Foundations and Applications of the Laplace-Beltrami Operator

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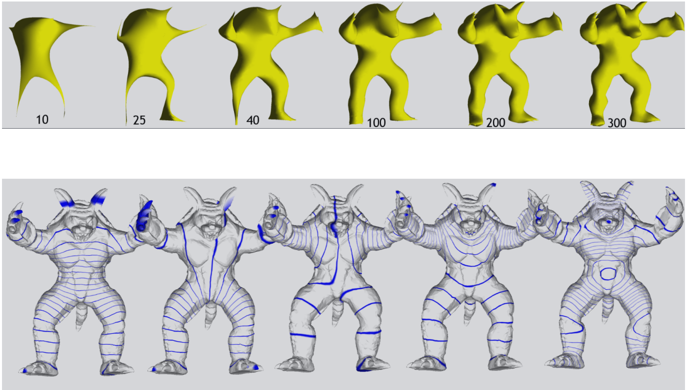
Motivation



Images from: Bruno Lévy, *Laplace-Beltrami eigenfunctions towards an algorithm that “understands" geometry*, 2006.

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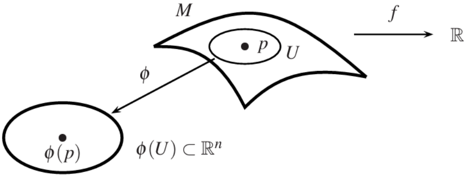
Manifolds

- Starting point: a locally Euclidean, Hausdorff and second-countable topological space $\mathbb{M}$
- Assume: $\mathbb{M}$ is *compact* and *embedded* in a Euclidean space
- Goal: do calculus and define differential operators on such an object



Differentiation

- Assume $\mathbb{M}$ is *smooth* or *differentiable*
- A function $f : \mathbb{M} \to \mathbb{R}$ is smooth at p when $f \circ \phi^{-1} : \phi(\mathcal{U}) \to \mathbb{R}$ is smooth at $\phi(p)$
- *Partial derivative* is $\frac{\partial f}{\partial x^i} : \phi(\mathcal{U}) \to \mathbb{R}$ such that for $p \in \mathbb{M}$ we have

$$\frac{\partial f}{\partial x^i}(p) = \frac{\partial(f \circ \phi^{-1})}{\partial r^i}(\phi(p)).$$

Geometry

- Want $\mathbb{M}$ to have geometry
- Example: take $\mathbb{M} = \mathbb{R}^n$ with standard coordinates and define

$$g_{\mathbf{p}}(\mathbf{a}, \mathbf{b}) = g_{\mathbf{p}}\left(\sum_{i=1}^{n} a_i \frac{\partial}{\partial x^i}, \sum_{j=1}^{n} b_j \frac{\partial}{\partial x^j}\right) = \sum_{k=1}^{n} a_k b_k = \mathbf{a}^\top \mathbf{b}$$

so that

$$\sum_{i,j} a_i b_j g_{ij} = \sum_{k=1}^{n} a_k b_k .$$

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- Across all basis vectors, we get a matrix $G \in \mathbb{R}^{n \times n}$.
- A *Riemannian metric* induces a norm.
- Need this to define an L^2 inner product, the gradient, and divergence.

Gradient and Divergence

Assume $\mathbb{M}$ smooth and Riemannian with metric G, and $f : \mathbb{M} \to \mathbb{R}$ smooth.

Definition

The gradient $\nabla : L^2(\mathbb{M}, G) \to \mathcal{T}\mathbb{M}$ in local coordinates as

$$\nabla_{\mathbb{M}} f = \sum_{i,j} g^{ij} \partial_i f \partial_j \text{ where } g^{ij} = [G^{-1}]_{ij}.$$

Let $\mathcal{F} : \mathbb{M} \to \mathcal{T}\mathbb{M}$ be a vector field such that $\mathcal{F} = \sum_i F_i \partial_i$.

Claim

If there exists an operator $div\mathcal{F}$ *satisfying* $\langle -div\mathcal{F}, f \rangle_{L^2(\mathbb{M},G)} = \langle \mathcal{F}, \nabla_{\mathbb{M}} f \rangle$ *then*

$$div\mathcal{F} = \frac{1}{\sqrt{\det G}} \partial_j \left(\sqrt{\det G} F^j \right).$$

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Definition

Assume $\mathbb{M}$ is a smooth, compact, m-dimensional Riemannian manifold embedded in $\mathbb{R}^l$, and f is a function from $\mathbb{M} \to \mathbb{R}$. It follows that the Laplace-Beltrami Operator is defined as

$$\Delta_{\mathbb{M}} f = -\text{div}(\nabla_{\mathbb{M}} f) = -\frac{1}{\sqrt{\det G}} \sum_j \partial_j \left(\sqrt{\det G} \sum_i g^{ij} \partial_i f \right).$$

