

Heat Kernel Signature

Discrete Differential Geometry - Project Writeup

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1. Introduction

In the mathematical study of heat conduction and diffusion, the fundamental guiding equation is called the heat equation, which is a parabolic partial differential equation that describes the distribution of heat or temperature in space over time [1]. The heat equation is also called the "diffusion equation", which models a wide variety of phenomena beyond heat, e.g., general dissipation phenomena (known to some scientists as "Fick's law"). For a heat/temperature distribution function $u(x, y, z, t)$ in 3D space (x, y, z) and with time variable t , the heat equation is

$$\frac{\partial u}{\partial t} - \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) = 0, \quad (1)$$

which can be generalized in any coordinate system as

$$\frac{\partial u}{\partial t} - \alpha \Delta u = 0, \quad (2)$$

where Δ is the Laplace operator and α is a positive constant which can be set to 1 as a mathematical treatment.

Suppose we have a compact Riemannian manifold M , then heat diffusion process over M is governed by the heat equation:

$$\Delta_M u(x, t) = \frac{\partial u(x, t)}{\partial t}, \quad (3)$$

where Δ_M is the Laplace-Beltrami operator of M . Given the Riemannian metric g of M , Δ_M in local coordinates can be expressed as

$$\Delta_M = - \frac{1}{|\sqrt{\det g}|} \sum_{i,j=1}^n \frac{\partial}{\partial x_i} \left(g^{ij} \sqrt{|\det g|} \frac{\partial}{\partial x_j} \right) \quad (4)$$

As introduced in the class, writing Δ_M in terms of exterior calculus leads to a much more concise expression and easy computation:

$$\Delta_M = \star d \star d + d \star d \star \quad (5)$$

where the $\star$ is the hodge star that encapsulates curvature information of M . Note that if M has boundary, additional boundary condition is applied as $u(x, t) = 0 \forall x \in \partial M$.

Let u_0 be the initial heat distribution on M ($u_0(x) = u(x, 0)$), then the solution of heat equation (3) has the form

$$u(x, t) = \int k_t(x, y) u_0(y) dy \quad (6)$$

where dy is the volume form at $y \in M$, and $k_t(x, y)$ is the so called heat kernel function. Intuitively, $k_t(x, y)$ can be thought as the total amount of heat transferred from y to x at time t if there is a unit amount of heat at y initially. In other words, $k_t(x, \cdot)$ is a solution to a Poisson problem with initial condition $k_0 = \delta_x$, where δ_x is Dirac delta function on point x and $\int_M \delta_x(z) dz = 1$.

Thus, if we multiply $h_t(x, y)$ with the initial heat distribution at y and integrate over the whole M , we will be able to get the heat distribution $u(x, t)$ at x at time t . Note that the heat kernel is not known to be in closed-form for most manifolds, but for simple cases like Euclidean space.

For a compact Riemannian manifold M , the heat kernel function has the eigendecomposition

$$k_t(x, y) = \sum_{i=0}^{\infty} e^{-\lambda_i t} \phi_i(x) \phi_i(y) \quad (7)$$

where λ_i and ϕ_i are the i^{th} eigenvalue and eigenfunction of Δ_M respectively, $\Delta \phi = \lambda \phi$.

The heat kernel function has a lot of nice properties as described in detail in [2]. The essential properties that we are interested in is its intrinsic property, informative property and multi-scale property. The intrinsic property means the heat kernel is invariant under isometric transformation, which is revealed in (4) that the Laplacian can be expressed in local coordinates as a function of metric. Thus if a Riemannian manifold is undergoing isometric deformation, the heat kernel of corresponding points on pre and post-deformation manifolds will be the same. The informative property implies that the heat kernel contains all the information about the intrinsic geometry of a Riemannian manifold M , and thus is able to fully characterize the shape of M up to isometry. The reason is a consequence of work in [3], which shows that

$$\lim_{t \rightarrow 0} t \log k_t(x, y) = -\frac{1}{4} d^2(x, y), \quad (8)$$

where $d(x, y)$ is the geodesic distance between points x and y . If the geodesic distance between all pairs of corresponding points on pre and post-deformation manifolds are identical, the two manifolds have the same intrinsic shape. Last, heat kernel is able to characterize local shape depending on the choice of the scale parameter t . As shown in Figure 1, $k_t(x, \cdot)$ and $k_t^D(x, \cdot)$ are the heat kernels of point x (black point in middle) computed from the entire horse shape and from the circled local region with BC $u(x, t) = 0 \forall x \in \partial M$ respectively. As t increases, the L_2 norm of heat kernels' difference on circled region increases correspondingly. However, for $t < 0.2$, the two heat kernel are nearly identical which implies that the under small t , heat kernel is able to characterize the local shape.

