



Heat Kernel Approximation on Kendall Shape Space

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Abstract: The heat kernel on Kendall shape subspaces is approximated by an expansion. The Kendall space is useful for representing the shapes associated with collections of landmarks' positions. The Minakshisundaram-Pleijel recursion formulas are used in order to calculate the closed-form approximations of the first and second coefficients of the heat kernel expansion. Prior to the exploitation of the recursion scheme, the expression of the Laplace-Beltrami operator is adapted to the targeted space using geodesic spherical and angular coordinates.

Keywords: Kendall shape space, heat kernel expansion, special orthogonal group, quotient space, shape recognition

1. Introduction

The heat kernel on the shape subspaces $\prod(\mathcal{X}_m^k)$, of the spaces \sum_m^k introduced by D.G. Kendall for $m \geq 3$ and $k \geq m + 2$, is approximated by means of expansion ^[1-9]. The latter is a time power-like series, for small enough values of time, that converges asymptotically to the minimal positive fundamental heat kernel solution $H(\prod(X), \prod(Y), t)$ of the parabolic partial differential equation on $\prod(\mathcal{X}_m^k)$ ^[10-16],

$$\Delta H(\prod(X), \prod(Y), t) = \frac{\partial H(\prod(X), \prod(Y), t)}{\partial t}. \tag{1}$$

Here, $\prod(X)$ and $\prod(Y)$ are two shapes in $\prod(\mathcal{X}_m^k)$, t is time, and Δ is the Laplace-Beltrami operator on $\prod(\mathcal{X}_m^k)$. In this paper, only both first coefficients of the expansion are calculated based on the Minakshisundaram-Pleijel recursion formulas ^[17, Chap. VI].

2. Preliminaries and methods

2.1 Kendall shape space

In Kendall shape theory, an object is initially represented by a configuration matrix in $\mathbb{R}^{m \times k}$ whose columns are the position vectors in \mathbb{R}^m of k landmarks, respectively. The landmarks are methodically selected from the object's boundary to capture its geometrical form. Usually, objects' shapes are structures in the plan or in the space where m equals two or three, respectively, though the Kendall theory is valid for any value of m which is larger or equal to two.

The shape is extracted through filtering out the effects of size, translation, and rotation from the initial configuration matrix. The elimination of translation and size effects leads to the pre-shape unit sphere \mathcal{S}_m^k of matrices X in $\mathbb{R}^{m \times (k-1)}$. Then, the shape map \prod eliminates the left action of rotations in the special orthogonal group $SO(m)$ to give rise to the shape space \sum_m^k . The latter coincides with the quotient space $\mathcal{S}_m^k/SO(m)$, where all the pre-shape matrices TX for T in $SO(m)$ correspond to the same shape $\prod(X)$.

The singular values decomposition plays a central role in Kendall theory. It helps to express any pre-shape X in \mathcal{X}_m^k as the three-factor product $U(\Lambda \ 0)V$. Here, U and V are elements of $SO(m)$ and $SO(k-1)$, respectively, and Λ is the diagonal matrix $\text{diag} \{ \lambda_1, \lambda_2, \dots, \lambda_m \}$ in $\mathbb{R}^{m \times m}$ such that $\lambda_i > \lambda_{i+1} > 0$ for $1 \leq i \leq m-1$ and the trace of Λ^2 is one. The pre-shapes of a given shape share the same singular values as well as the first m rows of V modulo rows' sign ^[1, Sect. 1.3].

The Riemannian metric as well as the differential structure have been determined on an open Riemannian manifold $\Pi(\mathcal{X}_m^k)$, whose dimension d_m^k is $m(k-1) - \frac{1}{2}m(m-1) - 1$, where \mathcal{X}_m^k is the open subset of \mathcal{S}_m^k defined hereafter,

$$\mathcal{X}_m^k = \{X \in \mathcal{S}_m^k : \lambda_1 > \dots > \lambda_{m-1} > \lambda_m > 0\}$$

2.2 Laplace-Beltrami operator

The Laplace-Beltrami operator on $\Pi(\mathcal{X}_m^k)$ involved in the heat equation in (1) is expressed as [1, Corollary 7.2],

$$\begin{aligned} \Delta = & \sum_{i=2}^m \frac{\partial^2}{\partial \lambda_i^2} - \sum_{i,j=2}^m \lambda_i \lambda_j \frac{\partial^2}{\partial \lambda_i \partial \lambda_j} - (m-1) \sum_{j=2}^m \lambda_j \frac{\partial}{\partial \lambda_j} \\ & + \sum_{i=1}^m \sum_{j=i+1}^{k-1} f(\lambda_i, \lambda_j) (\xi_{ij} \xi_{ij} - \nabla_{\xi_{ij}} \xi_{ij}), \end{aligned} \quad (2)$$

where $f(\lambda_i, \lambda_j)$ is a function of the indicated singular values, ∇ is the Levi-Civita connection, and

$$\left\{ \frac{\partial}{\partial \lambda_i} \right\}_{2 \leq i \leq m} \cup \{ \xi_{ij} \}_{1 \leq i \leq m, i < j \leq k-1}, \quad (3)$$

is the basis of the tangent space $\mathcal{T}_{\Pi(X)}(\Pi(\mathcal{X}_m^k))$ to $\Pi(\mathcal{X}_m^k)$ at the shape $\Pi(X)$; each vector ξ_{rs} is orthogonal to any other vector ξ_{ij} for $1 \leq i \leq m, i < j \leq k-1$, and to any vector $\frac{\partial}{\partial \lambda_i}$ for $2 \leq i \leq m$.

The latter basis is inherited from the basis,

$$\{ \tilde{\eta}_{ij} \}_{1 \leq i < j \leq m} \cup \left\{ \frac{\tilde{\partial}}{\tilde{\partial} \lambda_i} \right\}_{2 \leq i \leq m} \cup \{ \tilde{\xi}_{ij} \}_{1 \leq i \leq m, i < j \leq k-1}, \quad (4)$$

of the tangent space $\mathcal{T}_X(\mathcal{X}_m^k)$ to \mathcal{X}_m^k at any pre-shape X of $\Pi(X)$; the vectors $\tilde{\eta}_{ij}$, $\tilde{\xi}_{ij}$, and $\frac{\tilde{\partial}}{\tilde{\partial} \lambda_i}$ are linearly mapped onto the null, ξ_{ij} , and $\frac{\partial}{\partial \lambda_i}$ vectors, respectively, by the differential Π_* of Π at X . The standard coordinates matrices,

$$U \left(E_{ii} - \frac{\lambda_i}{\lambda_1} E_{11} \right) V, \quad 2 \leq i \leq m, \quad (5)$$

of the tangent vectors $\frac{\tilde{\partial}}{\tilde{\partial} \lambda_i}$ are of particular use in this paper, where each E_{jj} , for $1 \leq j \leq m$, is the matrix in $\mathbb{R}^{m \times (k-1)}$ whose (j, j) th entry is one and all of whose other entries are zero.

2.3 Exponential map and geodesic spherical coordinates

The exponential map is a differential geometry tool used to define the geodesic spherical coordinates that are important to carry out calculus and to describe diffusion processes on $\Pi(\mathcal{X}_m^k)$. The exponential map on $\Pi(\mathcal{X}_m^k)$ is defined based on the curve Γ_r introduced hereafter.

Thus first, let X be any pre-shape of a given shape $\Pi(X)$, and \tilde{T} a tangent vector to \mathcal{X}_m^k at X written in the basis (4) as,

$$\tilde{T} = \sum_{1 \leq i < j \leq m} \tilde{T}_{ij} \tilde{\eta}_{ij} + \sum_{i=2}^m T_i \frac{\tilde{\partial}}{\tilde{\partial} \lambda_i} + \sum_{i=1}^m \sum_{j=i+1}^{k-1} T_{ij} \tilde{\xi}_{ij}, \quad (6)$$

for some real number coordinates \tilde{T}_{ij} , T_i and T_{ij} ; $\Pi_*(\tilde{T})$ coincides always with the very same vector \mathcal{T} in (7) written in the basis (3) as,

$$\mathcal{T} = \sum_{i=2}^m T_i \frac{\partial}{\partial \lambda_i} + \sum_{i=1}^m \sum_{j=i+1}^{k-1} T_{ij} \xi_{ij}, \quad (7)$$

no matter the values of the coordinates \tilde{T}_{ij} .

Then, the following geodesic of pre-shapes in \mathcal{X}_m^k is used in Kendall shape theory to describe the differential structure of $\Pi(\mathcal{X}_m^k)$,

$$\tilde{\Gamma}_{\tilde{T}}(\epsilon) = U \exp(\epsilon A) (\cos(\epsilon) \Lambda + \sin(\epsilon) D \quad 0) \exp(\epsilon \tilde{B}) V. \quad (8)$$

Here, $\tilde{\Gamma}_{\tilde{T}}(0)$ is X , \tilde{T} is the tangent vector to $\tilde{\Gamma}_{\tilde{T}}$ at X as in (6), A and \tilde{B} are two skew-symmetric matrices in $\mathbb{R}^{m \times m}$ and $\mathbb{R}^{(k-1) \times (k-1)}$ respectively, and D is a diagonal matrix in $\mathbb{R}^{m \times m}$ such that the traces of ΛD and D^2 are zero and one respectively.

