} k_{TM}^{(N)}(s, y, y)^{1/2},
\]

where \(k_{TM}^{(N)}(t, x, x)\) is defined in (16). Due to Lemma 4.2(c), \(k_{TM}^{(N)}(t, x, x)\) is bounded, and thus the proof is finished. \(\square\)

With the above preparation, we are ready to introduce the vector spectral distance. Recall the following definitions. Suppose \((X, \delta)\) is a metric space, where \(\delta\) is the metric, and \(A, B \subseteq X\). 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 \(A, B \subseteq X\), we can define the Hausdorff distance, denoted as HD, associated with \(\delta\) by

\[
\text{HD}(A, B) = \inf \{ \epsilon : A \subseteq \mathcal{N}(B, \epsilon), B \subseteq \mathcal{N}(A, \epsilon) \},
\]

or equivalently

\[
\text{HD}(A, B) = \max \left\{ \sup_{x \in A} \inf_{y \in B} \delta(x, y), \sup_{y \in B} \inf_{x \in A} \delta(x, y) \right\}.
\]

(17) \(
\text{HD}(A, B) = \max \left\{ \sup_{x \in A} \inf_{y \in B} \delta(x, y), \sup_{y \in B} \inf_{x \in A} \delta(x, y) \right\}.
\)

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

\[
\text{span}\{\langle X_n, X_m \rangle : n, m \in \mathbb{N}, n \neq m \} = L^2(M) \setminus \{0\},
\]

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

Proof. Fix \(f \in L^2(M)\). If \(\int_M \langle X_n, X_m \rangle f(x) dx = \int_M \langle f X_n, X_m \rangle(x) dx = 0\) 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 \(f X_n = \sum_{k \in \mathbb{N}} \alpha_{n,k} X_k\), and hence we have

\[
0 = \int_M \langle X_n, X_m \rangle f dx = \sum_{k \in \mathbb{N}} \alpha_{n,k} \int_M \langle X_k, X_m \rangle dx = \alpha_{n,m}.
\]

As a result, we know \(f X_n = \alpha_{n,n} X_n\), which implies that \(f\) is constant. \(\square\)

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 \(K\) 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 \(\text{span}\{\nabla \langle X_{n_i}, X_{m_i} \rangle(x_0)\}_{n_i, m_i \in \mathbb{N}}\). 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 \(u_i = \int_M u \phi_i dx\) 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 \(\phi_i, i = K, K + 1, \ldots\), can be expanded by \(\{\langle X_{n_i}, X_{m_i} \rangle\}_{n_i, m_i \in \mathbb{N}, n_i \neq m}\), which leads to

\[
v = \sum_{i=K}^{\infty} v_i \sum_{n, m = 1}^{\infty} w_{i, n, m} \nabla \langle X_{n_i}, X_{m_i} \rangle(x_0) = \sum_{n, m = 1}^{\infty} \left( \sum_{i=K}^{\infty} v_i w_{i, n, m} \right) \nabla \langle X_{n_i}, X_{m_i} \rangle(x_0)
\]

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

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

for a given $a' \in \mathcal{B}(M', g')$. Thus there exists a sequence $(a_n)_{n=1}^{\infty}$ such that

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

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 $\text{HD}(V_t^{a_0}(M), V_t^{a_0}(M')) = 0$.

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 $V_t^{a_0}(M')$, we have

$$\text{Vol}(M)e^{-(\lambda_n + \lambda_m)t/2} \langle X_n(x), X_m(x) \rangle = \text{Vol}(M')e^{-(\lambda'_n + \lambda'_m)t/2} \langle X'_n(y'_i), X'_m(y'_i) \rangle$$

for all $n, m \geq 1$ and $x, y'_i \in M'$. There exists $x_t \in M$ s.t. for all $n, m \geq 1$

$$\text{Vol}(M)e^{-(\lambda_n + \lambda_m)t/2} \langle X_n(x_t), X_m(x_t) \rangle = \text{Vol}(M')e^{-(\lambda'_n + \lambda'_m)t/2} \langle X'_n(y'_i), X'_m(y'_i) \rangle$$

This defines $x_t$. Thus, we have

$$x_t \in M \quad \text{s.t.} \quad \lim_{t \to \infty} \text{HD}(V_t^{a_0}(M), V_t^{a_0}(M')) = 0.$$