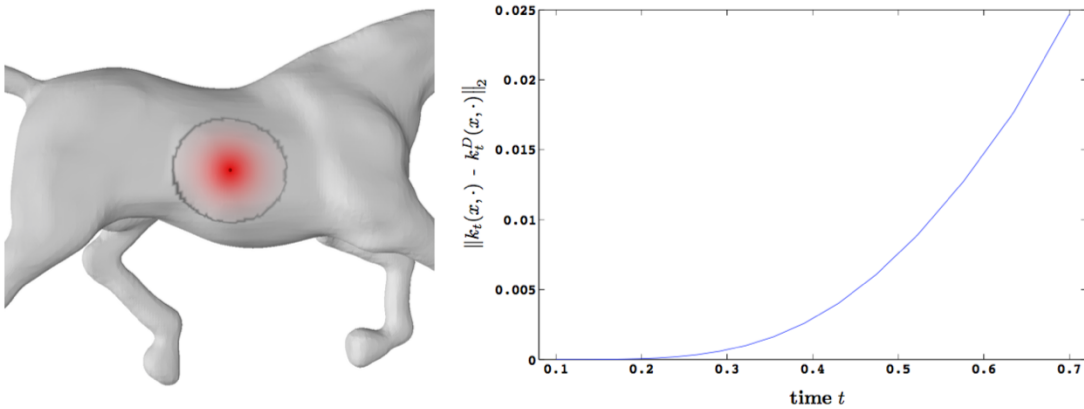


Figure 1^[2]

2. Heat kernel signature

2.1 Definition

With two essential properties mentioned above, the heat kernel becomes a very lucrative candidate for a point signature. However, one main defect of using the family of functions $\{k_t(x, \cdot)\}_{t>0}$ to characterize point x is its high computational complexity. For each point on M , its heat kernel $\{k_t(x, \cdot)\}_{t>0}$ is defined on the product of temporal and spatial domain $\mathbb{R}^+ \times M$. Thus, the full heat kernel of all points on M require $\mathbb{R}^+ \times M \times M$ space, not to mention the cost of matching the neighbors while comparing the heat kernels of two points.

The full heat kernel actually contains a lot of redundant information, and the change of heat kernel function in spatial domain is manifested by its change in time. An approach to overcome above difficulty is to reduce the dimensionality to temporal domain only and restrict heat kernel to its subset. Then, as proposed in [2], we have the heat kernel signature (HKS) which satisfies the requirements above.

Given a point x on the manifold M , its Heat Kernel Signature, $HKS(x)$, is defined to be a function over the temporal domain:

$$HKS(x): \mathbb{R}^+ \rightarrow \mathbb{R}, HKS(x, t) = k_t(x, x) \quad (9)$$

As proved in detail in [2], regardless of restricting the signature to the temporal domain and dropping the entire spatial domain, under mild assumptions, $\{k_t(x, x)\}_{t>0}$ keeps all of the information of $\{k_t(x, \cdot)\}_{t>0}$ (see Appendix).