Now, a shape curve $\Gamma_{\mathcal{T}}$ in $\Pi(\mathcal{X}_m^k)$ starting out at the shape $\Pi(X)$ in the direction of the tangent vector \mathcal{T} as in (7) is defined by,

$$\Gamma_{\mathcal{T}} = \Pi \circ \tilde{\Gamma}_{\tilde{T}}, \quad (9)$$

where $\tilde{\Gamma}_{\tilde{T}}$ is any pre-shape curve as in (6) such that $\Pi(\tilde{\Gamma}_{\tilde{T}}(0))$ and $\Pi_*(\tilde{T})$ are identical to $\Pi(X)$ and \mathcal{T} respectively. It is worth noting that, the coordinates \tilde{T}_{ij} of the tangent vector \tilde{T} in (6) are involved only in the left acting orthogonal matrix $U \exp(\epsilon \sum_{1 \leq i < j \leq m} \tilde{T}_{ij} S_{ij})$ in the expression of $\tilde{\Gamma}_{\tilde{T}}(\epsilon)$, so, $\tilde{\Gamma}_{\tilde{T}}(\epsilon)$ is always a pre-shape of the same shape $\Gamma_{\mathcal{T}}(\epsilon)$ for any values of \tilde{T}_{ij} . The shape curve $\Gamma_{\mathcal{T}}$ is a diffeomorphism that maps the product of specific open sets containing the diagonal matrix Λ and the first m rows of the orthogonal matrix V , onto an open neighbourhood of the shape $\Pi(X)$ [1, Sect. 7.2 and proof of Lemma 7.2].

In particular, when \mathcal{T} is unitary, $\Gamma_{\mathcal{T}}$ is equated with the exponential map $\exp_{\Pi(X)}(\epsilon \mathcal{T})$ on $\Pi(\mathcal{X}_m^k)$. In this case, the squared norm of \mathcal{T} is the sum of the squared norms of $\sum_{i=1}^m \sum_{j=i+1}^{k-1} T_{ij} \xi_{ij}$ and $\sum_{i=2}^m T_i \frac{\partial}{\partial \lambda_i}$, where the squared norms of the latter and of $\sum_{i=2}^m T_i \frac{\tilde{\partial}}{\tilde{\partial} \lambda_i}$ in (6) are identical since the vectors $\frac{\tilde{\partial}}{\tilde{\partial} \lambda_i}$ are isometrically mapped onto $\frac{\partial}{\partial \lambda_i}$, respectively. Here, the standard coordinates matrix of $\sum_{i=2}^m T_i \frac{\tilde{\partial}}{\tilde{\partial} \lambda_i}$ is $U(D \quad 0)V$, where D is the diagonal matrix,

$$\text{diag}\left\{-\frac{1}{\lambda_1} \sum_{i=2}^m T_i \lambda_i, T_2, T_3, \dots, T_{m-1}, T_m\right\}, \quad (10)$$

according to (5). Since the trace of D^2 is one, the vector $\sum_{i=2}^m T_i \frac{\partial}{\partial \lambda_i}$ is unitary. Thus, the coordinates T_{ij} in (7) are necessarily zero for all $1 \leq i \leq m$, $i < j \leq k-1$.

Finally, The geodesic spherical coordinates (ϵ, \mathcal{T}) , where \mathcal{T} is the unitary tangent vector $\sum_{i=2}^m T_i \frac{\partial}{\partial \lambda_i}$, help to define the geodesical sphere $\mathcal{S}(\Pi(X), \epsilon)$ in $\Pi(\mathcal{X}_m^k)$, centered at the shape $\Pi(X)$ and with radius ϵ , as the set of shapes $\exp_{\Pi(X)}(\epsilon \mathcal{T})$.

2.4 Heat kernel calculation

The Minakshisundaram-Pleijel recursion formulas are used to approximate the heat kernel $H(\Pi(X), \Pi(Y), t)$ on $\Pi(\mathcal{X}_m^k)$, by the expression hereafter,

$$\frac{1}{(4\pi t)^{d_m^k/2}} e^{-\arccos^2(\sum_{i=1}^m \lambda_i(YX^t))/4t} \{u_0(\epsilon, \mathcal{T}) + u_1(\epsilon, \mathcal{T})t\}, \quad (11)$$

for small time t and close enough shapes $\Pi(X)$ and $\Pi(Y)$, where the latter is the shape $\exp_{\Pi(X)}\left(\epsilon \sum_{i=2}^m \mathcal{T}_i \frac{\partial}{\partial \lambda_i}\right)$ [17, p.154].

Here, the $\lambda_i(YX^t)$ are the singular values of the matrix YX^t for any pre-shapes X and Y of the shapes $\Pi(X)$ and $\Pi(Y)$, respectively [1, Sect. 6.4].

Now, let $\sqrt{G}(\epsilon, \mathcal{T})$ be the determinant of the path of linear transformations on $\Pi(\mathcal{X}_m^k)$, which is equivalent to [17, p.317],

$$\epsilon^{d_m^k-1} - \frac{1}{6} \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^{d_m^k+1}. \quad (12)$$

Then, the expressions of the coefficients $u_0(\epsilon, \mathcal{T})$ and $u_1(\epsilon, \mathcal{T})$ are equivalent to [17, p.150],

$$\frac{1}{\sqrt{1 - \frac{1}{6} \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2}} \quad (13)$$

and

$$\frac{u_0(\epsilon, \mathcal{T})}{\epsilon} \int_0^\epsilon u_0(r, \mathcal{T}) \Delta u_0(r, \mathcal{T}) dr, \quad (14)$$

respectively. Here, the Ricci tensor is the bilinear symmetric form,

$$\text{Ric}(\mathcal{T}, \mathcal{T}) = \sum_{i,j=2}^m \text{Ric}\left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j}\right) \mathcal{T}_i \mathcal{T}_j, \quad (15)$$

that includes the terms $\text{Ric}\left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j}\right)$ for all $2 \leq i, j \leq m$, given in [1, Theorem 7.4] as hereafter,

$$\begin{aligned} \text{Ric}\left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j}\right) &= 3 \left\{ 2 \frac{\lambda_i^2}{(\lambda_i^2 + \lambda_1^2)^2} + \sum_{r=1, r \neq i}^m \frac{\lambda_r^2}{(\lambda_r^2 + \lambda_i^2)^2} \right. \\ &\left. + \frac{\lambda_i^2}{\lambda_1^2} \sum_{r=2}^m \frac{\lambda_r^2}{(\lambda_r^2 + \lambda_1^2)^2} \right\} + (d_m^k - 1) \left(1 + \frac{\lambda_i^2}{\lambda_1^2} \right) \end{aligned} \quad (16)$$

$$\begin{aligned} \text{Ric}\left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j}\right) &= 3\lambda_i \lambda_j \left\{ \frac{1}{(\lambda_i^2 + \lambda_1^2)^2} + \frac{1}{(\lambda_j^2 + \lambda_1^2)^2} + \frac{1}{(\lambda_i^2 + \lambda_j^2)^2} \right. \\ &\left. + \frac{1}{\lambda_1^2} \sum_{r=2}^m \frac{\lambda_r^2}{(\lambda_r^2 + \lambda_1^2)^2} + \frac{d_m^k - 1}{3\lambda_1^2} \right\}. \end{aligned} \quad (17)$$

So, it should be borne in mind that the intended heat kernel approximation is grounded on neglecting the higher order terms $u_i(\epsilon, T)^i$ for $i \geq 2$ within the general Minakshisundaram-Pleijel expansion, along with neglecting the term $O(\epsilon^{d_m+2})$ in the expression of the determinant of the path of linear transformation in (12).

3. Results

In the following subsections, the expression in (2) of the Laplace-Beltrami operator on $\prod(\mathcal{X}_m^k)$ is simplified and then reformulated using the geodesic spherical coordinates. After that, the second coefficient expressed in (14) of the heat kernel expansion in (11) is calculated using the Laplacian of the first coefficient in (13).

3.1 Simpler expression of the Laplace-Beltrami operator on $\prod(\mathcal{X}_m^k)$

Lemma 1 hereafter helps to simplify the expression of the Laplace-Beltrami operator on $\prod(\mathcal{X}_m^k)$ that becomes,

$$\Delta = \sum_{i=2}^m \frac{\partial^2}{\partial \lambda_i^2} - \sum_{i,j=2}^m \lambda_i \lambda_j \frac{\partial^2}{\partial \lambda_i \partial \lambda_j} - (m-1) \sum_{j=2}^m \lambda_j \frac{\partial}{\partial \lambda_j}. \quad (18)$$

since the differences $\xi_{ij} \xi_{ij} - \nabla_{\xi_{ij}} \xi_{ij}$ appearing in (2) are actually zero.

Lemma 1. The directional derivative $\xi_{ij} \xi_{ij}$ and the covariant derivative $\nabla_{\xi_{ij}} \xi_{ij}$, both of ξ_{ij} in the direction ξ_{ij} at any shape $\prod(X)$ in $\prod(\mathcal{X}_m^k)$, are identical for all $1 \leq i \leq m$, $i < j \leq k-1$.