Because $\{\{X_n(x), X_m(x)\}\}_{n,m=1}^{\infty}$ (resp. $\{\{X'_n(y), X_m(y)\}\}_{n,m=1}^{\infty}$) separate the points in the manifold by Theorem 3.1 the point $y'_i$ (resp. $x_t$) is uniquely defined and hence the corresponding map $f_t : x \to y'_i$ (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 $x, x_t$ and $y'_i, f_t(x), y'_i, f_t(x)$ are related by:

$$d_g(x, x_t) = \frac{(4\pi)^{d/2}}{d^{1/2}\text{Vol}(M)} \int_{\mathbb{R}^d} d_{\text{VDM},t}(x, x_t) \, (1 + O(t))$$

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 $C^\infty$ diffeomorphism. Define a map $F : M \times M' \to \mathbb{R}^d$ by

$$F(x, y') = (\langle X_n(x), X_m(x) \rangle - c_{n,m}(t) \langle X'_n(y), X'_m(y) \rangle)_{i=1}^{d},$$

where

$$c_{n,m}(t) = \frac{\text{Vol}(M')}{\text{Vol}(M)} e^{(\lambda_n + \lambda_m - \lambda'_n - \lambda'_m)t/2}.$$
Note that $F(h_t(y'), y') = 0$. Let $y'_0 = f_1(x_0)$. From Lemma 4.3 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 $f_1$ is smooth, too.

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

\[
0 = \text{Vol}(M)e^{-(\lambda_n + \lambda_m)t/2} \int_M \langle X_n(x), X_m(x) \rangle dV_M(x)
\]

\[
= \text{Vol}(M')e^{-(\lambda'_n + \lambda'_m)t/2} \int_M \langle X'_n(f_t(x)), X'_m(f_t(x)) \rangle dV_M(x)
\]

\[
= \text{Vol}(M')e^{-(\lambda'_n + \lambda'_m)t/2} \int_{M'} \langle X'_n(y), X'_m(y) \rangle a_t(y)dV_{M'}(y),
\]

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

\[
1 = \text{Vol}(M)e^{-\lambda_n t} \int_M \langle X_n(x), X_n(x) \rangle dV_M(x)
\]

\[
= \text{Vol}(M')e^{-\lambda'_n t} \int_M \langle X'_n(f_t(x)), X'_n(f_t(x)) \rangle dV_M(x)
\]

\[
= \text{Vol}(M')e^{-\lambda'_n t} \int_{M'} \langle X'_n(y), X'_n(y) \rangle a_t(y)dV_{M'}(y).
\]

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

\[
\int_{M'} \langle X'_n(y), X'_m(y) \rangle a_t(y)dV_{M'}(y) = 0,
\]

and when $n = m$,

\[
\int_{M'} \langle X'_n(y), X'_n(y) \rangle a_t(y)dV_{M'}(y) = 1.
\]

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 4.3 and (20) we conclude that $a_t(y)$ is constant from (20). From (21), we know $a_t(y) = 1$. Hence,

\[
\text{Vol}(M) = \int_M dV_M(x) = \int_{M'} (f_t)_*dV_{M'}(y) = \text{Vol}(M').
\]

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

\[
\langle X_n(x), X_m(x) \rangle = \langle X'_n(f_t(x)), X'_m(f_t(x)) \rangle.
\]

We now show that $f_t$ is an isometry. Fix $p \in M$. Note that since $f_t$ is a diffeomorph inism, 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 $d^if_t|_p E_i = a_i(p) E'_i(f_t(p))$, 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

\[
\begin{align*}
Z &= \sum_{n=1}^{\infty} \alpha_n X_n, \\
Z(p) &= 0, \quad \nabla Z(p) = 0, \quad \nabla^2 Z(p) = 0, \\
\nabla^2_{E_1, E_1} Z(p) &\neq 0, \\
\nabla^2_{E_1, E_1} Z(p) + \nabla^2_{E_2, E_2} Z(p) &= 0, \\
\nabla^2_{E_1, E_1} Z(p) &= 0 \text{ for all } l = 3, \ldots, d.
\end{align*}
\]

