Generalized Heat Kernel Signatures

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ABSTRACT

In this work we propose a generalization of the Heat Kernel Signature (HKS). The HKS is a point signature derived from the heat kernel of the Laplace-Beltrami operator of a surface. In the theory of exterior calculus on a Riemannian manifold, the Laplace-Beltrami operator of a surface is a special case of the Hodge Laplacian which acts on r-forms, i. e. the Hodge Laplacian on 0-forms (functions) is the Laplace-Beltrami operator. We investigate the usefulness of the heat kernel of the Hodge Laplacian on 1-forms (which can be seen as the vector Laplacian) to derive new point signatures which are invariant under isometric mappings. A similar approach used to obtain the HKS yields a symmetric tensor field of second order; for easier comparability we consider several scalar tensor invariants. Computed examples show that these new point signatures are especially interesting for surfaces with boundary.

Keywords: Shape analysis, Hodge Laplacian, heat kernel, discrete exterior calculus

1 INTRODUCTION

The identification of similarly shaped surfaces or parts of surfaces, represented as triangle meshes, is an important task in computational geometry. In this paper, we consider two surfaces as being similar if there is an isometry between them. For example, all meshes describing different poses of an animal are considered to be similar.

One approach to solve this problem makes use of spectral analysis of the Laplace-Beltrami operator Δ_0 of the surface. The Laplace-Beltrami operator Δ_0 describes diffusion processes, is by definition invariant under isometries, and is known to reveal many geometric properties of the surface.

In [8] the eigenvalues of the Laplace-Beltrami operator are proposed as a 'Shape-DNA'. If two surfaces are isometric, then the eigenvalues of the respective Laplace-Beltrami operators coincide. While one can construct counter examples to the converse of this statement, this does not seem to pose a problem in practice.

In contrast to this global characterization of surfaces, in [10] the eigenvalues and eigenfunctions of the Laplace-Beltrami operator are used to compute a point signature. This point signature is a function on the surface containing a scale parameter, and is called *Heat Kernel Signature*. For benchmarks evaluating the Heat Kernel Signature and other methods we refer the reader to [3], [4].

In this work we propose and investigate a generalization of the *Heat Kernel Signature*. The Laplace-Beltrami operator Δ_0 of a surface can be generalized to the Hodge Laplacian Δ_r which is an operator acting on r-forms. This operator is defined in the setting of exterior calculus in Section 2 and its heat kernel is introduced in Section 3. We can then derive a new isometry invariant point signature from the Hodge-Laplacian on 1-forms Δ_1 in Section 4. This yields a symmetric tensor field of second order containing a scale parameter. As it is difficult to compare and quantify such tensor fields, we consider several scalar valued tensor invariants for the purpose of surface analysis. To increase the reproducibility of the results shown in Section 6, we give some details about our implementation of this method in Section 5. For our discretization of Δ_1 we use the theory of discrete exterior calculus (DEC) which mimics the theory of exterior calculus on a discrete level.

2 MATHEMATICAL BACKGROUND

To generalize the Laplace-Beltrami operator and the heat kernel to r-forms it is beneficial to employ the theory of exterior calculus on a Riemannian manifold. We will give a short introduction to this topic in this section. An extensive introduction to exterior calculus can be found for example in the textbook [1].

For simplicity we restrict ourselves to a Riemannian manifold (M,g) of dimension 2. Readers who are not familiar with Riemannian manifolds may think of M being a surface embedded in $\mathbb{R}^3$. In this case the Riemannian metric g is given by the first fundamental form, i. e. g_p is the scalar product on the tangent space $T_p(M)$ at p which is induced by the standard scalar product on $\mathbb{R}^3$.

The set of r-forms on M is denoted by $\bigwedge^r(M)$, where $r = 0\dots2$. A 0-form on M is a smooth function from M to $\mathbb{R}$, consequently $\bigwedge^0(M) = C^\infty(M)$. A 1-form on

M is a smooth map which assigns each $p \in M$ a linear map from $T_p(M)$ to $\mathbb{R}$, i. e. an element of the dual space $(T_p(M))^*$ of $T_p(M)$. A 2-form α on M is a smooth map which assigns each $p \in M$ a bilinear form on $T_p(M)$ which is skew-symmetric, that is for each $p \in M$ and $v,w \in T_p(M)$ we have $\alpha_p(v,w) = -\alpha_p(w,v)$. We will later see that a 1-form can be identified with a vector field while a 2-form can be interpreted as a function on the manifold.

The Hodge-Laplace operator will now be defined in terms of local coordinates. Let (U,ϕ) be a chart with coordinate functions (x_1,x_2), i. e. $\phi(p) = (x_1(p),x_2(p)) \in \mathbb{R}^2$. The tangent vectors to the coordinate lines which are denoted by $\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}$, or shorter ∂_1, ∂_2, form a frame on U, i. e. $(\partial_1)_p, (\partial_2)_p$ is a basis of $T_p(M)$ for each $p \in U$. The differentials dx_1, dx_2 of x_1 and x_2 form a coframe on U, i. e. $(dx_1)_p, (dx_2)_p$ is a basis of $(T_p(M))^*$, and we have $dx_i(\partial_j) = \delta^i_j$. Thus, for any 1-form $\alpha \in \bigwedge^1(M)$ there are functions $f_1, f_2 \in \mathbb{C}^\infty(U)$ such that

$$\alpha|_U = f_1\, dx_1 + f_2\, dx_2 \ ,$$

where $f_1 = \alpha(\partial_1)$, $f_2 = \alpha(\partial_2)$.

The wedge prodcut $\wedge$ of two 1-forms α, β is defined pointwise at each $p \in M$ by

$$(\alpha_p \wedge \beta_p)(v,w) = \alpha_p(v)\beta_p(w) - \beta_p(v)\alpha_p(w)$$

for all $v,w \in T_p(M)$. A two form $\alpha \in \bigwedge^2(M)$ can thereby be represented by $\alpha|_U = f\, dx_1 \wedge dx_2$, where $f = \alpha(\partial_1, \partial_2) \in C^\infty(M)$.