Proof. According to [18, Theorem 2], the expression of the directional derivative $\xi_{ij} \xi_{ij}$ is,

$$\xi_{ij} \xi_{ij} = \sum_{r=2}^m \gamma_{ij,ij}^r \frac{\partial}{\partial \lambda_r} + \sum_{r=1}^m \sum_{s=r+1}^{k-1} \gamma_{ij,ij}^{rs} \xi_{rs}, \quad (19)$$

because for $1 \leq r < s \leq m$, the values of $\tilde{\gamma}_{ij,ij}^{rs}$ for $1 \leq i < j \leq m$ and $1 \leq i \leq m < j \leq k-1$ are linear combinations of the products $\delta_{ir} \delta_{is}$ and $\delta_{jr} \delta_{js}$ that are zero.

Now, the covariant derivative $\nabla_{\xi_{ij}} \xi_{ij}$ of the tangential vector field ξ_{ij} in the direction ξ_{ij} is a tangential vector field written as,

$$\nabla_{\xi_{ij}} \xi_{ij} = \sum_{r=2}^m \Gamma_{ij,ij}^r \frac{\partial}{\partial \lambda_r} + \sum_{r=1}^m \sum_{s=r+1}^{k-1} \Gamma_{ij,ij}^{rs} \xi_{rs}. \quad (20)$$

The Koszul formula leads to the equality between the double of $\langle \nabla_{\xi_{ij}} \xi_{ij}, \xi_{rs} \rangle$ and $2\xi_{ij} \langle \xi_{ij}, \xi_{rs} \rangle - \xi_{rs} \langle \xi_{ij}, \xi_{ij} \rangle - 2 \langle \xi_{ij}, [\xi_{ij}, \xi_{rs}] \rangle$, where the compatibility of the directional derivative with inner product and addition helps to deduce that $\langle \nabla_{\xi_{ij}} \xi_{ij}, \xi_{rs} \rangle$ and $\langle \xi_{ij} \xi_{ij}, \xi_{rs} \rangle$ are identical. So, according to (19) and (20), the Christoffel symbol $\Gamma_{ij,ij}^{rs}$ coincides with the scalar $\gamma_{ij,ij}^{rs}$ for $1 \leq r \leq m$, $r < s \leq k-1$. The identity between $\langle \nabla_{\xi_{ij}} \xi_{ij}, \frac{\partial}{\partial \lambda_r} \rangle$ and $\langle \xi_{ij} \xi_{ij}, \frac{\partial}{\partial \lambda_r} \rangle$ can be shown in a similar way. So, (19) and (20) lead to the next set of equations,

$$\sum_{r=2}^m \left\langle \frac{\partial}{\partial \lambda_{r'}} , \frac{\partial}{\partial \lambda_r} \right\rangle \Gamma_{ij,ij}^r = \sum_{r=2}^m \left\langle \frac{\partial}{\partial \lambda_{r'}} , \frac{\partial}{\partial \lambda_r} \right\rangle \gamma_{ij,ij}^r, \quad 2 \leq r' \leq m, \quad (21)$$

that are rewritten into the matrix equation $g(\Gamma_{ij,ij}^r)_{2 \leq r \leq m} = g(\gamma_{ij,ij}^r)_{2 \leq r \leq m}$, where g is the nonsingular metric matrix $\left(\left\langle \frac{\partial}{\partial \lambda_{r'}} , \frac{\partial}{\partial \lambda_r} \right\rangle \right)_{2 \leq r', r \leq m}$ [1, p.147], therefore the Christoffel symbol $\Gamma_{ij,ij}^r$ coincides with the scalar $\gamma_{ij,ij}^r$ for $2 \leq r \leq m$.

3.2 Laplace-Beltrami operator on $\mathbb{P}(\chi_m^k)$ in geodesic spherical coordinates

In Theorem 2, the partial derivatives $\frac{\partial}{\partial \lambda_i}$ and $\frac{\partial^2}{\partial \lambda_i \partial \lambda_j}$ in (18) are rewritten using the angular coordinates ϕ_ℓ in $[0, \pi[$ for $2 \leq \ell \leq m-2$, and ϕ_{m-1} in $[0, 2\pi[$. Mainly, Theorem 2 helps to restrict the Laplace-Beltrami operator in (18) to the geodesical sphere $\mathcal{S}(\mathbb{P}(X), \epsilon)$ in $\mathbb{P}(\chi_m^k)$ using the geodesic spherical coordinates $\left(\epsilon, \sum_{i=2}^m T_i \frac{\partial}{\partial \lambda_i}\right)$.

Theorem 2. Let $\mathbb{P}(X)$ be a shape in $\mathbb{P}(\chi_m^k)$, then for all $2 \leq i, j \leq m$,

$$\frac{\partial}{\partial \lambda_i} = \frac{1}{\sin(\epsilon)} \sum_{n=2}^i \sum_{\ell=2}^{\min\{n, m-1\}} \alpha_{n, \ell}^i \frac{\partial}{\partial \phi_\ell}, \quad (22)$$

and

$$\begin{aligned} \frac{\partial^2}{\partial \lambda_i \partial \lambda_j} &= \frac{1}{\sin^2(\epsilon)} \sum_{n=2}^i \sum_{v=2}^j \sum_{u=2}^{\min\{v, m-1\}} \sum_{\ell=2}^{\min\{n, m-1\}} \beta_{n, v, u, \ell}^{i, j} \frac{\partial^2}{\partial \phi_\ell} \\ &+ \frac{1}{\sin^2(\epsilon)} \sum_{n=2}^i \sum_{v=2}^j \sum_{u=2}^{\min\{v, m-1\}} \sum_{\ell=2}^{\min\{n, m-1\}} \alpha_{n, \ell}^i \alpha_{v, u}^j \frac{\partial^2}{\partial \phi_u \partial \phi_\ell}, \end{aligned} \quad (23)$$

where

$$\alpha_{n, \ell}^i = \frac{\partial \hat{T}_n}{\partial T_i} \frac{\partial \phi_\ell}{\partial \hat{T}_n}, \quad (24)$$

$$\beta_{n, v, u, \ell}^{i, j} = \alpha_{v, u}^j \frac{\partial \hat{T}_n}{\partial T_i} \frac{\partial^2 \phi_\ell}{\partial \phi_u \partial \hat{T}_n}, \quad (25)$$

$$\frac{\partial \hat{T}_m}{\partial T_m} = \frac{1}{\sqrt{1 - \lambda_m^2}}, \quad (26)$$

$$\frac{\partial \hat{T}_i}{\partial T_i} = \frac{\sqrt{\sum_{r=1}^i \lambda_r^2}}{\sqrt{\sum_{r=1}^{i-1} \lambda_r^2}}, \quad 2 \leq i \leq m-1, \quad (27)$$

$$\frac{\partial \hat{T}_n}{\partial T_i} = \frac{\lambda_n \lambda_i}{\sqrt{\sum_{r=1}^{n-1} \sum_{t=1}^n \lambda_r^2 \lambda_t^2}}, \quad 2 \leq n \leq i-1, \quad 3 \leq i \leq m, \quad (28)$$

$$\frac{\partial \phi_n}{\partial \hat{T}_n} = -\frac{\sin(\phi_n)}{\prod_{r=2}^{n-1} \sin(\phi_r)}, \quad (29)$$

$$\frac{\partial \phi_\ell}{\partial \hat{T}_n} = \frac{\prod_{r=\ell+1}^{n-1} \sin(\phi_r) \cos(\phi_\ell) \cos(\phi_n)}{\prod_{r=2}^{\ell-1} \sin(\phi_r)}, \quad \ell + 1 \leq n \leq m, \quad (30)$$

$$\frac{\partial^2 \phi_n}{\partial \phi_n \partial \hat{T}_n} = -\frac{\cos(\phi_n)}{\prod_{r=2}^{n-1} \sin(\phi_r)}, \quad (31)$$

$$\frac{\partial^2 \phi_n}{\partial \phi_u \partial \hat{T}_n} = \frac{\sin(\phi_n) \cos(\phi_u)}{\prod_{r=2}^{n-1} \sin(\phi_r) \sin(\phi_u)}, \quad 2 \leq u \leq n-1, \quad (32)$$

$$\frac{\partial^2 \phi_u}{\partial \phi_u \partial \hat{T}_n} = -\frac{\prod_{r=u}^{n-1} \sin(\phi_r) \cos(\phi_n)}{\prod_{r=2}^{u-1} \sin(\phi_r)}, \quad u + 1 \leq n \leq m, \quad (33)$$

$$\frac{\partial^2 \phi_\ell}{\partial \phi_u \partial \hat{T}_u} = -\frac{\prod_{r=\ell+1}^u \sin(\phi_r) \cos(\phi_\ell)}{\prod_{r=2}^{\ell-1} \sin(\phi_r)}, \quad \ell + 1 \leq u \leq m, \quad (34)$$

$$\frac{\partial^2 \phi_\ell}{\partial \phi_u \partial \hat{T}_n} = -\frac{\prod_{r=\ell+1}^{n-1} \sin(\phi_r) \cos(\phi_\ell) \cos(\phi_n) \cos(\phi_u)}{\prod_{r=2}^{\ell-1} \sin(\phi_r) \sin(\phi_u)}, \quad (35)$$

$\ell + 1 \leq n \leq m, \quad 2 \leq u \leq \ell - 1,$

$$\frac{\partial^2 \phi_\ell}{\partial \phi_u \partial \hat{T}_n} = \frac{\prod_{r=\ell+1}^{n-1} \sin(\phi_r) \cos(\phi_\ell) \cos(\phi_n) \cos(\phi_u)}{\prod_{r=2}^{\ell-1} \sin(\phi_r) \sin(\phi_u)}, \quad (36)$$

$\ell + 1 \leq n \leq m, \quad \ell + 1 \leq u \leq n - 1,$

$\frac{\partial \hat{T}_n}{\partial T_i}, \frac{\partial \phi_\ell}{\partial \hat{T}_n}$ and $\frac{\partial^2 \phi_\ell}{\partial \phi_u \partial \hat{T}_n}$ are zero otherwise.

