A Manifold Learning Approach to Boundary Value Problems

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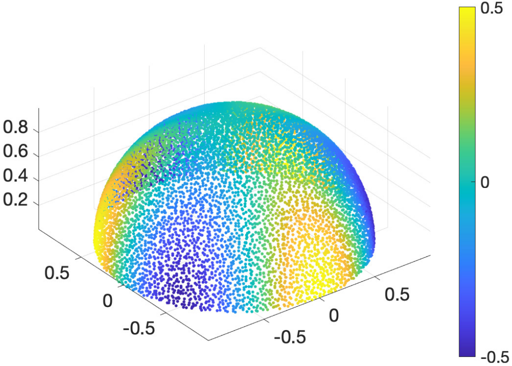
Slides developed with Ryan Vaughn

Boundary Value Problems on Embedded Manifolds

- Given points $\{x_i\}_{i=1}^N \subset \mathcal{M} \subset \mathbb{R}^d$
- Want to solve BVPs



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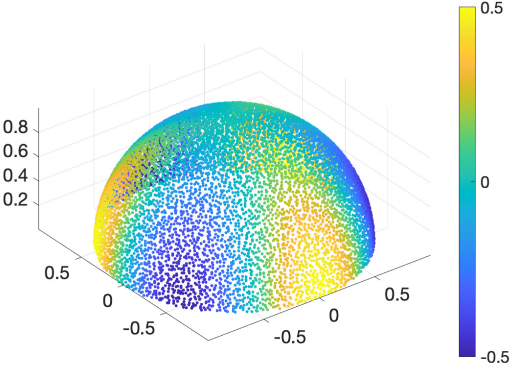
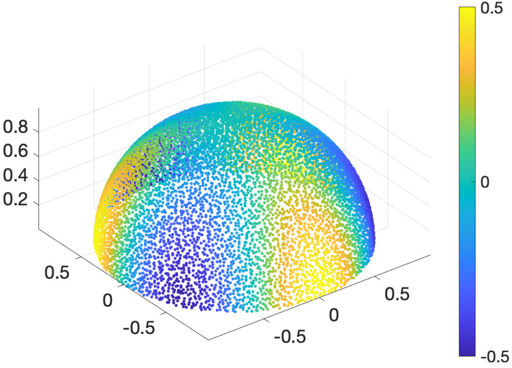
- Given points $\{x_i\}_{i=1}^N \subset \mathcal{M} \subset \mathbb{R}^d$
- Dimensions $m \equiv \dim(\mathcal{M})$ and d arbitrary



Boundary Value Problems on Embedded Manifolds

- Given points $\{x_i\}_{i=1}^{N} \subset \mathcal{M} \subset \mathbb{R}^d$
- Points come from a black-box:
  - hard to mesh
  - not uniformly distributed
  - location of boundary unknown



Mesh-free: Tools of the trade

Neumann Problem: Given $f \in H^1(\mathcal{M})^*$, $g \in L^2(\partial\mathcal{M})$,

$$\begin{cases} -\Delta u + u &= f \quad \text{in } \mathcal{M} \\ \nabla u \cdot \eta &= g \quad \text{on } \partial\mathcal{M} \end{cases}$$

η is the outward unit normal to $\partial\mathcal{M}$

Good news: Stokes' theorem still works on $\mathcal{M}$

$$-\int_{\mathcal{M}} v \Delta u \, dx = \int_{\mathcal{M}} \nabla v \cdot \nabla u \, dx - \int_{\partial\mathcal{M}} v \nabla u \cdot \eta \, ds$$

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Weak-sense formulation: $\forall v \in H^1(\Omega)$

$$\int_{\mathcal{M}} \nabla u \cdot \nabla v \, dx + \int_{\mathcal{M}} uv \, dx = \int_{\mathcal{M}} fv \, dx + \int_{\partial\mathcal{M}} gv \, ds$$

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Dirichlet Energy Volume Integral Boundary Integral

Key to Manifold Learning

- Given $f : \mathcal{M} \to \mathbb{R}$, want to estimate $\int_{\mathcal{M}} f(x)\,dx$
- Assume $\{x_i\}_{i=1}^N \subset \mathcal{M} \subset \mathbb{R}^d$ are sampled from distribution p