In the case that $\mathbb{M} = \mathbb{R}^n$,

$$\Delta_{\mathbb{M}} f = -\sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2}.$$

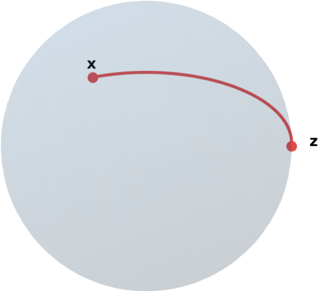
Self-Adjointness and Positive Semi-Definite

From the Divergence Theorem and the fact that $-\mathrm{div}$ is the adjoint of the gradient, we can find that the Laplace-Beltrami operator is both self-adjoint and positive semi-definite.

- eigenvalues are real and nonnegative
- eigenfunctions are orthogonal

Preservation of Locality

We're looking for functions $f : \mathbb{M} \to \mathbb{R}$ that map points close to each other.



Consider neighboring points $\mathbf{x},\mathbf{z} \in \mathbb{M}$ that map to $f(\mathbf{x})$, $f(\mathbf{z})$. Then

$$|f(\mathbf{x}) - f(\mathbf{z})| \leq d_{\mathbb{M}}(\mathbf{x},\mathbf{z}) \|\nabla f(\mathbf{x})\| + o(d_{\mathbb{M}}(\mathbf{x},\mathbf{z})).$$

Preservation of Locality

So minimizing Dirichlet energy gives us the best preservation of locality:

$$\underset{\|f\|_{L^2(\mathbb{M})}=1}{\arg\min} \int_{\mathbb{M}} \|\nabla f(\mathbf{x})\|^2$$

By Stokes' Theorem, $-\mathrm{div}$ and ∇ are adjoint, so for a vector field X we have $\int_{\mathbb{M}} \langle X, \nabla f \rangle = -\int_{\mathbb{M}} \mathrm{div}(X) f$. As a result, for $\Delta_{\mathbb{M}} f = -\mathrm{div}(\nabla f)$, we have:

$$\int_{\mathbb{M}} \|\nabla f\|^2 = \int_{\mathbb{M}} f \Delta_{\mathbb{M}} f.$$

Since $\Delta_{\mathbb{M}}$ is PSD and self-adjoint, a function f that minimizes $\int_{\mathbb{M}} \|\nabla f\|^2$ is an eigenfunction of $\Delta_{\mathbb{M}}$.

Preservation of Locality

Choose the first m eigenfunctions $f_1, \ldots, f_m$ corresponding to the lowest m eigenvalues (excluding $\lambda_0 = 0$)

Map $\mathbf{x} \mapsto (f_1(\mathbf{x}), \ldots, f_m(\mathbf{x})) \in \mathbb{R}^m$

Since f_i minimizes $\int_{\mathbb{M}} \|\nabla f\|^2$ subject to orthogonality, nearby points on $\mathbb{M}$ map to nearby points in $\mathbb{R}^m$.

In the discrete case, eigenvectors of the graph Laplacian L converge to eigenfunctions of $\Delta_{\mathbb{M}}$.

Nodal Sets and Domains

- Given an eigenfunction $v \in L^2(\mathbb{M}, G)$ of $\Delta_{\mathbb{M}}$, its *nodal set* is

$$\mathcal{N} = \{x \in \mathbb{M} : v(x) = 0\}.$$

- Nodal sets inform on the geometry of the underlying manifold:
  - Nodal sets partition the manifold into nodal domains
  - The n^{th} eigenfunction can have no more than n nodal domains.
  - The nodal sets are curves intersecting at constant angles.

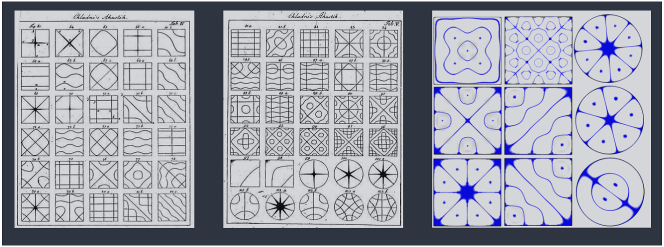
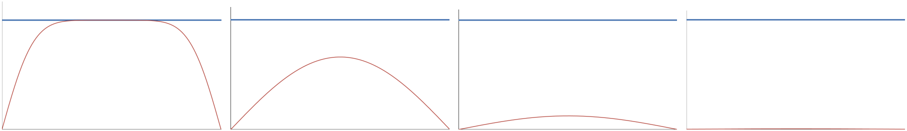


Figure: Nodal sets experimentally (Chladni, 1787) and by code (Lévy, 2006).