2.2 Relation to curvature

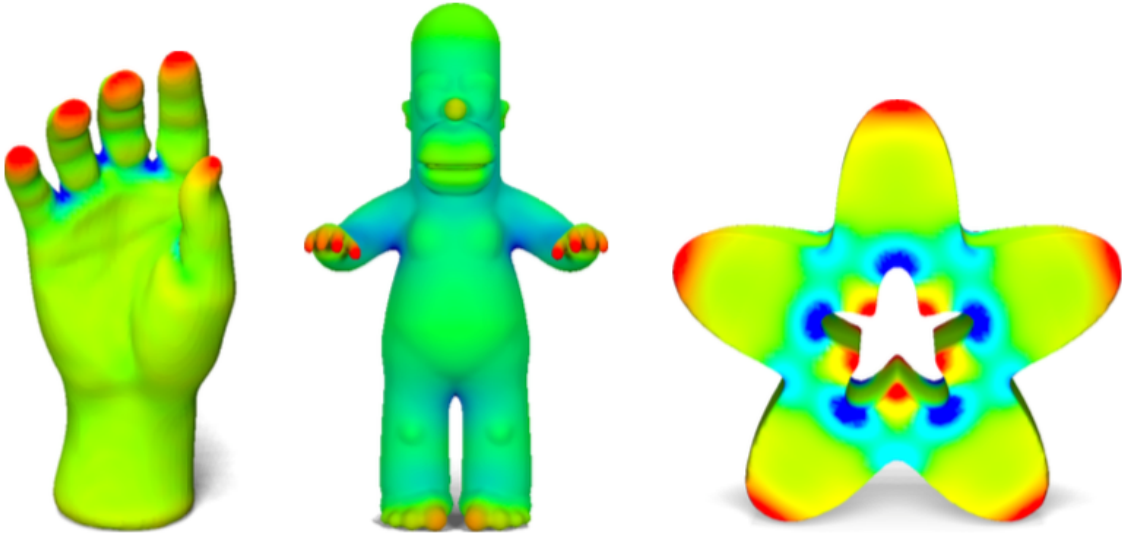


Figure 2^[2]

The $HKS(x, t)$ defined above has very close relation to the local curvature of region around point x . Given a small fixed t , Figure 2^[2] shows the values of heat kernel function $k_t(x, x)$ on three models respectively. The function values are mapped from blue (lowest) to red (highest)

on the three model respectively. As shown in the figure, the regions with large Gaussian curvatures generally have high heat kernel function value while the regions with small (negative) curvatures have low function values. An intuitive explanation for the consistency between Gaussian curvature and heat kernel function value is the rate of the heat diffusion. As discussed in class (Figure 3), the scalar curvature S (twice the Gaussian curvature) on a Riemannian manifold measures the deviation of the volume of a geodesic ball B_g from the volume of a Euclidean Ball $B_{\mathbb{R}^n}$ of equal radius, thus region with small scalar curvature has larger B_g . As a consequence, heat tends to diffuse faster in region with small curvature (large adjacent area) than in region with large curvature. Therefore, with small fixed t , points locally keep more heat in large curvature region and thus have higher heat kernel function value.

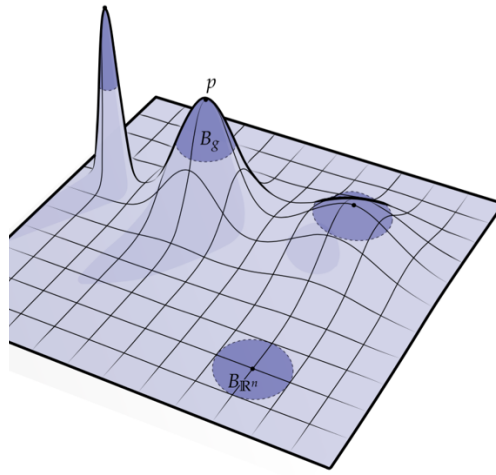


Figure 3^[5]

3. Discretization

The discretized version of heat kernel is computed via the discretized Laplace-Beltrami operator. In [2], to circumvent the limitations of requiring well-shaped mesh and possibly repeated eigenvalues, authors used the mesh Laplace operator[7] as an estimation of the Laplace-Beltrami operator. For now, without consideration for practice, let's just use the cotangent-weight Laplace operator in our discussion.

Given a scalar function ϕ defined on discretized surface M . The cotangent-weight Laplacian is defined as

$$(\Delta\phi)_i = \frac{1}{2A_i} \sum_j (\cot \alpha_j + \cot \beta_j) (\phi_i - \phi_j) \quad (10)$$

where α_j and β_j are angles opposite to edge between vertex i and j as shown in figure below. A_i is one third the area of all triangles adjacent to vertex i which works as a normalization factor as proposed in [6]. The Laplacian value on vertex i is obtained by summing cotangent value of α_j and β_j over all the immediate neighbors of vertex i as shown in Figure 4^[5].