There is an isomorphism between vector fields and 1-forms on M which is called flat operator and denoted by $^\flat$. For a vector field v it is defined by $v^\flat_p(\cdot) = g(v_p, \cdot)$ at each $p \in M$. Its inverse is the sharp operator $^\sharp$. If e_1, e_2 is an orthonormal basis of $T_p(M)$ and $\varepsilon_1, \varepsilon_2$ its dual basis we have $(\lambda_1 e_1 + \lambda_2 e_2)^\flat = \lambda_1 \varepsilon_1 + \lambda_2 \varepsilon_2$, where $\lambda_1, \lambda_2 \in \mathbb{R}$.

The differential d takes a function f on M to the 1-form

$$d_0 f = \frac{\partial f}{\partial x_1} dx_1 = \frac{\partial f}{\partial x_2} dx_2 \ ,$$

i. e. d_0 maps 0-forms to 1-forms. One may think of d_0 as ∇. We will denote d also by d_0 and define the map d_1 taking 1-forms to 2-forms by

$$d_1\,(f_1\, dx_1 + f_2\, dx_2) = \left(\frac{\partial f_2}{\partial x_1} - \frac{\partial f_1}{\partial x_2}\right) dx_1 \wedge dx_2 \ .$$

d_1 can be interpreted as $\nabla\times$. The maps d_0 and d_1 are referred to as *exterior derivative*.

Next we will define the maps δ_1 and δ_2 which take 1-forms to 0-forms and 2-forms to 1-forms, respectively, and are also called *codifferential*. These maps depend, in contrast to d_0 and d_1, on the metric of M. We set $g_{ij} = g\left(\frac{\partial}{\partial x_i}, \frac{\partial}{\partial x_j}\right)$ and $G = \sqrt{\det[g_{ij}]}$. For simplicity we use orthogonal coordinates, that is $[g_{ij}]$ is a diagonal matrix. This is not a restriction, since any point $p \in M$ is contained in a chart with this property. The *Hodge star operator* $*_r$ is a map taking r-forms to $(2-r)$-forms, $r = 0, \ldots, 2$, defined by

$$*_0 f = G f\, dx \wedge dy \ ,$$
$$*_1(f_1\, dx_1 + f_2\, dx_1) = -g_{22} G f_2\, dx_1 + g_{11} G f_1\, dx_2 \ ,$$
$$*_2(f\, dx_1 \wedge dx_2) = \frac{f}{G} \ .$$

Now δ_1 and δ_2 are defined by

$$\delta_1 = -*_2\, d_1 *_1 \ , \quad \delta_2 = -*_1\, d_0 *_2 \ ,$$

which can be rewritten to

$$\delta_1\,(f_1\, dx_1 + f_2\, dx_2) = -\frac{1}{G}\left(\frac{\partial g_{11} G f_1}{\partial x_1} + \frac{\partial g_{22} G f_2}{\partial x_2}\right),$$
$$\delta_2(f\, dx_1 \wedge dx_2) = g_{22} G \frac{\partial \frac{f}{G}}{\partial x_2} dx_1 - g_{11} G \frac{\partial \frac{f}{G}}{\partial x_1} dx_2 \ .$$

One may think of $-\delta_1$ as $\nabla\cdot$ and $-\delta_1$ as $\nabla^\perp$.

The *Hodge Laplacian* $\Delta_r : \bigwedge^r(M) \to \bigwedge^r(M)$, where $r = 0, \ldots, 2$, is now defined by

$$\Delta_0 = \delta_1 d_0 \ ,$$
$$\Delta_1 = \delta_2 d_1 + d_0 \delta_1 \ ,$$
$$\Delta_2 = d_1 \delta_2 \ .$$

Sometimes Δ_r is also called Laplace-de Rham operator or just Laplacian, where Δ_0 is also referred to as Laplace-Beltrami operator. If $M = \mathbb{R}^2$ with standard coordinates we have $g_{11} = g_{22} = G = 1$, thus $-\Delta_0$ coincides with the well-known definition of the Laplacian on $\mathbb{R}^2$, i. e. $\Delta_0 = \frac{\partial^2}{\partial^2 x_1} + \frac{\partial^2}{\partial^2 x_2}$.

3 HEAT KERNEL

The basic properties of heat diffusion on a Riemannian manifold will be introduced in this section. Of special interest for us is the heat kernel and its generalization to 1-forms. In Section 4 we will derive point signatures from the heat kernel for 1-forms in a similar way as the Heat Kernel Signature is derived from the heat kernel for functions. For details on the heat kernel for r-forms see [9].

Let (M,g) be a 2-dimensional, compact, oriented Riemannian manifold. Given an initial heat distribution $f(p) = f(0,p) \in C^\infty(M)$ on M, considered to be perfectly insulated, the heat distribution $f(t,p) \in C^\infty(M)$ at time t is governed by the *heat equation*

$$(\partial_t + \Delta_0) f(t,p) = 0 \ .$$

The function $k^0(t,p,q) \in C^\infty(\mathbb{R}^+ \times M \times M)$ such that for all $f \in C^\infty(M)$

$$(\partial_t + (\Delta_0)_p) k^0(t,p,q) = 0 \ ,$$
$$\lim_{t \to 0} \int k^0(t,p,q) f(q)\, dq = f(p) \ ,$$

is called *heat kernel*. $(\Delta_0)_p$ denotes the Laplacian acting in the p variable. Using the heat kernel one can define the *heat operator* H_t for $t > 0$ by

$$H_t f(p) = \int_M k^0(t,p,q) f(q)\, dq \ .$$

One can show that $f(t,p) = H_t f(p)$ solves the Heat equation, thus H_t maps an initial heat distribution to the heat distribution at time t. The heat kernel can be computed from the eigenvalues λ_i and the corresponding eigenfunctions ϕ_i of Δ_0 by the formula