(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 \(\nabla'\). We claim that

\[
\begin{align*}
Z' &= \sum_{n=1}^{\infty} \alpha_n X'_n, \\
Z'(f_t(p)) &= 0, \quad \nabla' Z'(f_t(p)) = 0, \quad \nabla'^2 Z'(f_t(p)) = 0, \\
\nabla'^2_{E'_1, E'_1} Z'(f_t(p)) &\neq 0, \\
\nabla'^2_{E'_1, E'_1} Z'(f_t(p)) + \nabla'^2_{E'_2, E'_2} Z'(f_t(p)) &= 0, \\
\nabla'^2_{E'_1, E'_1} Z'(f_t(p)) &= 0 \text{ for all } l = 3, \ldots, d.
\end{align*}
\]

(25)

By (23), we know

\[
\langle Z'(f_t(p)), Z'(f_t(p)) \rangle = \sum_{k,l=1}^{\infty} \alpha_k \alpha_l \langle X'_k(f_t(p)), X'_l(f_t(p)) \rangle
\]

\[
= \sum_{k,l=1}^{\infty} \alpha_k \alpha_l \langle X_k(p), X_l(p) \rangle = \langle Z(p), Z(p) \rangle = 0
\]

and

\[
\langle \nabla'^2 Z'(f_t(p)), \nabla'^2 Z'(f_t(p)) \rangle = \sum_{k,l=1}^{\infty} \alpha_k \lambda'_k \alpha_l \lambda'_l \langle X'_k(f_t(p)), X'_l(f_t(p)) \rangle
\]

\[
= \sum_{k,l=1}^{\infty} \alpha_k \lambda_k \alpha_l \lambda_l \langle X_k(p), X_l(p) \rangle = \langle \nabla^2 Z(p), \nabla^2 Z(p) \rangle = 0,
\]

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

\[
\frac{d^2}{dt^2}|_{t=0} \langle Z, Z \rangle (\gamma(t)) = \frac{d}{dt}|_{t=0} \langle \nabla V Z, Z \rangle (\gamma(t))
\]

\[
= 2 \langle \nabla V \nabla V Z, Z(p) \rangle + \langle \nabla V Z, \nabla V V Z(p) \rangle = 2 \langle \nabla V Z, \nabla V V Z(p) \rangle,
\]

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

\[
\frac{d^2}{dt^2}|_{t=0} \langle Z, Z \rangle (\gamma(t))
\]

\[
= \frac{d^2}{dt^2}|_{t=0} \langle Z', Z' \rangle (f_t \circ \gamma(t))
\]

\[
= 2 \frac{d}{dt}|_{t=0} \langle \nabla_{f_t \circ \gamma} Z', Z' \rangle (f_t \circ \gamma(t))
\]

\[
= 2 \langle \nabla_{f_t \circ \gamma} \nabla_{f_t \circ \gamma} Z', Z' \rangle (f_t(p)) + \langle \nabla_{f_t \circ \gamma} Z', \nabla_{f_t \circ \gamma} Z' \rangle (f_t(p))
\]

\[
= 2 \langle \nabla_{f_t \circ \gamma} Z', \nabla_{f_t \circ \gamma} Z' \rangle (f_t(p))
\]
Thus, we have shown the claim (25).

which implies $\nabla' f_i, v Z'(f_i(p)) = 0$. Since $f_i$ is diffeomorphic and $v$ is arbitrary, we conclude that $\nabla' Z'(f_i(p)) = 0$.

Next choose the same curve $\gamma$ and take the fourth order derivative:

$$\frac{d^4}{dt^4}\vert_{t=0} \langle Z, Z \rangle(\gamma(t))$$

$$= 2\langle \nabla' f_i, v \nabla' f_i, v \nabla' f_i, v \nabla' f_i, v Z', Z' \rangle(f_i(p))$$

$$+ 8\langle \nabla' f_i, v \nabla' f_i, v \nabla' f_i, v Z', Z' \rangle(f_i(p))$$

$$+ 6\langle \nabla' f_i, v \nabla' f_i, v \nabla' f_i, v Z' \rangle(f_i(p))$$

$$= 6\langle \nabla' f_i, v \nabla' f_i, v Z' \rangle(f_i(p))$$

$$= 6\langle \nabla^2 f_i, v, v Z' \rangle(f_i(p))$$

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 $Z'(f_i(p)) = 0$ and $\nabla' Z'(f_i(p)) = 0$ we have

$$\frac{d^4}{dt^4}\vert_{t=0} \langle Z, Z \rangle(\gamma(t))$$

where $Z(\gamma(t)) = 0$.