Proof. Both tangent components $\sum_{i=2}^m T_i \frac{\partial}{\partial \lambda_i}$ and $\sum_{i=2}^m T_i \frac{\tilde{\partial}}{\partial \tilde{\lambda}_i}$, in (7) and (6), respectively, are unitary (Sect. Preliminaries and methods). Besides, the squared norm of $\sum_{i=2}^m T_i \frac{\tilde{\partial}}{\partial \tilde{\lambda}_i}$ equals the sum $\sum_{i=2}^m \hat{T}_i^2$ for the coordinates \hat{T}_i , where,

$$\hat{T}_i = \frac{\sqrt{\sum_{r=1}^i \lambda_r^2}}{\sqrt{\sum_{r=1}^{i-1} \lambda_r^2}} T_i + \frac{\lambda_i}{\sqrt{\sum_{r=1}^{i-1} \sum_{t=1}^i \lambda_r^2 \lambda_t^2}} \sum_{r=i+1}^m \lambda_r T_r, \quad 2 \leq i \leq m-1, \quad (37)$$

and

$$\hat{T}_m = \frac{1}{\sqrt{1 - \lambda_m^2}} T_m, \quad (38)$$

as stated in [19, Lemma 2]. Therefore, the coordinates \hat{T}_i can be written as,

$$\hat{T}_i = \prod_{\ell=2}^{i-1} \sin(\phi_\ell) \cos(\phi_i), \quad 2 \leq i \leq m-1, \quad (39)$$

and

$$\hat{T}_m = \prod_{\ell=2}^{m-1} \sin(\phi_\ell) \quad (40)$$

using the angular coordinates ϕ_i ; these latter can be retrieved from the coordinates \hat{T}_i through,

$$\phi_\ell = \operatorname{arccot} \left(\frac{\hat{T}_\ell}{\sqrt{\sum_{i=\ell+1}^m \hat{T}_i^2}} \right), \quad 2 \leq \ell \leq m-2, \quad \sum_{i=\ell+1}^m \hat{T}_i^2 \neq 0, \quad (41)$$

and

$$\phi_{m-1} = 2 \operatorname{arccot} \left(\frac{\hat{T}_{m-1} + \sqrt{\hat{T}_{m-1}^2 + \hat{T}_m^2}}{\hat{T}_m} \right), \quad \hat{T}_m \neq 0, \quad (42)$$

where, each angle ϕ_ℓ for $2 \leq \ell \leq m-2$ is zero if $\sum_{i=\ell+1}^m \hat{T}_i^2$ is zero and $\hat{T}_\ell > 0$, and the angle ϕ_{m-1} is zero if the coordinate \hat{T}_m is zero and $\hat{T}_{m-1} > 0$.

Next, let $\lambda_i(\Pi(X))$ and λ_i for $1 \leq i \leq m$ be the singular values of the pre-shapes of $\Pi(X)$ and $\exp_{\Pi(X)}(\in \mathcal{T})$, respectively; the $\lambda_i(\Pi(X))$ are constant since $\Pi(X)$ is held fixed. Then, the value of each λ_i varies linearly with the coordinate \mathcal{T}_i according to $\cos(\in)\lambda_i(\Pi(X)) + \sin(\in)\mathcal{T}_i$ for $2 \leq i \leq m$. So, for strictly positive values of \in , the term $\frac{\partial \mathcal{T}_i}{\partial \lambda_i}$ coincides with $\frac{1}{\sin(\in)}$. The chain rule helps to express $\frac{\partial}{\partial \lambda_i}$ as $\frac{\partial \mathcal{T}_i}{\partial \lambda_i} \frac{\partial}{\partial \mathcal{T}_i}$, that is $\frac{1}{\sin(\in)} \frac{\partial}{\partial \mathcal{T}_i}$ for $2 \leq i \leq m$. The chain rule helps also to write the partial derivatives,

$$\frac{\partial}{\partial \mathcal{T}_i} = \sum_{n=2}^i \sum_{\ell=2}^{\min\{n, m-1\}} \frac{\partial \hat{T}_n}{\partial \mathcal{T}_i} \frac{\partial \phi_\ell}{\partial \hat{T}_n} \frac{\partial}{\partial \phi_\ell} \quad 2 \leq i \leq m, \quad (43)$$

where $\frac{\partial \hat{T}_n}{\partial \lambda_i}$ are calculated using (37) and (38), and $\frac{\partial \phi_\ell}{\partial \hat{T}_n}$ are calculated using (41), (42), as well as the identity between $\sum_{i=\ell+1}^m \hat{T}_i^2$ and $\prod_{r=2}^\ell \sin^2(\phi_r)$; the terms $\frac{\partial \hat{T}_n}{\partial \mathcal{T}_i}$ for $i+1 \leq n \leq m$, $2 \leq i \leq m-1$ and $\frac{\partial \phi_\ell}{\partial \hat{T}_n}$ for $2 \leq n \leq \ell-1$, are zero. Now, $\frac{\partial}{\partial \lambda_i}$ is used to calculate $\frac{\partial^2}{\partial \lambda_j \partial \lambda_i}$ for $2 \leq i, j \leq m$ at $\Pi(X)$ as,

$$\frac{1}{\sin^2(\in)} \sum_{j=v+2}^i \sum_{u=2}^{\min\{v, m-1\}} \sum_{n=2}^i \sum_{\ell=2}^{\min\{n, m-1\}} \frac{\partial \hat{T}_v}{\partial \mathcal{T}_j} \frac{\partial \phi_u}{\partial \hat{T}_v} \frac{\partial \hat{T}_n}{\partial \mathcal{T}_i} \frac{\partial}{\partial \phi_u} \left(\frac{\partial \phi_\ell}{\partial \hat{T}_n} \frac{\partial}{\partial \phi_\ell} \right), \quad (44)$$

due to the independence of $\frac{\partial \hat{T}_n}{\partial \lambda_i}$ from the angles ϕ_i ; the calculation of $\frac{\partial^2 \phi_\ell}{\partial \phi_u \partial \hat{T}_n}$ is achieved by applying $\frac{\partial}{\partial \phi_u}$ to the already computed terms $\frac{\partial \phi_\ell}{\partial \hat{T}_n}$.

3.3 Calculation of the coefficient $u_1(\epsilon, \mathcal{T})$

In Theorem 3, the Laplacian of the coefficient $u_0(\epsilon, \mathcal{T})$ is established since it is needed for calculating $u_1(\epsilon, \mathcal{T})$.

Theorem 3. Let $\Pi(X)$ be a shape in $\Pi(\mathcal{X}_m^k)$ and let \mathcal{T} be a unitary tangent vector to $\Pi(\mathcal{X}_m^k)$ at $\Pi(X)$. Then, the expression of $\Delta u_0(\epsilon, \mathcal{T})$ is

$$\begin{aligned} \Delta u_0(\epsilon, \mathcal{T}) &= \mathcal{A}(\epsilon, \mathcal{T}) + \sum_{i=2}^m \frac{\partial^2 u_0(\epsilon, \mathcal{T})}{\partial \lambda_i^2} \\ &\quad - \sum_{i,j=2}^m \lambda_i \lambda_j \frac{\partial^2 u_0(\epsilon, \mathcal{T})}{\partial \lambda_i \partial \lambda_j} - (m-1) \sum_{i=2}^m \lambda_i \frac{\partial u_0(\epsilon, \mathcal{T})}{\partial \lambda_i}, \end{aligned} \quad (45)$$

where

$$\frac{\partial u_0(\epsilon, \mathcal{T})}{\partial \lambda_i} = K^i(\mathcal{T}) \mathcal{B}(\epsilon, \mathcal{T}), \quad (46)$$

$$K^i(\mathcal{T}) = \sum_{n=2}^i \sum_{\ell=2}^{\min\{n, m-1\}} \kappa_{n,\ell}^i, \quad (47)$$

$$\kappa_{n,\ell}^i = \alpha_{n,\ell}^i \frac{\partial \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_\ell}, \quad (48)$$

such that $\alpha_{n,\ell}^i$ is defined in (24),

$$\frac{\partial^2 u_0(\epsilon, \mathcal{T})}{\partial \lambda_i \partial \lambda_j} = K_2^{i,j}(\mathcal{T}) \mathcal{C}(\epsilon, \mathcal{T}) + K_1^{i,j}(\mathcal{T}) \mathcal{D}(\epsilon, \mathcal{T}), \quad (49)$$