$$k^0(t,p,q) = \sum_i e^{-\lambda_i t} \phi_i(p)\phi_i(q) \ .$$

Next we will generalize the heat kernel to 1-forms which results in a so-called double 1-form. A double 1-form is a smooth map which assigns each $(p,q) \in M \times M$ a bilinear map $T_pM \times T_qM \to \mathbb{R}$. Consequently, if β is a double form on M, $v \in T_p(M)$, $w \in T_q(M)$, then $q \mapsto \beta(p,q)(v,\cdot)$ and $p \mapsto \beta(p,q)(\cdot,w)$ are 1-forms on M. The heat kernel for 1-forms is now a double form $k^1(t,p,q)$ depending smoothly on an additional parameter t, which satisfies for each $\alpha \in \bigwedge^k(M)$

$$(\partial_t + (\Delta_1)_p) k^1(t,p,q) = 0 \ ,$$
$$\lim_{t\to 0} \int_M k^1(t,p,q) \left(\cdot, \alpha^\sharp(q)\right) dq = \alpha(p)(\cdot) \ .$$

Note that, given $\alpha \in \bigwedge^1(M)$ and $p,q \in M$ we obtain a bilinear map $T_p(M) \times T_q(M) \to \mathbb{R}$ by multiplying $\alpha(p)$ and $\alpha(q)$; thus

$$(p,q) \mapsto \alpha(p)(\cdot)\, \alpha(q)(\cdot)$$

is a double form. Similarly to the heat kernel for functions, we can compute the heat kernel for 1-forms from the eigenvalues λ_i and the eigenforms α_i of Δ_1 by

$$k^1(t,p,q)(\cdot,\cdot) = \sum_i e^{-\lambda_i t} \alpha_i(p)(\cdot)\, \alpha_i(q)(\cdot) \ .$$

4 POINT SIGNATURES FROM THE HEAT KERNEL FOR 1-FORMS

In this section we will derive new point signatures from the heat kernel of 1-forms. This is done in a similar way as the Heat Kernel Signature is derived from the heat kernel for functions (0-forms). The main difference is that this approach does not result in a time-dependent function for the heat kernel of 1-forms, instead we obtain a time-dependent tensor field. Thus, to obtain comparable values, we consider scalar tensor invariants. In this way we obtain several point signatures which are especially interesting for manifolds with boundary, as we will see in Section 6.

The Heat Kernel Signature at p is defined by

$$t \mapsto k^0(t,p,p) \ ,$$

i. e. a function $\mathbb{R}^+ \to \mathbb{R}$ is assigned to each point $p \in M$. It is shown in [10] that two points p,q have similar shaped neighborhoods if $\{k(t,p,p)\}_{t>0}$ and $\{k(t,q,q)\}_{t>0}$ coincide.

The analogous definition for the heat kernel for 1-forms,

$$t \mapsto k^1(t,p,p) \ ,$$

assigns each point $p \in M$ a bilinear form on $T_p(M)$ or equivalently a symmetric covariant tensor of second order. Comparing covariant tensors of second order on $T_p(M)$ and $T_q(M)$ is not possible unless we have a meaningful map between $T_p(M)$ and $T_q(M)$. It is therefore difficult to compare $\{k^1(t,p,p)\}_{t>0}$ and $\{k^1(t,q,q)\}_{t>0}$ directly. However, we can consider scalar tensor invariants which are independent of the chosen orthonormal basis of the tangent space.

If e_1, e_2 is an orthonormal basis of $T_p(M)$ we can assign to each bilinear form β a matrix $B = (b_{ij})$, where $b_{ij} = \beta(e_i, e_j)$, $i, j = 1, 2$. Now B is the matrix representation of β with respect to the orthonormal basis e_1, e_2 and the eigenvalues of β are defined to be the eigenvalues of B. If $\tilde{e}_1, \tilde{e}_2$ is another orthonormal basis and S the orthogonal matrix satisfying $\tilde{e}_1 = Se_1, \tilde{e}_2 = Se_2$, then the corresponding matrix representation $\tilde{B}$ of α is given by $\tilde{B} = SBS^T$, and with that the definition of the eigenvalues of β is independent of a certain orthonormal basis. Consequently, if λ_1 is the larger and λ_2 the smaller eigenvalue of β, quantities like λ_1 or λ_2 or combinations of it like the trace $\mathrm{tr}(\beta) = \mathrm{tr}(B) = \lambda_1 + \lambda_2$ or the determinant $\det(\beta) = \det(B) = \lambda_1\lambda_2$ are scalar tensor invariants. Using such tensor invariants we obtain point signatures like $\{\mathrm{tr}(k^1(t,p,p))\}_{t>0}$ which can be compared similarly as the Heat Kernel Signature, see [10] for details.

5 NUMERICAL REALIZATION

To compute our point signatures we need a matrix representation of the bilinear forms $k^1(t,p,p)$. We will use the equation

$$k^1(t,p,p)(\cdot,\cdot) = \sum_i e^{-\lambda_i t} \alpha_i(p)(\cdot)\, \alpha_i(p)(\cdot) \ , \quad (1)$$

where λ_i and α_i are the eigenvalues and eigenforms of Δ_1. For the computation of the eigenvalues and eigenforms we use the theory of discrete exterior calculus (DEC), which mimics the theory of exterior calculus on surfaces approximated as triangle meshes. A short introduction to DEC is given in Subsection 5.1.

Unfortunately the computation of the eigenvalues and eigenforms of Δ_1 using DEC is not straightforward. The common definitions work only for very special triangulations. We propose a solution to this problem in Subsection 5.2. Moreover we explain a way to realize the product $\alpha_i(p)(\cdot)\, \alpha_i(p)(\cdot)$ of two eigenforms which is not obvious for discrete r-forms.