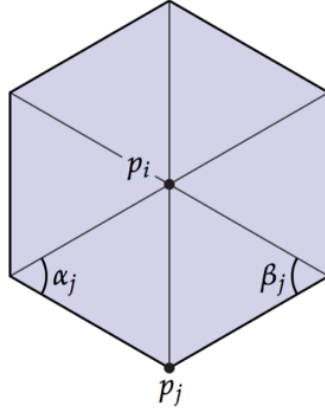


Figure 4^[5]

Based on the above formulation, the discretized Laplace-Beltrami operator is in the form of a sparse matrix $L = A^{-1}W$, where A is a diagonal matrix, whose element $A(i, i)$ represents the area associated with vertex i as the A_i in equation (10), and W is a symmetric semi-definite matrix constructed from the cotangent scheme.

Suppose u_t is a time dependent function defined on vertices, then $u_t(x)$ is the amount of heat on vertex x at time t . Equivalent to equation (3), the discretized version of heat equation is:

$$Lu_t = \frac{\partial u_t}{\partial t} \quad (11)$$

the solution to the equation above has the form $u_t = e^{-tL}u_0$ where u_0 is the initial heat distribution and e^{-tL} is a matrix exponential

$$e^{-tL} = \sum_{i=0}^{\infty} \frac{(-tL)^i}{i!} \quad (12)$$

The e^{-tL} can be interpreted as a heat operator and can be written in the form $e^{-tL} = K_t A = \sum_y k_t(x, y)u_0(y)A(y)$ which is the discretized version of equation (4). Each entry of matrix K_t represents the heat kernel of a pair of vertices. Entries of K_t has the form

$$K_t(x, y) = \sum_{i=1}^n e^{-\lambda_i t} \phi_i(x) \phi_i(y) \quad (13)$$

which is identical to equation (7) in the smooth settings. As $K_t(x, y)$ represents the heat kernel between vertex x and vertex y , the heat kernel signature of vertex x is simply the corresponding diagonal element of K_t .

$$HKS(x, t) = K_t(x, x) \quad (14)$$

Note that the computation for large heat kernel by matrix exponential can be extremely expensive. Thus in practice, it's more efficient to compute the diagonal entries directly from eigendecomposition, and just use the largest several eigenvalues and eigenvectors as e^{-tL} will gradually damp out "high frequencies".

4. Related applications in computation

4.1 Geodesics in heat

As shown in equation (8), the heat kernel has close relation to computing the pairwise geodesic distance a Riemannian manifold which can determine the Riemannian metric (intrinsic geometry) as we discussed in class. However, the equation is not widely used in the computation of geodesic distances. Limitation arises from the difficulty in reconstructing heat kernel precisely in numerical computation. Based on same core concept of heat kernel, works in [4] proposed the so called heat method for computing geodesic distance. Instead of calculating the distance through

$$d(x, y) = \lim_{t \rightarrow 0} \sqrt{-4t \log k_t(x, y)} \quad (15)$$

authors ask the gradient of temperature field ∇u_t to point in the right direction. The general pipeline can be described as

- Integrate the heat flow $\frac{\partial u}{\partial t} = \Delta u$ for some fixed time t .
- Evaluate the vector field $X = -\nabla u / |\nabla u|$ (normalizing to unit vectors and only ask for directions)
- Solve the Poisson equation $\Delta \phi = \nabla \cdot X$ (reconstruct the temperature field)

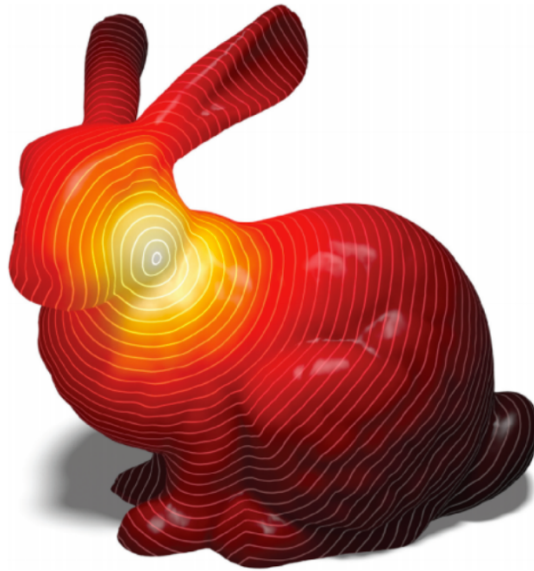


Figure 5^[4]