Connection to the Heat Equation



The heat equation problem is $\left(\frac{\partial}{\partial t} + \Delta_{\mathbb{M}}\right) u = 0$.

- $u(t,x)$: the heat distribution at time t
- $f : \mathbb{M} \to \mathbb{R}$: initial heat distribution.

Solution: $u(t,x) = \int_{\mathbb{M}} H_t(x,y) f(y)$

- H_t : the heat kernel or Green's function for the equation

$$\Delta_{\mathbb{M}}(f(x)) = -\Delta_{\mathbb{M}} u(x,0) = -\left(\frac{\partial}{\partial t}\left[\int_{\mathbb{M}} H_t(x,y) f(y)\right]\right)_{t=0}.$$

Connections to the Heat Equation

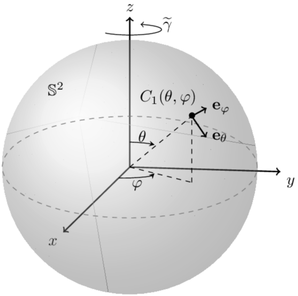
We use PDE approximations to simplify the LBO:
$H_t \approx (4\pi t)^{-m/2} e^{-\frac{\|x-y\|^2}{4t}}(\phi(x,y) + O(t))$, the Gaussian, where $\phi(x,y)$ is smooth with $\phi(x,x) = 1$.
When x and y are close to each other and t is small,

$$H_t \approx (4\pi t)^{-\frac{m}{2}} e^{-\frac{\|x-y\|^2}{4t}}.$$

This leads to the approximation

$$\Delta_{\mathbb{M}}(f(x)) \approx \frac{1}{t}\left(f(x) - (4\pi t)^{-\frac{m}{2}} \int_{\mathbb{M}} e^{-\frac{\|x-y\|^2}{4t}} f(y)dy\right).$$

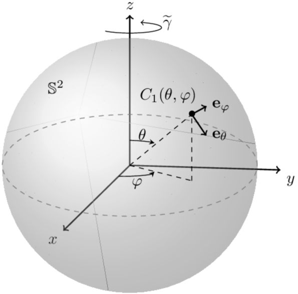
Example: S^2



On S^2, we get a special result for the Laplace-Beltrami Operator using the azimuthal angle and colatitude:

$$\Delta_{S^2} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left\{\sin\theta\frac{\partial}{\partial\theta}\right\} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}.$$

Example: S^2



Using this definition of the LBO, we find the solutions to the eigenfunction problem Δ_{S^2} to be

$$\lambda = \frac{1}{\|Y\|^2} \int_{S^2} \left(\left| \frac{dY}{d\theta} \right|^2 + \frac{1}{\sin^2 \theta} \left| \frac{dY}{d\varphi} \right|^2 \right) d\mu.$$

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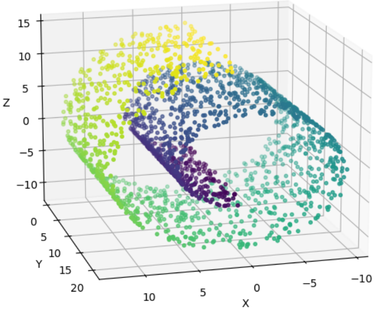
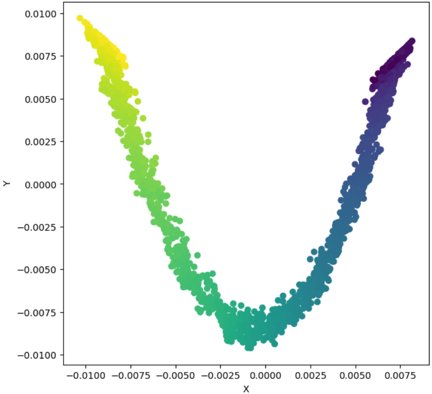
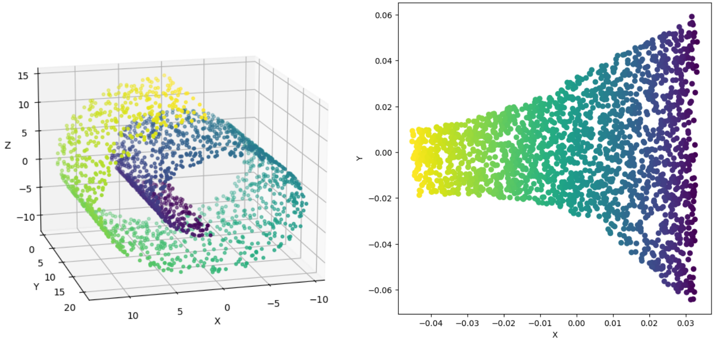
Laplacian Eigenmaps