5.1 Discrete Exterior Calculus

DEC deals with discrete forms which are defined on on a triangle mesh as an approximation of a surface. Additionally counterparts of operators like the exterior derivative and the Hodge star operator are defined for discrete forms. This enables us to define a discrete Hodge Laplacian. Thus DEC mimics the theory of smooth r-forms on surfaces. For details on DEC we refer the reader to [7], which is the most extensive source, as well as to [5] and [6].

Let K be a triangle mesh with vertex set $V = \{v_i\}$, edge set $E = \{e_i\}$ and triangle set $T = \{t_i\}$. We assume that all triangles and edges have a fixed orientation. The orientation of a vertex is always positive; the orientation of an edge e_i is given by an order of vertices $e = [v_i v_j]$; the orientation of a triangle t is given by a cyclic order of vertices $t = [v_i v_j v_k]$. If v is a vertex of the edge $e = [v_i v_j]$, the orientations of v and e are said to agree if $v = v_j$ and disagree if $v = v_i$. Similarly, given an edge e of a triangle t, the orientations of e and t are said to agree (disagree) if the vertices of e occur in the same (opposite) order in t.

Discrete 0-forms, 1-forms and 2-forms are defined to be functions from V, E and T to $\mathbb{R}$, respectively. The function values should be understood as the integral of a continuous 0-form, 1-form or 2-form over a vertex, edge or triangle, respectively. Note that reversing the orientation of vertices, edges or triangles changes the sign of the associated integral values, thus the same holds for discrete r-forms. Of course, this definition of discrete r-forms does not allow a point-wise evaluation.

However, it is possible to interpolate discrete r-forms by Whitney forms which are piecewise linear r-forms on the triangles. Whitney 0-forms are the so-called hat functions, i. e. ϕ_{v_i} is the piecewise linear function with $\phi_{v_i}(v_j) = \delta^i_j$. For an edge $e = [v_i, v_j]$ the Whitney 1-form ϕ_e is supported on the triangles adjacent to e and given by $\phi_e = \phi_{v_i} d\phi_{v_j} - \phi_{v_j} d\phi_{v_i}$. Note that ϕ_e is piecewise linear on each triangle, but discontinuous on the edge. However, the integral of both parts of ϕ_e over e is 1. We also have that the integral of ϕ_e is 0 over each edge different from e. There is a similar definition for Whitney 2-forms which we omit here. The Whitney interpolant $\mathscr{I}\alpha$ of a discrete 0-form α is now given by

$$\mathscr{I}\alpha = \sum_{i=1,\dots,|V|} \alpha(v_i)\phi_{v_i} \quad .$$

The Whitney interpolant for discrete 1-forms and 2-forms is defined analogously.

0-forms, 1-forms and 2-forms can be seen as vectors in $\mathbb{R}^{|V|}$, $\mathbb{R}^{|E|}$ and $\mathbb{R}^{|T|}$. Thus operators like the exterior derivative, the hodge star operator and the codifferential are defined as matrices. To define the discrete exterior derivate we need to define the boundary operator first. The boundary operator ∂_1 is given by the matrix of dimension $|V| \times |E|$ with the entries

$$(\partial_1)_{ij} = \begin{cases} 1 \ , & \text{orientations of } v_i \text{ and } e_j \text{ agree} \ , \\ -1 \ , & \text{orientations of } v_i \text{ and } e_j \text{ disagree} \ , \end{cases}$$

if v_i is a vertex of the edge e_j and zero otherwise. The boundary operator ∂_2 is now defined analogously by

$$(\partial_1)_{ij} = \begin{cases} 1 \ , & \text{orientations of } e_i \text{ and } t_j \text{ agree} \ , \\ -1 \ , & \text{orientations of } e_i \text{ and } t_j \text{ disagree} \ , \end{cases}$$

if the e_j is an edge of the triangle t_j and zero otherwise. The discrete exterior derivate is now defined to be the transpose of the boundary operator, i. e.

$$d_0 = (\partial_1)^T \quad , \quad d_1 = (\partial_2)^T \quad .$$

Thus, as for smooth r-forms we have that d_0 maps 0-forms to 1-forms, and d_1 maps 1-forms to 2-forms.

While the hodge star operator $*_r$ in the continuous case maps r-forms to $(2-r)$-forms, the discrete hodge star operator maps a discrete r-form to a so-called dual $(2-r)$-form which is defined on the dual mesh. We assume for the moment that every triangle $t \in T$ contains its circumcenter. Then the (circumcentric) dual mesh is a cell decomposition of K where the cells are constructed as follows: The dual 0-cell $\star t$ of a triangle $t \in T$ is the circumcenter of t. The dual 1-cell $\star e$ of an edge $e \in E$ consists of the two line segments connecting the circumcenters of the triangles adjacent to e and the midpoint of e. The dual 2-cell $\star v$ of a vertex $v \in V$ is the area around v which is bounded by the dual 1-cells of the edges adjacent to v. Note that the dual mesh coincides with the Voronoi tesselation of K corresponding to the vertex set V, see [2] for details.

A dual r-form is now a map which assigns each dual r-cell a real number. Thus dual 0-forms, 1-forms and 2-forms can be represented as vectors in $\mathbb{R}^{|T|}$, $\mathbb{R}^{|E|}$ and $\mathbb{R}^{|V|}$. The exterior derivative on dual 0-forms and dual 1-forms is defined by the matrices

$$d_0^{Dual} = d_1^T = \partial_2 \quad , \quad d_1^{Dual} = -d_0^T = -\partial_1 \quad .$$

The discrete Hodge star operator $*_r$ which maps r-forms to dual $2-r$ forms is given by square matrices

$$*_0 \in \mathbb{R}^{|V|\times|V|} \quad , \quad *_1 \in \mathbb{R}^{|E|\times|E|} \quad , \quad *_2 \in \mathbb{R}^{|T|\times|T|} \quad .$$

Unfortunately there is no unique way to define the entries of these matrices. A possible choice for $*_0$, $*_1$ and $*_2$ are diagonal matrices with entries given by

$$(*_0)_{ii} = \frac{|\star v_i|}{|v_i|} \quad , \quad (*_1)_{ii} = \frac{|\star e_i|}{|e_i|} \quad , \quad (*_2)_{ii} = \frac{|\star t_i|}{|t_i|} \quad ,$$

where $|v| = 1$, $|e|$ is the length of e, $|t|$ is the area of t and analogously for dual cells. Since this is the common definition in DEC, see [7] and [5] for example, we also denote this Hodge star by $*_r^{DEC}$.