$$K_1^{i,j}(\mathcal{T}) = \sum_{n=2}^i \sum_{\ell=2}^{\min\{n, m-1\}} \sum_{v=2}^j \sum_{u=2}^{\min\{v, m-1\}} \kappa_{n,\ell}^i \kappa_{v,u}^j, \quad (50)$$

$$K_2^{i,j}(\mathcal{T}) = \sum_{n=2}^i \sum_{v=2}^j \sum_{u=2}^{\min\{v, m-1\}} \sum_{\ell=2}^{\min\{n, m-1\}} \kappa_{n,v,u,\ell}^{i,j}, \quad (51)$$

$$\kappa_{n,v,u,\ell}^{i,j} = \beta_{n,v,u,\ell}^{i,j} \frac{\partial \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_\ell} + \alpha_{n,\ell}^i \alpha_{v,u}^j \frac{\partial^2 \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_u \partial \phi_\ell}, \quad (52)$$

such that $\beta_{n,v,u,\ell}^{i,j}$ is defined in (25),

$$\mathcal{A}(\epsilon, \mathcal{T}) = \frac{\sqrt{6 \text{Ric}(\mathcal{T}, \mathcal{T}) (6d_m^k - (d_m^k - 1) \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)}}{(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)^{5/2}}, \quad (53)$$

$$\mathcal{B}(\epsilon, \mathcal{T}) = \frac{\sqrt{6} \epsilon^2}{2 \sin(\epsilon) (6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)^{3/2}}, \quad (54)$$

$$\mathcal{C}(\epsilon, \mathcal{T}) = \frac{\mathcal{B}(\epsilon, \mathcal{T})}{\sin(\epsilon)}, \quad (55)$$

$$\mathcal{D}(\epsilon, \mathcal{T}) = \frac{3\mathcal{B}(\epsilon, \mathcal{T}) \epsilon^2}{2 \sin(\epsilon) (6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)}, \quad (56)$$

$$\frac{\partial \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_\ell} = 2 \sum_{i,j=2}^m \text{Ric} \left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j} \right) \frac{\partial \mathcal{T}_i}{\partial \phi_\ell} \mathcal{T}_j, \quad (57)$$

$$\frac{\partial^2 \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_u \partial \phi_\ell} = 2 \sum_{i,j=2}^m \text{Ric} \left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j} \right) \left(\frac{\partial^2 \mathcal{T}_i}{\partial \phi_u \partial \phi_\ell} \mathcal{T}_j + \frac{\partial \mathcal{T}_i}{\partial \phi_\ell} \frac{\partial \mathcal{T}_j}{\partial \phi_u} \right), \quad (58)$$

$$\frac{\partial \mathcal{T}_m}{\partial \phi_\ell} = \sqrt{1 - \lambda_m^2} \prod_{p=2, p \neq \ell}^{m-1} \sin(\phi_p) \cos(\phi_\ell), \quad (59)$$

$$\begin{aligned} \frac{\partial \mathcal{T}_\ell}{\partial \phi_\ell} &= -\frac{\sqrt{\sum_{r=1}^{\ell-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^{\ell} \lambda_r^2}} \prod_{p=2}^{\ell} \sin(\phi_p) - \lambda_\ell \left\{ \sum_{s=\ell+1}^{m-1} \frac{\lambda_s \prod_{p=2, p \neq \ell}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \right. \\ &+ \left. \frac{\lambda_m}{\sqrt{1 - \lambda_m^2}} \prod_{p=2, p \neq \ell}^{m-1} \sin(\phi_p) \right\} \cos(\phi_\ell), \quad 2 \leq \ell \leq m-1, \end{aligned} \quad (60)$$

$$\begin{aligned} \frac{\partial \mathcal{T}_i}{\partial \phi_\ell} &= \left(\frac{\sqrt{\sum_{r=1}^{i-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^i \lambda_r^2}} \prod_{p=2, p \neq \ell}^{i-1} \sin(\phi_p) \cos(\phi_i) - \lambda_i \left\{ \sum_{s=i+1}^{m-1} \frac{\lambda_s \prod_{p=2, p \neq \ell}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \right. \right. \\ &+ \left. \left. \frac{\lambda_m}{\sqrt{1 - \lambda_m^2}} \prod_{p=2, p \neq \ell}^{m-1} \sin(\phi_p) \right\} \right) \cos(\phi_\ell), \quad 2 \leq i \leq m-1, \ell < i, \end{aligned} \quad (61)$$

$$\begin{aligned} \frac{\partial \mathcal{T}_i}{\partial \phi_\ell} &= \lambda_i \left(\frac{\lambda_\ell \prod_{p=2}^{\ell} \sin(\phi_p)}{\sqrt{\sum_{r=1}^{\ell-1} \sum_{t=1}^{\ell} \lambda_r^2 \lambda_t^2}} - \left\{ \sum_{s=\ell+1}^{m-1} \frac{\lambda_s \prod_{p=2, p \neq \ell}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \right. \right. \\ &+ \left. \left. \frac{\lambda_m}{\sqrt{1 - \lambda_m^2}} \prod_{p=2, p \neq \ell}^{m-1} \sin(\phi_p) \right\} \right) \cos(\phi_\ell), \quad 2 \leq i \leq m-1, \ell > i, \end{aligned} \quad (62)$$

$$\frac{\partial^2 \mathcal{T}_m}{\partial \phi_\ell^2} = -\sqrt{1-\lambda_m^2} \Pi_{p=2}^{m-1} \sin(\phi_p), \quad (63)$$

$$\frac{\partial^2 \mathcal{T}_m}{\partial \phi_u \partial \phi_\ell} = \sqrt{1-\lambda_m^2} \Pi_{p=2, p \neq \ell, p \neq u}^{m-1} \sin(\phi_p) \cos(\phi_u) \cos(\phi_\ell), \quad u \neq \ell, \quad (64)$$

$$\begin{aligned} \frac{\partial^2 \mathcal{T}_\ell}{\partial \phi_\ell^2} &= -\frac{\sqrt{\sum_{r=1}^{\ell-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^{\ell} \lambda_r^2}} \Pi_{p=2}^{\ell} \sin(\phi_p) \cos(\phi_\ell) + \lambda_\ell \sum_{s=\ell+1}^{m-1} \frac{\lambda_s \Pi_{p=2}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \\ &+ \frac{\lambda_\ell \lambda_m}{\sqrt{1-\lambda_m^2}} \Pi_{p=2}^{m-1} \sin(\phi_p), \quad 2 \leq \ell \leq m-1, \end{aligned} \quad (65)$$

$$\begin{aligned} \frac{\partial^2 \mathcal{T}_\ell}{\partial \phi_u \partial \phi_\ell} &= -\left(\frac{\sqrt{\sum_{r=1}^{\ell-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^{\ell} \lambda_r^2}} \Pi_{p=2, p \neq u}^{\ell} \sin(\phi_p) \right) + \lambda_\ell \left\{ \sum_{s=\ell+1}^{m-1} \frac{\lambda_s \Pi_{p=2, p \neq \ell, p \neq u}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \right. \\ &+ \left. \frac{\lambda_m}{\sqrt{1-\lambda_m^2}} \Pi_{p=2, p \neq \ell, p \neq u}^{m-1} \sin(\phi_p) \right\} \cos(\phi_\ell) \cos(\phi_u), \quad 2 \leq \ell \leq m-1, \quad u < \ell, \end{aligned} \quad (66)$$

$$\begin{aligned} \frac{\partial^2 \mathcal{T}_\ell}{\partial \phi_u \partial \phi_\ell} &= \lambda_\ell \left(\frac{\lambda_u \Pi_{p=2, p \neq \ell}^u \sin(\phi_p)}{\sqrt{\sum_{r=1}^{u-1} \sum_{t=1}^u \lambda_r^2 \lambda_t^2}} - \left\{ \sum_{s=u+1}^{m-1} \frac{\lambda_s \Pi_{p=2, p \neq \ell, p \neq u}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \right. \right. \\ &+ \left. \left. \frac{\lambda_m}{\sqrt{1-\lambda_m^2}} \Pi_{p=2, p \neq \ell, p \neq u}^{m-1} \sin(\phi_p) \right\} \cos(\phi_u) \right) \cos(\phi_\ell), \quad 2 \leq \ell \leq m-1, \quad \ell < u, \end{aligned} \quad (67)$$

$$\begin{aligned} \frac{\partial^2 \mathcal{T}_i}{\partial \phi_\ell^2} &= -\frac{\sqrt{\sum_{r=1}^{i-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^i \lambda_r^2}} \Pi_{p=2}^{i-1} \sin(\phi_p) \cos(\phi_i) + \lambda_i \sum_{s=i+1}^{m-1} \frac{\lambda_s \Pi_{p=2}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \\ &+ \frac{\lambda_i \lambda_m}{\sqrt{1-\lambda_m^2}} \Pi_{p=2}^{m-1} \sin(\phi_p), \quad 2 \leq i \leq m-1, \quad \ell < i, \end{aligned} \quad (68)$$