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(x_i) = \mathbb{E}_{X\sim p}[f(X)] = \int_{\mathcal{M}} f(x)p(x)\,dx$$

- Step one is estimate the density p so we can compute:

$$\frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{p(x_i)} = \int_{\mathcal{M}} f(x)\,dx + \mathcal{O}(N^{-1/2})$$

Key to Manifold Learning

- $L^2(\mathcal{M})$ inner product $\Rightarrow$ diagonal matrix $D_{ii} = \frac{1}{Np(x_i)}$

$$\vec{g}^\top D\vec{f} = \frac{1}{N}\sum_{i=1}^{N}\frac{g(x_i)f(x_i)}{p(x_i)} = \langle f, g\rangle_{L^2} + \mathcal{O}(N^{-1/2})$$

Estimating the density

- Select a kernel function, eg. $k_\epsilon(x,y) = e^{-||x-y||^2/\epsilon^2}$
- Define a kernel matrix $K_{ij} = \frac{k_\epsilon(x_i,x_j)}{m_0 \epsilon^m N}$

$$
\begin{aligned}
(K\vec{f})_i &\equiv \frac{\epsilon^{-m}}{m_0 N} \sum_{j=1}^{N} k_\epsilon(x_i,x_j) f(x_j) \\
&= \frac{\epsilon^{-m}}{m_0} \int_{\mathcal{M}} k_\epsilon(x_i,y) f(y) p(y)\, dy + \mathcal{O}(\epsilon^{-m} N^{-1/2}) \\
&= f(x_i) p(x_i) + \mathcal{O}(\epsilon, \epsilon^{-m} N^{-1/2})
\end{aligned}
$$

- Setting $f \equiv 1$ we have

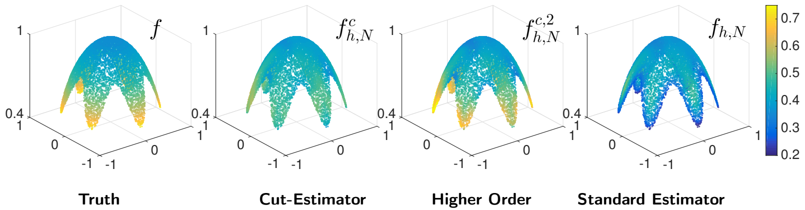
$$
p_i = \sum_{j=1}^{N} K_{ij} = p(x_i) + \mathcal{O}(\epsilon, \epsilon^{-m} N^{-1/2})
$$

Density estimation on manifold $\mathcal{M} \subset \mathbb{R}^d$ without boundary

$$\begin{aligned}
\mathbb{E}\left[\sum_{j=1}^{N} K_{ij}\right] &= \frac{1}{m_0\epsilon^d}\int_{y\in\mathcal{M}} h\left(\frac{||x-y||^2}{\epsilon^2}\right) p(y)\, dV(y) \\
(\text{decay of } h) &= \frac{1}{m_0\epsilon^d}\int_{||x-y||<\epsilon^\alpha} h\left(\frac{||x-y||^2}{\epsilon^2}\right) p(y)\, dV(y) \\
(y = \exp_x(\epsilon s)) &= \frac{1}{m_0}\int_{||\epsilon s||<\epsilon^\alpha} h\left(||s||^2 + \mathcal{O}(\epsilon^2 s_i^4)\right) p(\exp_x(\epsilon s))\,(1+\mathcal{O}(\epsilon^2 s_i^2))ds \\
(\text{Taylor}) &= \frac{1}{m_0}\int_{||s||<\epsilon^{\alpha-1}} h\left(||s||^2\right)\left(p(x)+\epsilon\nabla p(x)\cdot s\right)\, ds + \mathcal{O}(\epsilon^2) \\
(\text{symmetry}) &= \frac{1}{m_0}\int_{||s||<\epsilon^{\alpha-1}} h\left(||s||^2\right) p(x)\, ds + \mathcal{O}(\epsilon^2) \\
(\alpha<1) &= p(x)\frac{1}{m_0}\int_{\mathbb{R}^d} h\left(||s||^2\right)\, ds + \mathcal{O}(\epsilon^2) \\
&= p(x) + \mathcal{O}(\epsilon^2)
\end{aligned}$$