Another possible definition, suggested in [6], is to define $(*_0)_{ij}$ as the the L^2-inner product of the Whitney 0-forms ϕ_{v_i} and ϕ_{v_j}, and analogously for $*_1$ and $*_2$ using Whitney 1-forms and 2-forms corresponding to edges and triangles, respectively. For more details and an explicit computation of the entries of $*_r^{Whit}$ we refer to [11]. We denote this Hodge star operator also by $*_r^{Whit}$ in allusion to the use of Whitney forms. The advantages and disadvantages of $*^{DEC}$ and $*^{Whit}$ in view of spectral analysis of the Hodge Laplacian will be discussed in Subsection 5.2.

To map dual $(2-r)$-forms to discrete r-forms we need an inverse Hodge star operator $*_{2-r}^{Dual}$. An obvious choice would be $*^{-1}$ but in this case the property $*_r *_{2-r} \alpha = (-1)^{r(2-r)}\alpha$ which we have for a smooth r-form α would not hold. Instead $*_{2-r}^{Dual}$ is defined by

$$*_{2-r}^{Dual} = (-1)^{r(2-r)}(*_r)^{-1} \quad .$$

Now, similarly as for smooth r-forms, we define the discrete codifferential which maps discrete r-forms to discrete $(r-1)$-forms for $r = 1,2$ by

$$\delta_1 = -*_2^{Dual}\, d_1^{Dual} *_1 \quad ,$$
$$\delta_2 = -*_1^{Dual}\, d_0^{Dual} *_2 \quad .$$

This enables us to define the discrete Hodge Laplacian Δ_r just the same way as in the smooth case by

$$\Delta_0 = \delta_1 d_0 \quad ,$$
$$\Delta_1 = \delta_2 d_1 + d_0 \delta_1 \quad ,$$
$$\Delta_2 = d_1 \delta_2 \quad .$$

Thus Δ_r can be assembled from the boundary operator and the discrete Hodge star operator by

$$\Delta_0 = *_0^{-1} \partial_1 *_1 \partial_1^T \quad ,$$
$$\Delta_1 = *_1^{-1} \partial_2 *_2 \partial_2^T + \partial_1^T *_0^{-1} \partial_1 *_1 \quad ,$$
$$\Delta_2 = \partial_2^T *_1^{-1} \partial_2 *_2 \quad .$$

5.2 Numerical Computation of the Point Signatures

To compute $k^1(t,p,p)$ using the formula (1) we need to compute the eigenvalues and eigenforms of Δ_1 in a first step. We will see that we need certain combinations of the Hodge star operators $*_r^{DEC}$ and $*_r^{Whit}$ to accomplish this. In a second step we need to compute the products of two eigenforms $\alpha_i(p)(\cdot)\,\alpha_i(p)(\cdot)$. Since DEC does not provide such a product, we use Whitney forms to interpolate smooth r-forms from discrete r-forms. This results in matrix representations of $\alpha_i(p)(\cdot)\,\alpha_i(p)(\cdot)$ which can be summed easily.

To compute the eigenvalues of Δ_1 we need to solve the eigenvalue problem

$$\Delta_1 \alpha = \left(*_1^{-1} \partial_2 *_2 \partial_2^T + \partial_1^T *_0^{-1} \partial_1 *_1\right) \alpha = \lambda \alpha \quad ,$$

or alternatively the generalized eigenvalue problem

$$\left(\partial_2 *_2 \partial_2^T + *_1 \partial_1^T *_0^{-1} \partial_1 *_1\right) \alpha = \lambda *_1 \alpha \quad .$$

The advantage of the generalized eigenvalue problem is that one does not need the inverse of $*_1$, but only needs the inverse of $*_0$. However, to solve such a generalized eigenvalue problem with usual numerical methods, e. g. by using the command `eigs` in Matlab, the matrix on the right hand side, i. e. $*_1$, must be symmetric positive definite. Moreover we need to compute the inverse of $*_0$. So, which of the matrices $*_r^{DEC}$, $*_r^{Whit}$, $r = 0,\dots,2$, are invertible, which are also symmetric positive definite?

Since $*_1^{DEC}$ is a diagonal matrix with diagonal entries given by

$$(*_1)_{ii} = \frac{|\star e_i|}{|e_i|} \quad ,$$

it is invertible if and only if $|\star e_i|/|e_i| \neq 0$ for $i = 1,\dots,|E|$; if $|\star e_i|/|e_i| > 0$ for $i = 1,\dots,|E|$ it is also positive definite. The length $|e|$ of an edge is obviously always positive. For the length $|\star e|$ of the dual 1-cell of an edge e this is possibly not the case. Of course, if we assume that the circumcenter of each $t \in T$ is contained in t, as in the previous section, the length of $\star e$ is the sum of the lengths of the two line segments connecting the circumcenters of the two triangles adjacent to e with the midpoint of e and thus positive. But this is not a viable assumption in applications. One can solve this problem in the following way: Let t be a triangle adjacent to e. If t and the circumcenter of t lie on different sides of the line containing e, then the according line segment counts negative. Thus the length $|\star e|$ of a dual 1-cell $\star e$ can be negative; this is the case if and only if this edge violates the local Delaunay property and consequently the entries of $*^{DEC}$ are only nonnegative if K is an (intrinsic) Delaunay triangulation, see [2] for details on Delaunay triangulations of triangle meshes. Since it is a very strong condition to assume that K is a Delaunay triangulation and moreover not sufficient for positive definiteness of $*^{DEC}$, only positive semidefiniteness, we cannot assume that $*_1^{DEC}$ is invertible or even positive definite.