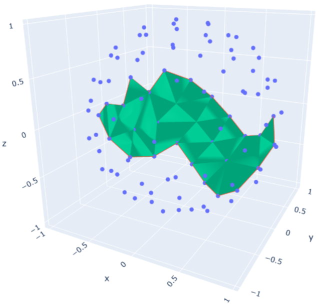
- Create a graph G, where nodes are data points and edges are weights established by the nodes' proximity.
- Solve $Lf = \lambda Df$, where $D_{ii} = \sum_j W_{ji}$ and $L = D - W$ (W the weight matrix).

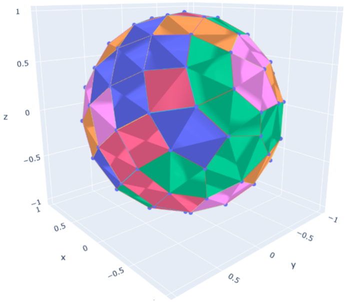
Local Linear Embedding



- Find each data point's n nearest neighbors and assembles a weight matrix W by choosing W_{ij} to minimize $\sum_{i=1}^{\ell} \|\mathbf{x}_i - \sum_{j=1}^{n} W_{ij}\mathbf{x}_{i_j}\|$ for all data points $\mathbf{x}_i \in \mathbb{R}^k$.
- With $E = (I - W)^\top (I - W)$, under conditions, the problem becomes the eigenfunction problem $Ef = \frac{1}{2}\Delta_{\mathbb{M}}^2 f$.

Persistent Homology





- Learn topological invariants of a manifold from a point cloud.
- Persistent homology can be used as a regularization for Laplace-Beltrami manifold learning (Zhang et. al., 2025).
- Variants can be used for dimensionality reduction (De Silva and Vejdemo-Johansson, 2009).

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We explored:

- Modeling heat diffusion on a manifold
- Helmholtz equation and geometry processing
- Laplacian autoencoders

Heat Equation on a Manifold

Consider a Möbius strip of width w approximated on a triangle mesh:

$$\mathbf{r}(u,v) = \begin{pmatrix} (1 + v\cos\frac{u}{2})\cos u \\ (1 + v\cos\frac{u}{2})\sin u \\ v\sin\frac{u}{2} \end{pmatrix}$$

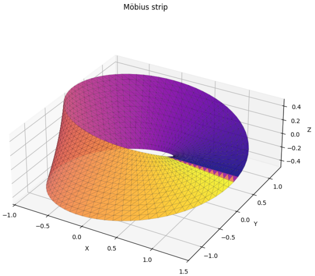
$u \in [0, 2\pi),\ v \in [-w, w].$

Heat equation with Neumann BCs:

$$u_t = \Delta_{\mathbb{M}} u, \quad \nabla_{\mathbb{M}} u \cdot \hat{\mathbf{n}}\big|_{\partial\mathbb{M}} = 0$$

Weak form:

$$\int_{\mathbb{M}} v\, u_t = -\int_{\mathbb{M}} \nabla_{\mathbb{M}} v \cdot \nabla_{\mathbb{M}} u$$



Heat Equation on a Manifold

Weak form with test function v and Neumann BCs:

$$\int_{\mathbb{M}} v\, u_t \; = - \int_{\mathbb{M}} \nabla_{\mathbb{M}} v \cdot \nabla_{\mathbb{M}} u$$

Apply Galerkin projection onto $V_h = \mathrm{span}\{\phi_1, \ldots, \phi_N\}$ $(\phi_j(\mathbf{p}_i) = \delta_{ij})$ with $u_h(\mathbf{x}, t) = \sum_j u_j(t)\, \phi_j(\mathbf{x})$, set $v = \phi_i$:

$$\sum_j \dot{u}_j(t) \underbrace{\int_{\mathbb{M}} \phi_i \phi_j}_{M_{ij}} = - \sum_j u_j(t) \underbrace{\int_{\mathbb{M}} \nabla_{\mathbb{M}} \phi_i \cdot \nabla_{\mathbb{M}} \phi_j}_{L_{ij}}$$

Matrix ODE:

$$M\dot{\mathbf{u}} = -L\mathbf{u}$$

Heat Equation on a Manifold

Solve $M\dot{\mathbf{u}} = -L\mathbf{u}$ with implicit Euler:

$$\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{\Delta t} \approx -M^{-1} L\mathbf{u}_{n+1}$$