Since $v$ is arbitrary, we have

$$\langle \nabla^2 E_i, E_i Z, \nabla^2 E_i, E_i Z \rangle(p) = \langle \nabla' f_i, E_i f_i, E_i Z', \nabla' f_i, E_i f_i, E_i Z' \rangle(f_i(p)).$$

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 $\gamma$ so that $\gamma'(0) = E_i$, where $i = 1, \ldots, d$, we have

$$\frac{d^2}{dt^2}\vert_{t=0} \langle Z, Y \rangle(\gamma(t))$$

$$= \langle \nabla E_i, E_i Z, Y \rangle(p) + 2\langle \nabla E_i, Z, E_i Y \rangle(p) + \langle Z, \nabla E_i, E_i Y \rangle(p)$$

$$= \langle \nabla^2 E_i, E_i Z, Y \rangle(p)$$

(26)
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

$$\frac{d^2}{dt^2}|_{t=0} \langle Z, Y \rangle (\gamma(t))$$

$$= \frac{d^2}{dt^2}|_{t=0} \langle Z', Y' \rangle (f \circ \gamma(t))$$

$$= \langle \nabla_{f_*, E_*, f_*, E}^2 Z', Y' \rangle (f_i(p))$$

$$= a_i(p)^2 \langle \nabla_{E_i', E_i'}^2 Z', Y' \rangle (f_i(p))$$

(27)

From (26) and (27), we have

$$\langle \nabla_{E_i', E_i'}^2 Z, Y \rangle (p) = a_i(p)^2 \langle \nabla_{E_i', E_i'}^2 Z', Y' \rangle (f_i(p)).$$

Hence, by the assumption of $Z$ we have

$$0 = \langle \nabla^2 Z, Y \rangle (p) = \langle \nabla_{E_1, E_1}^2 Z + \nabla_{E_2, E_2}^2 Z, Y \rangle (p)$$

$$= a_1(p)^2 \langle \nabla_{E_1', E_1'}^2 Z', Y' \rangle (f_i(p)) + a_2(p)^2 \langle \nabla_{E_2', E_2'}^2 Z', Y' \rangle (f_i(p)).$$

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

$$a_1(p)^2 \langle \nabla_{E_1', E_1'}^2 Z'(f_i(p)) + a_2(p)^2 \langle \nabla_{E_2', E_2'}^2 Z'(f_i(p)) = 0.$$

Combining with the fact that

$$\langle \nabla_{E_1', E_1'}^2 Z'(f_i(p)) = \langle \nabla_{E_2', E_2'}^2 Z'(f_i(p)) = 0$$

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

By repeating the arguments from (26) 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 $W = \sum_{i=1}^{\infty} \beta_i X_i$, $W(p) = 0$, $\nabla W(p) = 0$ and $\nabla^2 W(p) \neq 0$. Construct $W' = \sum_{i=1}^{\infty} \beta_i X_i'$. By the same argument, we know $W'(f_i(p)) = 0$ and $\nabla W'(f_i(p)) = 0$.

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

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

and

$$\frac{d^2}{dt^2}|_{t=0} \langle W, Y \rangle (\gamma(t)) = \frac{d^2}{dt^2}|_{t=0} \langle W', Y' \rangle (f \circ \gamma(t))$$

$$= \langle \nabla_{f_*, E_*, f_*, E}^2 W', Y' \rangle (f_i(p)) = a(p)^2 \langle \nabla_{E_i', E_i'}^2 W', Y' \rangle (f_i(p)).$$

Thus we have

$$a(p)^2 \langle \nabla^2 W', Y' \rangle = a(p)^2 \langle \sum_{i=1}^{d} \nabla_{E_i', E_i'}^2 W', Y' \rangle = \langle \sum_{i=1}^{d} \nabla_{E_i, E_i}^2 W, Y \rangle = \langle \nabla^2 W, Y \rangle.$$
which gives us \( a(p) = 1 \) and hence \( f_t \) is isometric. We have thus finished the proof.