Similarly $*_0^{DEC}$ is positive definite if $|\star v_i| > 0$ for $i = 1,\dots,|V|$. The computation of the area $|\star v|$ of a dual 2-cell $\star v$ is shown in Figure 1, for details we refer the reader to [11]. Note that $|\star v|$ can be positive even if K is not a Delaunay triangulation; $|\star v|$ is only negative for rather degenerate meshes. Thus we can assume that $*_0^{DEC}$ is positive definite and thus invertible. Finally, $*_2^{DEC}$ is obviously positive definite.

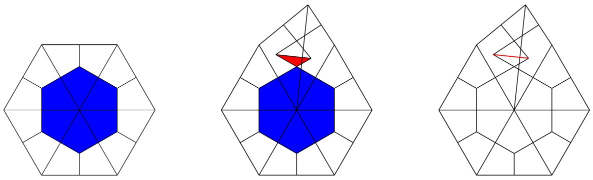

Figure 1: Primal and dual meshes. The left mesh is Delaunay, whereas the other meshes are not Delaunay. The middle mesh shows a dual 0-cell whose area is given by the blue area minus the red area. The red line in the right mesh shows a dual 1-cell with negative length.

The positive definiteness of $*_r^{Whit}$ follows from the fact that $\alpha^T *_r^{Whit} \beta$ is the L^2-inner product of the Whitney interpolants $\mathscr{I}\alpha$ and $\mathscr{I}\beta$ of two discrete r-forms α, β, thus

$$\alpha^T *_r^{Whit} \alpha > 0$$

for any r-form $\alpha \neq 0$. Consequently $*_r^{Whit}$ is also invertible, but unfortunately we cannot use the inverse of $*_r^{Whit}$. The reason for this is that $*_k^{Whit}$ is not diagonal (unless $r = 2$) and thus the inverse is in general not a sparse matrix which is a mandatory condition for large meshes.

As a consequence, to solve the generalized eigenvalue problem for Δ_1, we have to use $(*_0^{DEC})^{-1}$ and $*_1^{Whit}$ on the right hand side. For $*_1$ on the left hand side we can choose either $*_1^{DEC}$ or $*_1^{Whit}$, both work properly as the numerical tests in [11] show. For $*_2$ there is nothing to choose, since $*_2^{DEC} = *_2^{Whit}$.

We now discuss the computation of the matrix representation of $k^1(t,p,p)$ from the eigenvalues and eigenforms of Δ_1 using the formula

$$k^1(t,p,p)(\cdot,\cdot) = \sum_i e^{-\lambda_i t} \alpha_i(p)(\cdot)\,\alpha_i(p)(\cdot) \quad .$$

One difficulty is to compute the product of the eigenforms α_i of Δ_1. The α_i are only available as discrete 1-forms, but unfortunately DEC does not provide such a product. To overcome this problem we interpolate the discrete 1-forms using Whitney forms. The resulting smooth forms can be multiplied easily. Though, as noted in the previous subsection, the Whitney forms are only continuous within the triangles, thus it is not possible to evaluate the resulting tensors on the vertices. Instead, we evaluate the tensors on the barycenters of the triangles.

We proceed with a detailed description of the computation of the matrix representation of $k^1(t,p,p)$. Let $t = [v_i v_j v_k]$ be a triangle, while the orientation of the edges is given by $e_i = [v_j v_k]$, $e_j = [v_k v_i]$ and $e_k = [v_i v_j]$. Using the orthonormal basis

$$e_1 = \frac{v_j - v_i}{\|v_j - v_i\|} \quad , \quad e_2 = \frac{(v_k - v_i) - \langle v_k - v_i \,, e_1\rangle\, e_1}{\|(v_k - v_i) - \langle v_k - v_i \,, e_1\rangle\, e_1\|}$$

and choosing v_i as origin we obtain

$$v_i = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad , \quad v_j = \begin{pmatrix} x_j \\ 0 \end{pmatrix} \quad , \quad v_k = \begin{pmatrix} x_k \\ y_k \end{pmatrix} \quad ,$$

where $x_j = \langle v_j \,, e_1\rangle$, $x_k = \langle v_k \,, e_1\rangle$, $y_k = \langle v_k \,, e_2\rangle$. Now easy calculations show for the hat functions $\phi_{v_i}, \phi_{v_j}, \phi_{v_k}$ that

$$(d\phi_i)^\sharp = \begin{pmatrix} -\frac{1}{x_j} \\ \frac{x_k}{x_j y_k} - \frac{1}{y_k} \end{pmatrix} \quad ,$$

$$(d\phi_j)^\sharp = \begin{pmatrix} \frac{1}{x_j} \\ -\frac{x_k}{x_j y_k} \end{pmatrix} \quad ,$$

$$(d\phi_k)^\sharp = \begin{pmatrix} 0 \\ \frac{1}{y_k} \end{pmatrix} \quad ,$$

where we used the sharp operator to identify 1-forms with vectorfields. Let now α be an eigenform of Δ_1, then the Whitney interpolant $\mathscr{I}\beta$ at the barycenter p of T is given by

$$(\mathscr{I}\alpha)(p) = \frac{1}{3}(\alpha(e_k)(d\phi_{v_j} - d\phi_{v_i}) + \alpha(e_i)(d\phi_{v_k} - d\phi_{v_j}) + \alpha(e_{v_j})(d\phi_{v_i} - d\phi_{v_k})) \quad .$$