$$\begin{aligned} \frac{\partial^2 \mathcal{T}_i}{\partial \phi_\ell^2} &= \lambda_i \left(\frac{\lambda_\ell \Pi_{p=2}^{\ell-1} \sin(\phi_p) \cos(\phi_\ell)}{\sqrt{\sum_{r=1}^{\ell-1} \sum_{t=1}^{\ell} \lambda_r^2 \lambda_t^2}} + \sum_{s=\ell+1}^{m-1} \frac{\lambda_s \Pi_{p=2}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \right. \\ &+ \left. \frac{\lambda_m}{\sqrt{1-\lambda_m^2}} \Pi_{p=2}^{m-1} \sin(\phi_p) \right), \quad 2 \leq i \leq m-1, \quad \ell > i, \end{aligned} \quad (69)$$

$$\begin{aligned} \frac{\partial^2 \mathcal{T}_i}{\partial \phi_u \partial \phi_\ell} &= \left(\frac{\sqrt{\sum_{r=1}^{i-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^i \lambda_r^2}} \prod_{p=2, p \neq \ell, p \neq u}^{i-1} \sin(\phi_p) \cos(\phi_i) \right. \\ &- \lambda_i \left\{ \sum_{s=i+1}^{m-1} \frac{\lambda_s}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \prod_{p=2, p \neq \ell, p \neq u}^{s-1} \sin(\phi_p) \cos(\phi_s) \right. \\ &\left. \left. + \frac{\lambda_m}{\sqrt{1-\lambda_m^2}} \prod_{p=2, p \neq \ell, p \neq u}^{m-1} \sin(\phi_p) \right\} \right) \cos(\phi_u) \cos(\phi_\ell), \quad 2 \leq i \leq m-1, \ell \neq u < i, \end{aligned} \quad (70)$$

$$\begin{aligned} \frac{\partial^2 \mathcal{T}_i}{\partial \phi_u \partial \phi_\ell} &= \lambda_i \left(\frac{\lambda_\ell \prod_{p=2, p \neq u}^\ell \sin(\phi_p)}{\sqrt{\sum_{r=1}^{\ell-1} \sum_{t=1}^\ell \lambda_r^2 \lambda_t^2}} - \left\{ \sum_{s=\ell+1}^{m-1} \frac{\lambda_s \prod_{p=2, p \neq \ell, p \neq u}^{s-1} \sin(\phi_p) \cos(\phi_s)}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \right. \right. \\ &\left. \left. + \frac{\lambda_m}{\sqrt{1-\lambda_m^2}} \prod_{p=2, p \neq \ell, p \neq u}^{m-1} \sin(\phi_p) \right\} \cos(\phi_\ell) \right) \cos(\phi_u), \quad (71) \\ &2 \leq i \leq m-1, (u \neq i) < \ell \text{ or } (\ell \neq i) < u. \end{aligned}$$

Proof. The Laplacian of $u_0(\epsilon, \mathcal{T})$ in (13) is computed as the sum of the two terms $\frac{1}{\sqrt{G}} \frac{\partial}{\partial \epsilon} \left(\sqrt{G} \frac{\partial u_0(\epsilon, \mathcal{T})}{\partial \epsilon} \right)$ and $\Delta_{\mathcal{S}(\Pi(X), \epsilon)} u_0(\epsilon, \mathcal{T})$, where $\Delta_{\mathcal{S}(\Pi(X), \epsilon)}$ is the restriction of the Laplace-Beltrami operator in (18) to the geodesical sphere $\mathcal{S}(\Pi(X), \epsilon)$ in $\Pi(\mathcal{X}_m^k)$ through Theorem 2^[17, p.149].

The first term involves, $\frac{\partial u_0(\epsilon, \mathcal{T})}{\partial \epsilon}$ that is $\frac{\sqrt{6} \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon}{(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)}$, and \sqrt{G} in (12), so it equals $\frac{\sqrt{6} \text{Ric}(\mathcal{T}, \mathcal{T}) (6d_m^k - (d_m^k - 1) \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)}{(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)^{5/2}}$. Next, according to (22) and (23), the second term involves $\frac{\partial u_0(\epsilon, \mathcal{T})}{\partial \phi_\ell}$ and $\frac{\partial^2 u_0(\epsilon, \mathcal{T})}{\partial \phi_u \partial \phi_\ell}$ hereafter,

$$\frac{\partial u_0(\epsilon, \mathcal{T})}{\partial \phi_\ell} = \frac{\sqrt{6} \epsilon^2}{2(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)^{3/2}} \frac{\partial \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_\ell}, \quad (72)$$

$$\begin{aligned} \frac{\partial^2 u_0(\epsilon, \mathcal{T})}{\partial \phi_u \partial \phi_\ell} &= \frac{3\sqrt{6} \epsilon^4}{4(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)^{5/2}} \frac{\partial \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_u} \frac{\partial \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_\ell} \\ &+ \frac{\sqrt{6} \epsilon^2}{2(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2)^{3/2}} \frac{\partial^2 \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_u \partial \phi_\ell}, \end{aligned} \quad (73)$$

where,

$$\frac{\partial \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_\ell} = 2 \sum_{i,j=2}^m \text{Ric} \left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j} \right) \frac{\partial \mathcal{T}_i}{\partial \phi_\ell} \mathcal{T}_j, \quad (74)$$

$$\frac{\partial^2 \text{Ric}(\mathcal{T}, \mathcal{T})}{\partial \phi_u \partial \phi_\ell} = 2 \sum_{i,j=2}^m \text{Ric} \left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j} \right) \left(\frac{\partial^2 \mathcal{T}_i}{\partial \phi_u \partial \phi_\ell} \mathcal{T}_j + \frac{\partial \mathcal{T}_i}{\partial \phi_\ell} \frac{\partial \mathcal{T}_j}{\partial \phi_u} \right). \quad (75)$$

Now, the following reciprocal relations,

$$\mathcal{T}_i = \frac{\sqrt{\sum_{r=1}^{i-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^i \lambda_r^2}} \hat{\mathcal{T}}_i - \lambda_i \left(\sum_{s=i+1}^{m-1} \frac{\lambda_s}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \hat{\mathcal{T}}_s + \frac{\lambda_m}{\sqrt{1-\lambda_m^2}} \hat{\mathcal{T}}_m \right), \quad (76)$$

$$2 \leq i \leq m-1,$$

and

$$\mathcal{T}_m = \sqrt{1-\lambda_m^2} \hat{\mathcal{T}}_m, \quad (77)$$

of (37) and (38), respectively, are considered ^[19, Lemma 3], and consecutively the coordinates $\hat{\mathcal{T}}_s$ are replaced with their expressions in (39) and (40) to get,

$$\mathcal{T}_i = \frac{\sqrt{\sum_{r=1}^{i-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^i \lambda_r^2}} \prod_{\ell=2}^{i-1} \sin(\phi_\ell) \cos(\phi_i) - \lambda_i \left(\sum_{s=i+1}^{m-1} \frac{\lambda_s}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} \prod_{\ell=2}^{s-1} \sin(\phi_\ell) \cos(\phi_s) \right. \\ \left. + \frac{\lambda_m}{\sqrt{1-\lambda_m^2}} \prod_{\ell=2}^{m-1} \sin(\phi_\ell) \right), \quad 2 \leq i \leq m-1, \quad (78)$$

and

$$\mathcal{T}_m = \sqrt{1-\lambda_m^2} \prod_{\ell=2}^{m-1} \sin(\phi_\ell). \quad (79)$$

Then, the calculus of the partial derivatives $\frac{\partial \mathcal{T}_i}{\partial \phi_\ell}$ and $\frac{\partial^2 \mathcal{T}_i}{\partial \phi_u \partial \phi_\ell}$ appearing in (74) and (75) is achieved using (78) and (79).

The term $\Delta u_0(0, T)$ is defined through the continuous extension at $(0, T)$ of the functions $\mathcal{B}(\epsilon, T)$, $\mathcal{C}(\epsilon, T)$, and $\mathcal{D}(\epsilon, T)$ since they converge to zero, $\frac{1}{12}$, and zero, respectively, when ϵ converges to zero.

Finally, the expression of the coefficient $u_1(\epsilon, T)$ is obtained in Corollary 4 hereafter.