\[ \Box \]

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

\[
\|V_t^a(x)\|_{h_1}^2 := \text{Vol}(M)^2 \sum_{i,j \geq 1} (1 + t^{i/d} + j^{i/d}) e^{-(\lambda_i + \lambda_j)t} \langle X_i(x), X_j(x) \rangle^2 \\
\leq A(d,k,D) \text{Vol}(M)^2 \sum_{i,j \geq 1} (1 + \lambda_i + \lambda_j) e^{-(\lambda_i + \lambda_j)t} \langle X_i(x), X_j(x) \rangle^2 \\
\leq A(d,k,D) E(d,k,D) t^{-d} (F(0,d) + t^{-1} F(1,d)),
\]

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 \( \ell^2 \) by Rellich’s Theorem. Denote the closure of \( K_0 \) in \( \ell^2 \) by \( K \). Denote the set of all non-empty closed subsets of \( K \) by \( \mathcal{F}(K) \), equipped with the Hausdorff distance \( \text{HD} \) associated with the canonical metric on \( \ell^2 \). By Lemma 1.1 the metric space \( (\mathcal{F}(K), \text{HD}) \) is precompact.

By Theorem 3.1 since \( M \) is compact, \( V_t^a(M) \) is compact inside \( \ell^2 \) 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 \( \text{HD} \) 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,

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

Here we view \( V_t^a(M) \) as a point in the set \( E \). By Lemma 1.3 \( V_t(M) \) is a closed subset of \( E \) with related to the Hausdorff distance \( \text{HD} \). Indeed, by the closeness of \( \mathcal{B}(M,g) \) and Lemma 4.3 we have

\[
\text{HD}(V_t^a(M), V_t^b(M)) \leq 2 \text{Vol}(M)^2 d_{\mathcal{B}(M,g)}(a,b) \sup_{x \in M} |K_t^{(N)}(t,x,x)|,
\]

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 \( h_{\text{HD}} \) associated with the distance HD. By Lemma 1.1 again, we conclude that \( \mathcal{F}(E) \) is precompact with related to the distance \( h_{\text{HD}} \). 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 \( h_{\text{HD}} \).
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,
\[ d_t(M, M') = d_{HD}(V_t(M), V_t(M')) , \]
and we conclude the proof.

\[ \square \]

6. Acknowledgements

The author acknowledges the support partially by FHWA grant DTFH61-08-C-00028 and partially by Award Number FA9550-09-1-0551 from AFOSR. He acknowledges Professor Charlie Fefferman and Professor Amit Singer for their time and inspiring and helpful discussions; in particular Professor Amit Singer, who introduced him the massive data analysis field. He also acknowledges the valuable discussion with Professor Gérard Besson and Richard Bamler.

References

[1] P. Bérard. Spectral Geometry: Direct and Inverse Problems. Springer, 1986.
[2] P. Bérard, G. Besson, and S. Gallot. Embedding riemannian manifolds by their heat kernel. Geometric and functional analysis, 4(4):373, 1994.
[3] R. R. Coifman and S. Lafon. Diffusion maps. Applied and Computational Harmonic Analysis, 21(1):5–30, 2006.
[4] P. Gilkey. The Index Theorem and the Heat Equation. Princeton, 1974.
[5] R. Hadani and A. Singer. Representation theoretic patterns in three dimensional cryo-electron microscopy II – the class averaging problem. Foundations of Computational Mathematics (FoCM), 11(5):589–616, 2011.
[6] P. Jones, M. Maggioni, and R. Schul. Manifold parametrizations by eigenfunctions of the laplacian and heat kernels. PNAS, 105(6):1803–1808, 2008.
[7] A. Singer and H.-T. Wu. Vector diffusion maps and the connection laplacian. Communications on Pure and Applied Mathematics, 65(8):1067–1144, 2010.
[8] A. Singer and H.-T. Wu. Orientability and diffusion map. Applied and Computational Harmonic Analysis, 31(1):44–58, 2011.
[9] A. Singer, Z. Zhao, Y. Shkolnisky, and R. Hadani. Viewing angle classification of cryo-electron microscopy images using eigenvectors. SIAM Journal on Imaging Sciences, 4(2):543–572, 2011.