The matrix representaion of $\mathscr{I}\alpha(p)(\cdot)\,\mathscr{I}\alpha(p)(\cdot)$ is now given by

$$\Big((\mathscr{I}\alpha)^\sharp(p)\Big)\Big((\mathscr{I}\alpha)^\sharp(p)\Big)^T \quad ,$$

and the matrix representation of $k^1(t,p,p)$ by

$$\sum_i e^{-\lambda_i t}\Big((\mathscr{I}\alpha_i)^\sharp(p)\Big)\Big((\mathscr{I}\alpha_i)^\sharp(p)\Big)^T \quad . \qquad (2)$$

6 RESULTS

In this section we visualize our point signatures with colormaps; small values are represented by blue and high values by red. The surfaces we investigate are the trim-star model, the armadillo model and the Caesar model, provided by the AIM@SHAPE Shape Repository, a surface representing a mandible produced by M. Zinser, Universitätsklinik Köln, and a square. Plots of the point signatures for these surfaces are given for different time values and compared with the Heat Kernel Signature.

We approximate the sum in equation 2 by the first 100 summands, i. e. we have to compute the 100 smallest eigenvalues and the corresponding eigenvectors of Δ_1. The number of summands needed depends on the surface. In our examples more summands show no significant improvement. The computation of the eigenvalues and eigenvectors of Δ_1, for which we use Matlab, needs most time, everything else can be done interactively. Timings are shown in Table 1; for comparison we also give timings for the computation of 100

Model	Vertices	Δ_1	Δ_0
Mandible	11495	39.9	8.9
Trim-star	5192	17.2	7.6
Square	4096	13.4	3.4
Caesar	4717	15.0	3.0

Table 1: Timings in seconds for the computation of 100 eigenvalues and eigenvectors of Δ_1 and Δ_0.

eigenvalues and eigenvectors of Δ_0, which are needed to compute the HKS.

To avoid readjusting the colormap for different values of t we plot the function

$$\frac{\operatorname{tr}\left(k^1(t,p,p)\right)}{\int_M \operatorname{tr}\left(k^1(t,p,p)\right)dp} \ ,$$

rather than $\operatorname{tr}\left(k^1(t,p,p)\right)$, and analogously for other invariants. Such a normalization is also used in [10] to ensure that different values of t contribute approximately equally when comparing two signatures.

In the case of a closed surface the smaller and the larger eigenvalue of $k^1(t,p,p)$ have very similar values for all $p \in M$ and all $t > 0$. The behavior of $\operatorname{tr}\left(k^1(t,p,p)\right)$ and $\det\left(k^1(t,p,p)\right)$ corresponds to this observation. Thus, whichever invariant we use, we obtain nearly the same information from the resulting point signature. A comparison of $\operatorname{tr}\left(k^1(t,p,p)\right)$ and the Heat Kernel Signature is shown in Figures 2 and 3. Despite the fact that the Heat Kernel Signature has high values where $\operatorname{tr}\left(e^1(t,p,p)\right)$ has low values and vice versa, both point signatures show a similar behavior for small values of t. In contrast, for large values of t their behavior is very different.

We should note here that Δ_0 has a single zero eigenvalue and the corresponding eigenfunction is constant. Thus we have

$$\lim_{t\to\infty} k^0(t,p,p) = \lim_{t\to\infty} \sum_i e^{-\lambda_i t}\phi_i(p)\phi_i(p) = \phi_0^2(p) \ ,$$

i. e. the Heat Kernel Signature converges to a constant function which is different to zero. In contrast, Δ_1 has $2g$ eigenforms to the eigenvalue zero, where g is the genus of the surface. Now the limit

$$\lim_{t\to\infty} k^1(t,p,q)(\cdot,\cdot) = \lim_{t\to\infty} \sum_i e^{-\lambda_i t}\alpha_i(p)(\cdot)\,\alpha_i(p)(\cdot)$$

is zero for surfaces with $g = 0$ and nonzero for surfaces with $g > 0$.

Thus, for the mandible model in Figure 2 $\operatorname{tr}\left(k^1(t,p,p)\right)$ converges to zero, while it does not converge to zero for the trim-star in Figure 3. However, as a consequence of our normalization, the limit zero is not visible in Figure 2, we rather see how $\operatorname{tr}\left(k^1(t,p,p)\right)$ approaches zero.

To demonstrate the isometry invariance of $k^1(t,p,p)$ Figure 4 shows $\operatorname{tr}\left(k^1(t,p,p)\right)$ for different poses of the armadillo modell.

In contrast to closed surfaces the smaller and the larger eigenvalue of $k^1(t,p,p)$ behave differently for surfaces with boundary. Consequently we also have a different behavior of $\operatorname{tr}\left(k^1(t,p,p)\right)$ and $\det\left(k^1(t,p,p)\right)$, see Figure 5 for a square and Figure 6 for a model of the head of Julius Caesar. While $\operatorname{tr}\left(k^1(t,p,p)\right)$ and the Heat Kernel Signature show a similar behavior for small t in the case of a closed surface, for surfaces with boundary this is only true away from the boundary, see again Figures 5 and 6. The Heat Kernel Signature seems to be much more influenced by the boundary as $\operatorname{tr}\left(k^1(t,p,p)\right)$. We should note here that we used for the computation of the Heat Kernel Signature eigenfunctions satisfying Neumann boundary conditions, i. e. for any eigenfunction ϕ we have

$$\frac{\partial\phi}{\partial n}(p) = 0 \ , \quad p \in \partial M \ ,$$

where ∂M denotes the boundary of M and n denotes the normal to the boundary. If we would use Dirichlet boundary conditions instead, i. e.

$$\phi(p) = 0 \ , \quad p \in \partial M \ ,$$

the influence of the boundary to the Heat Kernel Signature would be even bigger.