4.2 Heat Kernel Embedding of Graphs

The work in [8] investigate the use of heat kernels as a means of embedding the individual nodes of a graph on a manifold in a vector space. The heat kernel of the graph is found by exponentiating the Laplacian eigen-system over time. Spectral representation of the heat kernel can be used to compute both Euclidean and geodesic distances between nodes. Thus the resulting pattern of distances can be used to embed the nodes of the graph on a manifold using multidimensional scaling. And the distribution of embedded points are used to characterize the graph and perform graph clustering as shown in Figure 6.

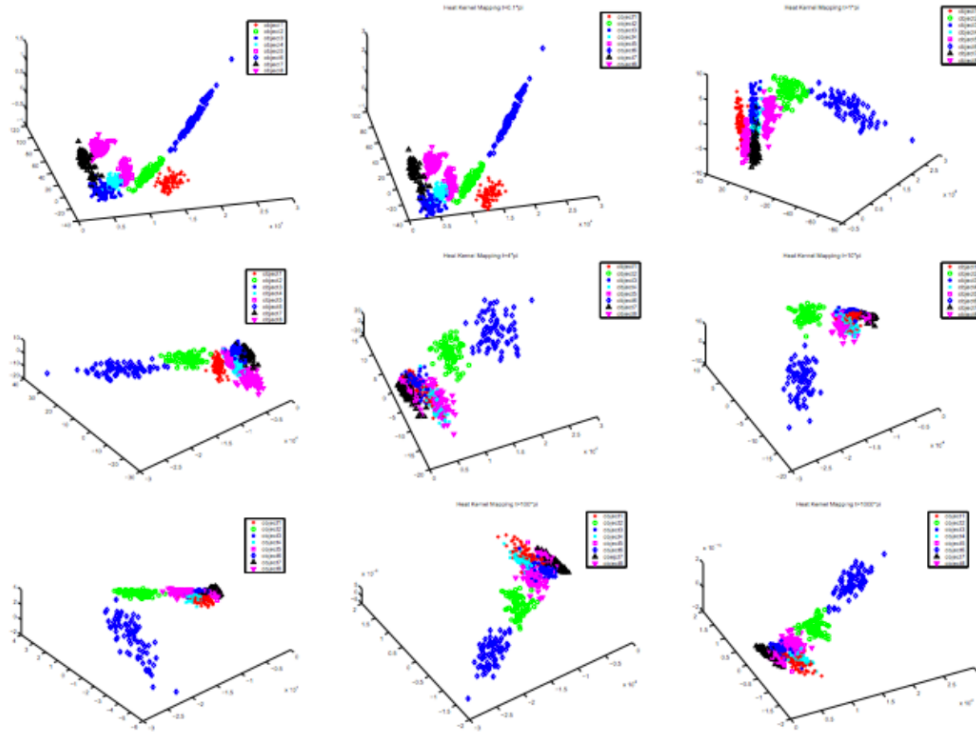


Figure 6^[8]

5. Project implementation

For the code implementation part of this course project, I would like to implement the computation of HKS by following the pipeline described in [2], and apply it on several geometric models. The details will involve computing the HKS of different feature vertices at different time step, comparing HKS of the same geometric models under isometric transformation, and comparing the HKS of different geometric models at the same scale. An example as Figure 7 would be a terrific showcase for multi scale property of HKS, where the chosen points are similar under local scale while the difference only appears at large time step.