Corollary 4. Under the same assumptions of Theorem 3, the expression of $u_1(\epsilon, T)$ is

$$\mathcal{I}(\epsilon, T) + \left(\sum_{i=2}^m K_2^{i,i}(T) - \sum_{i,j=2}^m \lambda_i \lambda_j K_2^{i,j}(T) \right) \mathcal{J}(\epsilon, T) \\ + \left(\sum_{i=2}^m K_1^{i,i}(T) - \sum_{i,j=2}^m \lambda_i \lambda_j K_1^{i,j}(T) \right) \mathcal{K}(\epsilon, T) \\ - \sum_{i=2}^m \lambda_i K^i(T) \mathcal{L}(\epsilon, T), \quad (80)$$

where $K^i(T)$, $K_1^{i,j}(T)$ and $K_2^{i,j}(T)$ are defined in (47), (50), and (51), respectively, and

$$\mathcal{I}(\epsilon, \mathcal{T}) = \frac{\sqrt{6} \left(6 + 24d_m^k + (1 - 4d_m^k) \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2 \right) \text{Ric}(\mathcal{T}, \mathcal{T})}{8 \left(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2 \right)^{5/2}} + \frac{(4d_m^k - 1) \sqrt{\text{Ric}(\mathcal{T}, \mathcal{T})}}{48 \epsilon \sqrt{6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2}} \text{atanh} \left(\frac{\sqrt{\text{Ric}(\mathcal{T}, \mathcal{T})} \epsilon}{\sqrt{6}} \right), \quad (81)$$

$$\mathcal{J}(\epsilon, \mathcal{T}) = \frac{3\sqrt{6}}{\epsilon \sqrt{6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2}} \int_0^\epsilon \frac{r^2}{\sin^2(r) \left(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) r^2 \right)^2} dr, \quad (82)$$

$$\mathcal{K}(\epsilon, \mathcal{T}) = \frac{9\sqrt{6}}{2 \epsilon \sqrt{6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2}} \int_0^\epsilon \frac{r^4}{\sin^2(r) \left(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) r^2 \right)^3} dr, \quad (83)$$

$$\mathcal{L}(\epsilon, \mathcal{T}) = \frac{3\sqrt{6}(m-1)}{\epsilon \sqrt{6 - \text{Ric}(\mathcal{T}, \mathcal{T}) \epsilon^2}} \int_0^\epsilon \frac{r^2}{\sin^2(r) \left(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) r^2 \right)^2} dr. \quad (84)$$

Proof. It is clear that the term $u_0(r, \mathcal{T}) \Delta u_0(r, \mathcal{T})$, in the expression (14) of $u_1(\epsilon, \mathcal{T})$, is a continuous function of r as ascertained by Theorem 3 (notice that $u_1(0, \mathcal{T})$ equals $u_0^2(0, \mathcal{T}) \Delta u_0(0, \mathcal{T})$). So, (13) and (45) are used to write $u_0(r, \mathcal{T}) \Delta u_0(r, \mathcal{T})$ as,

$$\frac{\sqrt{6}}{\sqrt{6 - \text{Ric}(\mathcal{T}, \mathcal{T}) r^2}} \left(\frac{\sqrt{6} \text{Ric}(\mathcal{T}, \mathcal{T}) \{ 6d_m^k - (d_m^k - 1) \text{Ric}(\mathcal{T}, \mathcal{T}) r^2 \}}{\left(6 - \text{Ric}(\mathcal{T}, \mathcal{T}) r^2 \right)^{5/2}} + \sum_{i=2}^m \frac{\partial^2 u_0(r, \mathcal{T})}{\partial \lambda_i^2} - \sum_{i,j=2}^m \lambda_i \lambda_j \frac{\partial^2 u_0(r, \mathcal{T})}{\partial \lambda_i \partial \lambda_j} - (m-1) \sum_{i=2}^m \lambda_i \frac{\partial u_0(r, \mathcal{T})}{\partial \lambda_i} \right).$$

Then, both $\int_0^\epsilon \frac{\sqrt{6}}{\sqrt{6 - \text{Ric}(\mathcal{T}, \mathcal{T}) r^2}} \frac{\partial u_0(r, \mathcal{T})}{\partial \lambda_i} dr$ and $\int_0^\epsilon \frac{\sqrt{6}}{\sqrt{6 - \text{Ric}(\mathcal{T}, \mathcal{T}) r^2}} \frac{\partial^2 u_0(r, \mathcal{T})}{\partial \lambda_i \partial \lambda_j} dr$ are computed using (46) and (49), respectively, where the parameter ϵ should be within closed intervals corresponding to compact subspaces of $\prod(\mathcal{X}_m^k)$.

4. Discussion

The heat kernel approximation proposed in (11) can be extended straightforwardly to the subspace $\sum_m^k \setminus \Pi(\mathcal{D}_{m-1})$ of shapes in \sum_m^k whose pre-shapes' singular values λ_i , for $1 \leq i \leq m$, remain strictly positive, yet they are not necessarily different anymore; here, \mathcal{D}_{m-1} is the set, defined in Kendall theory, of pre-shapes where λ_m is fixed to zero. The extension is based on the fact that the already used differential operators and functions, involving unitary tangent vectors, are still valid for $\sum_m^k \setminus \Pi(\mathcal{D}_{m-1})$ since none of them includes terms that are inversely proportional to singular values differences. Essentially, the established expressions of the Laplace-Beltrami operator, the exponential map, the determinant of the path of linear transformations, the Ricci tensor for $\prod(\mathcal{X}_m^k)$, as well as the coefficients $u_0(\epsilon, \mathcal{T})$ and $u_1(\epsilon, \mathcal{T})$, are all well defined on $\sum_m^k \setminus \Pi(\mathcal{D}_{m-1})$.

The Kendall space has been exploited in several objects' recognition approaches^[20-23], a fact that emphasizes the need for tools, like the heat kernel closed-form established in this paper, to better measure the similarity between shapes.

Indeed, heat kernel can be interpreted as density probability function or also as inner product in various approaches of machine learning for shapes recognition. It should be recalled that the motivation for the establishment of the heat kernel expression in (11) has been the need to solve the problem of shape classification within the framework of Kendall shape space. In general, given a set of N training shapes $(\Pi(S_i), C_i)$ for $1 \leq i \leq N$, where C_i are labels designating classes, then the consequent question of interest is naturally what would be the class of an unseen shape $\Pi(S)$? For the special case of two classes C_1 and C_2 , the shapes' classifier C is a function that maps any shape $\Pi(S)$ in $\Pi(\mathcal{X}_m^k)$ to one of the two classes. The Reproducing Kernel Hilbert Space (RKHS) of the linear combinations of the functions $H(\Pi(S_i), \cdot, t)$, is commonly used to seek the classifier $C(\cdot)$ amongst the functions $\sum_{i=1}^N c_i H(\Pi(S_i), \cdot, t)$ in RKHS for some scalars c_i in \mathbb{R} ; according to the Representer theorem, C minimizes the error functional $\frac{1}{N} \sum_{i=1}^N (C(\Pi(S_i)) - C_i)^2 + \psi \sum_{i=1}^N c_i^2 H(\Pi(S_i), \Pi(S_i), t)$ where C_i are integer labels and ψ is some regularization scalar parameter^[40, 41]. It is interesting to notice that theoretically, the manifold metric can help to perform shapes' classification more easily, but in practice this kind of classification is too sensitive to noise, hence the importance of the heat kernel based classifiers that are robust^[42]. Besides, the heat kernel is a Mercer one that makes it useful for statistical learning; the geodesic distance does not have this property of course^[11]. Consequently, the heat kernel is appropriate for constructing nonlinear support vector machines for shapes' classification^[43].

It is worth noting that to better grasp the significance of the heat kernel closed-form approximation in (11) it should be reminded that the straightforward resolution of heat equations is only feasible for a restricted set of classical manifolds^[24-27], other approaches provide merely bounds of the heat kernel^[28-38]. Furthermore, number of closed-form expressions have been proposed in the literature to calculate the heat kernel on hyperspheres like \mathcal{S}_m^k . For instance, the heat kernel $h(X, Y, t)$ on \mathcal{S}_m^k , endowed with a distance d and for any pre-shapes X and Y , can be approximated by the following expression obtained from [39, p. 16],

$$\frac{e^{-d^2(X,Y)/2t}}{\sqrt{2\pi t}^{m(k-1)}} \left(\frac{\sqrt{d(X,Y)}}{\sqrt{\sin(d(X,Y))}} \right)^{m(k-1)-1}$$

since the principal curvatures of $m(k-1)-1$ equal one. The heat kernel $h(X, Y, t)$ can also be written as the sum

$$\sum_{i \geq 1} e_i(X) e_i(Y) e^{-v_i t},$$

where e_i and v_i are the eigenfunctions and eigenvalues of the Laplacian on the hypersphere^[17]; other heat kernel calculation techniques are based upon recurrence relations of derivatives^[14]. Despite the elegance of all of these closed-form expressions, they do not help to easily infer closed-form expressions for the heat kernel on the quotient space \sum_m^k , as done in this paper. Indeed, given a manifold M , the closed-form of the heat kernel $H_{M/G_I}(p, q, t)$ on the quotient space M/G_I coincides with the sum of the heat kernels $h_M(p, g_I \bullet q, t)$ of M for all isometries g_I in the discontinuous group G_I ^[17, p.155], p and q are in M , and $g_I \bullet q$ are the actions of the isometries g_I on q ; in the present research the orthogonal group $SO(m)$ is a continuous Lie group.