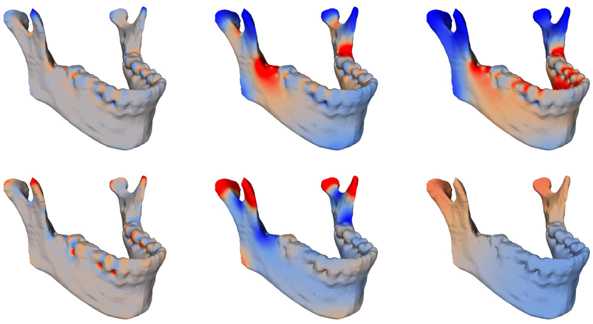

Figure 2: $\operatorname{tr}(k^1(t,p,p))$ (top) and Heat Kernel Signature (bottom) for increasing values of t.

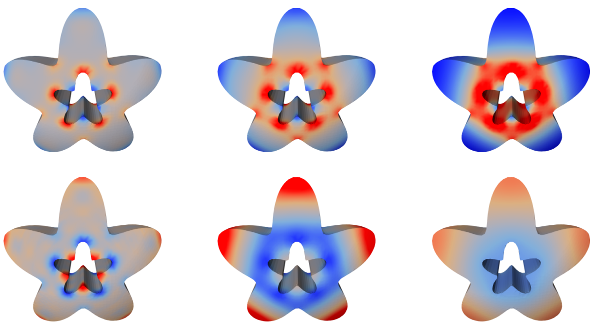

Figure 3: $\operatorname{tr}(k^1(t,p,p))$ (top) and Heat Kernel Signature (bottom) for increasing values of t.

7 CONCLUSION

In this work we derived new point signatures from the heat kernel for 1-forms. We imitated the way in which

Figure 4: $\mathrm{tr}(k^1(t,p,p))$ of the armadillo modell in different poses.

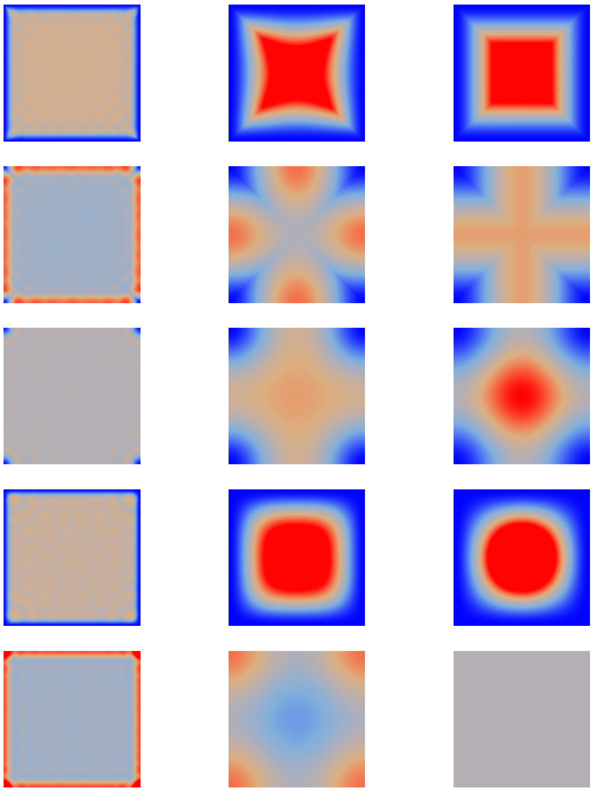

Figure 5: from top to bottom: smaller eigenvalue of $k^1(t,p,p)$, larger eigenvalue of $k^1(t,p,p)$, $\mathrm{tr}(k^1(t,p,p))$, $\det(k^1(t,p,p))$ and Heat Kernel signature for increasing values of t.

the Heat Kernel Signature is derived from the Heat Kernel of 0-forms. Since this yields a time-dependent tensor field of second order, we obtain several point signatures by considering tensor invariants like the eigenvalues, the trace and the determinant. In the case of surfaces without boundary both eigenvalues have very similar values; the trace and the determinant behave accordingly. For small time values the behavior of both eigenvalues is quite similar to the Heat Kernel Signature, but it differs for large time values. In contrast to this, the behavior of the eigenvalues is very different for surfaces with boundary, even for small time values. Thus all considered tensor invariants differ significantly from the Heat Kernel Signature. This property might bring improvements for the analysis of surfaces with boundary, compared to the Heat Kernel Signature with

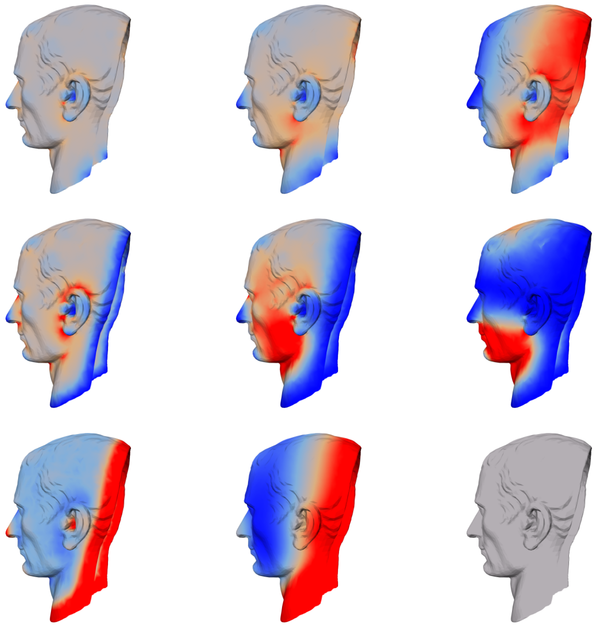

Figure 6: from top to bottom: $\mathrm{tr}(k^1(t,p,p))$, $\det(k^1(t,p,p))$ and Heat Kernel Signature for increasing values of t.

Dirichlet or Neumann boundary conditions; a further examination is left for future work.

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