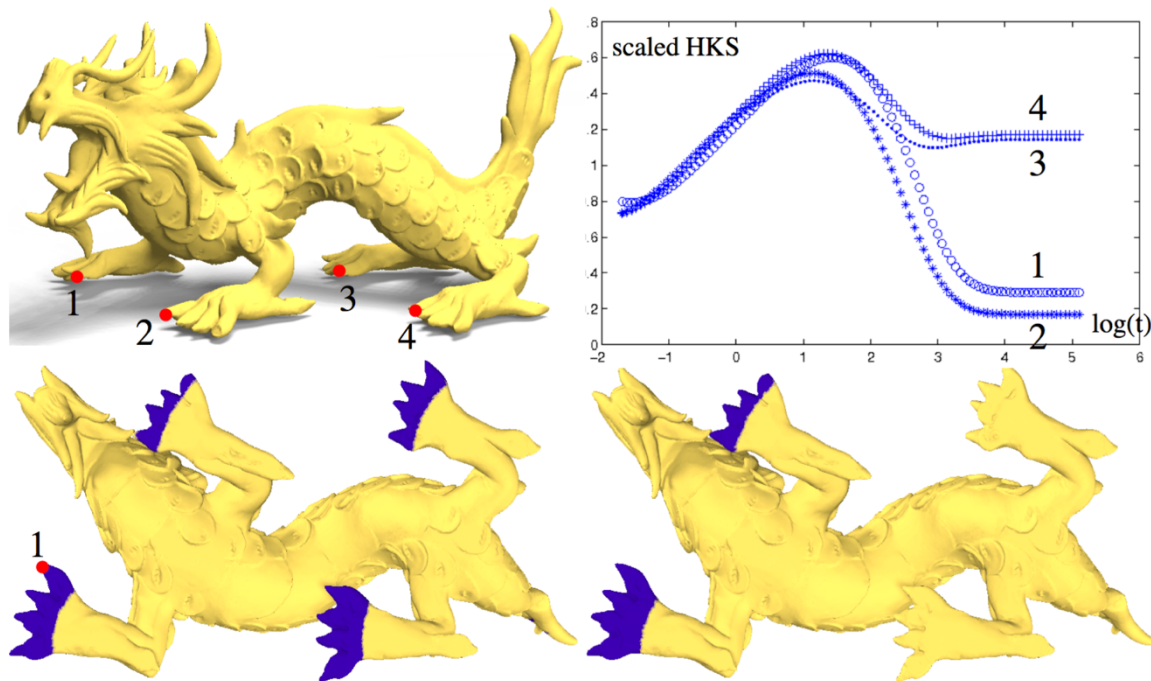


Figure 7^[2]

Besides the planned parts above, testing on special cases can also be part of the implementation if time allows. According to [2], if the Laplace-Beltrami operator is implemented as the naïve cotangent-weight Laplacian, there might be problems caused by ill-shape mesh as cotangent of large angle create negative weight on adjacent vertices while computing the Laplacian. So testing on mesh with large angle might help to develop more sense about these arguments, and thus give a more thorough understanding of the HKS.

6. Reference

- [1] https://en.wikipedia.org/wiki/Heat_equation
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[8] Xiao Bai, Richard C. Wilson, Edwin R. Hancock. Manifold Embedding of Graphs Using the Heat Kernel. Mathematics of Surfaces XI, Volume 3604 of the series Lecture Notes in Computer Science pp 34-49.

7. Appendix

For symmetrical shape with repeated eigenvalues, e.g. the sphere below, HKS can be the same for several different points on the surface, whereas the f is not an isometric transformation. Thus in such situation, heat kernel cannot be fully recovered from HKS and HKS does lose some information about the shape.

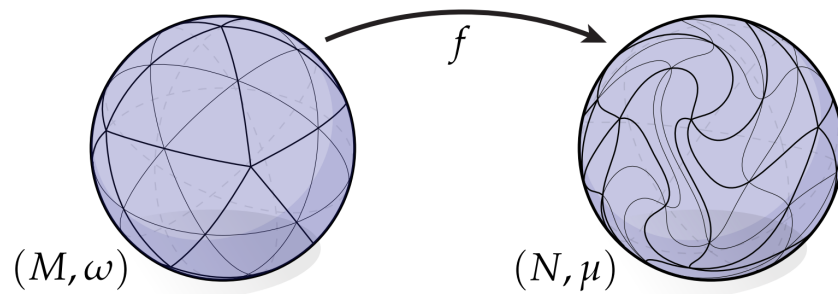


Figure 8^[5]