The present discussion is ended with an analysis of the values of the parameter ϵ . Indeed, the latter should fulfill number of conditions in order to keep consistent the results presented so far. First, the values of ϵ in (8) should be in the interval $[0, \epsilon_\lambda]$ defined in [19, Lemma 4] to keep the pre-shape curves $\tilde{\Gamma}_\epsilon(\epsilon)$ within \mathcal{X}_m^k . Besides, the parameter ϵ should be necessarily strictly smaller than the local injectivity radius $\arccos\left(\sqrt{1 - \lambda_{m-1}^2 - \lambda_m^2}\right)$ of $\Pi(\mathcal{X}_m^k)$ at a shape $\Pi(X)$ to accurately define exponential map (Sect. Preliminaries and methods) and to exploit the Minakshisundaram-Pleijel recursion formulas^[19, Lemma 1]; the spaces $\sum_m^k \setminus \Pi(\mathcal{D}_{m-1})$ and $\Pi(\mathcal{X}_m^k)$ share the previous expression of the local injectivity radius. This injectivity radius based upper bound is necessary yet not sufficient because the heat kernel expansion is defined on compact subspaces of $\Pi(\mathcal{X}_m^k)$. Furthermore, in (13) that defines the first coefficient of the heat kernel expansion, the parameter ϵ should be strictly smaller than

$$\frac{\sqrt{6}}{\sqrt{\sum_{i,j=2}^m \text{Ric}\left(\frac{\partial}{\partial \lambda_i}, \frac{\partial}{\partial \lambda_j}\right) \epsilon_i \epsilon_j}}, \quad (85)$$

where the real numbers,

$$\epsilon_i = \frac{\sqrt{\sum_{r=1}^{i-1} \lambda_r^2}}{\sqrt{\sum_{r=1}^i \lambda_r^2}} + \lambda_i \left(\sum_{s=i+1}^{m-1} \frac{\lambda_s}{\sqrt{\sum_{r=1}^{s-1} \sum_{t=1}^s \lambda_r^2 \lambda_t^2}} + \frac{\lambda_m}{\sqrt{1-\lambda_m^2}} \right), \quad 2 \leq i \leq m-1 \quad (86)$$

and

$$\epsilon_m = \sqrt{1-\lambda_m^2}. \quad (87)$$

are the upper bounds of the absolute values of the coordinates T_i in (15) that have been already written above as (78) and (79).

5. Conclusion

The Minakshisundaram-Pleijel recursion formulas proved to be useful in the case of the Kendall shape spaces Σ_m^k , for $m \geq 3$ and $k \geq m + 2$, that are homeomorphic neither to each other nor to any known spaces. They helped to establish the closed-form approximations of the first and second coefficients of the heat kernel expansion. The obtained expression of the heat kernel in (11) represents a potential interest in machine learning for objects recognition since it helps to get more robust and accurate shape similarity measurements. The latter is evaluated through interpreting the heat kernel as density probability functions and inner products in Bayesian and kernel-based machine learning approaches, respectively.

References

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- [1] Kendall DG, Barden D, Carne TK, Le H. *Shape and shape theory*. England: John Wiley & Sons Ltd; 1999. p.309.
 - [2] Kendall DG. The diffusion of shape. *Adv. Appl. Probab.* 1977; 9(3): 428-430.
 - [3] Kendall DG. Shape manifolds, procrustean metrics, and complex projective spaces. *Bull. Lond. Math. Soc.* 1984; 16(2): 81-121.
 - [4] Kendall DG. Exact distributions for shapes of random triangles in convex sets. *Adv. Appl. Probab.* 1985; 17(2): 308-329.
 - [5] Kendall DG. Further developments and applications of the statistical theory of shape. *Theory Probab. Appl.* 1986; 31(3): 407-412.
 - [6] Kendall DG. A survey of the statistical theory of shape. *Statist. Sci.* 1989; 4(2): 87-99.
 - [7] Le H, Kendall DG. The riemannian structure of euclidean shape spaces: a novel environment for statistics. *Ann. Statist.* 1993; 21(3): 1225-1271.
 - [8] Kendall DG, Le H. The structure and explicit determination of convex polygonally shape-densities. *Adv. Appl. Probab.* 1987; 19(4): 896-916.
 - [9] Mtibaa R, Khan S. Tangential vector fields on Kendall shape space. *J. Adv. Math. Stud.* 2018; 11(3): 520-527.
 - [10] Dryden EB, Gordon CS, Greenwald SJ, Webb DL. Asymptotic expansion of the heat kernel for orbifolds. *Michigan Math. J.* 2008; 56(1): 205-238.
 - [11] Lafferty J, Lebanon G. Diffusion kernels on statistical manifolds. *J. Mach. Learn. Res.* 2005; 6: 129-163.
 - [12] Dowker JS. Heat kernel expansion on a generalized cone. *J. Math. Phys.* 1989; 30(4): 770-773.
 - [13] Dowker JS. Heat-kernel expansion on a polyhedron. *Phys. Rev. D.* 1987; 36(2): 620-622.
 - [14] Nagase M. Expressions of the heat kernels on spheres by elementary functions and their recurrence relations. *Saitama Math. J.* 2010; 27: 25-34.

- [15] Lue PC. The asymptotic expansion for the trace of the heat kernel on a generalized surface of revolution. *Trans. Amer. Math. Soc.* 1982; 273(1): 93-110.
- [16] Vassilevich DV. Heat kernel expansion : user's manual. *Phys. Rep.* 2003; 388(5-6): 279-362.
- [17] Chavel I. *Eigenvalues in Riemannian geometry*. United States of America: Academic Press Inc; 1984. p.379.
- [18] Mtibaa R, Khan S. Directional derivatives on Kendall shape space. *Nonlinear Studies*. 2020; 27(1): 25-52.
- [19] Mtibaa R, Khan S. Injectivity radius and geometric bound on Kendall shape space. *Nonlinear Studies*. 2019; 26(3): 663-691.
- [20] Rouahi H. Allah, Mtibaa R, Zagrouba E. Bayesian approach in Kendall shape space for plant species classification. In: Alexandre L, Salvador Sánchez J, Rodrigues J. *Pattern Recognition and Image Analysis IbPRIA (Lecture Notes in Computer Science 10255)*. Springer, Cham; 2017. p.322-331.
- [21] Han Y. Recognize objects with three kinds of information in landmarks. *Pattern Recognition*. 2013; 46(11): 2860-2873.
- [22] Han Y, Wang B, Idesawa M, Shimai H. Recognition of multiple configurations of objects with limited data. *Pattern Recognition*. 2010; 43(4): 1467-1475.
- [23] Han Y, Koike H, Idesawa M. Recognizing objects with multiple configurations. *Pattern Anal. Appl.* 2014; 17(1): 195-209.
- [24] Guoqiang W, Yi H. The heat kernels on some classical manifolds and classical domains. *Acta Math. Sinica New Series*. 1991; 7(4): 324-341.
- [25] Fischer HR, Jungster JJ, Williams FL. The heat kernel on the two-sphere. *Adv. Math.* 1984; 54(2): 226-232.
- [26] Grigor'yan A, Noguchi M. The heat kernel on hyperbolic space. *Bull. Lond. Math. Soc.* 1998; 30(6): 643-650.
- [27] Ding H. Heat kernels of lorentz cones. *Canad. Math. Bull.* 1999; 42(2): 169-173.
- [28] Grigor'yan A. Gaussian upper bounds for the heat kernel on arbitrary manifolds. *J. Differential Geom.* 1997; 45(1): 33-52.
- [29] Grigor'yan A. Heat kernel upper bounds on a complete non-compact manifold. *Rev. Mat. Iberoam.* 1994; 10(2): 395-452.
- [30] Grigor'yan A, Telcs A. Two-sided estimates of heat kernels on metric measure spaces. *Ann. Probab.* 2012; 40(3): 1212-1284.
- [31] Grigor'yan A, Ishiwata S. Heat kernel estimates on a connected sum of two copies of \mathbb{R}^n along a surface of revolution. *Global and Stochastic Analysis*. 2015; 2(1): 29-65.
- [32] Nowaka A, Sjögren P, Szarek TZ. Sharp estimates of the spherical heat kernel. *J. Math. Pures. Appl.* 2019; 129: 23-33.
- [33] Rose C. Heat kernel upper bound on Riemannian manifolds with locally uniform ricci curvature integral bounds. *J. Geom. Anal.* 2017; 27(2): 1737-1750.
- [34] Barilari D, Boscain U, Neel RW. Small-time heat kernel asymptotics at the sub-riemannian cut locus. *J. Differential Geom.* 2012; 92(3): 373-416.
- [35] Bernicota F, Coulhomb T, Frey D. Gaussian heat kernel bounds through elliptic Moser iteration. *J. Math. Pures. Appl.* 2016; 106(6): 995-1037.
- [36] Saloff-Coste L. The heat kernel and its estimates. *Adv. Stud. Pure Math.* 2010; 57: 405-436.
- [37] Pivarski M, Saloff-Coste L. Small time heat kernel behavior on Riemannian complexes. *New York J. Math.* 2008; 14: 459-494.
- [38] Cheng SY, Li P, Yau S-T. On the upper estimate of the heat kernel of a complete riemannian manifold. *Amer. J. Math.* 1981; 103(5): 1021-1063.
- [39] Molchanov SA. Diffusion processes and riemannian geometry. *Russian Math. Surveys*. 1975; 30(1): 1-63.
- [40] Burges CJC, Scholkopf B, Smola AJ. *Advances in kernel methods: support vector learning*. The MIT Press; 1999.
- [41] Wahba G. Spline models for observational data. CBMS-NSF regional conference series in applied mathematics. *SIAM, Philadelphia, PA*. 1990.
- [42] Belkin M, Niyogi P. Semi-supervised learning on riemannian manifolds. *Machine Learning*. 2004; 56: 209-239.
- [43] Burges CJC. A tutorial on support vector machines for pattern recognition. *Data mining and knowledge discovery*. 1998; 2: 121-167.