Density estimation on manifold $\mathcal{M} \subset \mathbb{R}^d$ with boundary

Requires estimating the distance to boundary function



(Berry & Sauer, [1])

Kernel integral operator

$$\int_{\mathcal{M}} \nabla u \cdot \nabla v \, dx + \int_{\mathcal{M}} uv \, dx = \int_{\mathcal{M}} fv \, dx + \int_{\partial\mathcal{M}} gv \, ds$$

Dirichlet Energy Volume Integral Boundary Integral

- Kernel, $K \Rightarrow$ Density, $p_i \approx p(x_i) \Rightarrow$ Volume, $D_{ii} = \frac{1}{Np_i}$
- To get Dirichlet Energy and Boundary Integral we dig deeper into kernel integral asymptotics

Diffusion Maps (w/o Boundary)

Proposition (Coifman, Lafon 2006 [2])

Let $\mathcal{M}$ be a compact Riemannian manifold without boundary and let ϵ be sufficiently small. Then we have uniformly in the variable ϵ :

$$\mathcal{K}_\epsilon f(x) \equiv \epsilon^{-m} \int_{\mathcal{M}} k_\epsilon(x, y) f(y)\, dy$$
$$= m_0 f(x) + \epsilon^2 m_2 \Big(f(x)\omega(x) - \Delta f(x) \Big) + \mathcal{O}(\epsilon^3)$$

where m_0 and m_2 are constants depending on k and $\omega(x)$ is a function depending on the curvature of $\mathcal{M}$.

(Uniformity in ϵ is crucial.)

New Result (w/ Boundary)

Theorem (R. Vaughn, [8])

For ϵ sufficiently small, let $\text{dist}(x, \partial\mathcal{M}) < \epsilon$*. Then:*

$$\mathcal{K}_\epsilon f(x) = m_0^\partial(x) f(x) + \epsilon m_1^\partial(x) \left(\langle \nabla f, \eta_x \rangle_g - \frac{m-1}{2} H(x) f(x) \right) + \mathcal{O}(\epsilon^2)$$

where $m_0^\partial(x)$ and $m_2^\partial(x)$ are functions of the distance to the boundary and $H(x)$ is the mean curvature of the hypersurface parallel to ∂M intersecting x.

Isolating the Laplacian

$$\mathcal{K}_\epsilon f(x) = f(x) + \epsilon m_1(\nabla f(x) \cdot \eta + H(x)f(x)) + \epsilon^2 m_2(\omega(x)f(x) - \Delta f(x))$$

$$f(x)\mathcal{K}_\epsilon 1(x) = f(x) + \epsilon m_1 H(x)f(x) + \epsilon^2 m_2 \omega(x)f(x)$$

Subtract...

$$\mathcal{L}_\epsilon f(x) \equiv \mathcal{K}_\epsilon f(x) - f(x)\mathcal{K}_\epsilon 1(x)$$

$$= -\epsilon m_1 \nabla f(x) \cdot \eta + \epsilon^2 m_2 \Delta f(x)$$

The long-standing mystery...

$$\frac{1}{m_2\epsilon^2}\mathcal{L}_\epsilon f(x) = \frac{\epsilon^{-m}}{m_2\epsilon^2}\int_{\mathcal{M}} k_\epsilon(x,y)f(y) - k_\epsilon(x,y)f(x)\,dy$$

$$= \Delta f(x) - \frac{c\nabla f(x)\cdot\eta}{\epsilon} + \mathcal{O}(\epsilon)$$

Diffusion Maps Problems at the Boundary

Elements of proof:

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  Normal coordinate charts shrink near the boundary.
- ~~Expand $\mathcal{K}_\epsilon$ in Riemannian normal coordinates.~~
  Can't apply Taylor's theorem without coordinates.
- ~~Use radial symmetry of the domain to cancel all odd terms.~~
  Even if we could, the coordinates would be nonsymmetric.
  - Addressed by "symmetrizing" normal coordinates near the boundary in [3, 4] and others.

Diffusion Maps Solution at the Boundary

Solution: Use different coordinates near the boundary.

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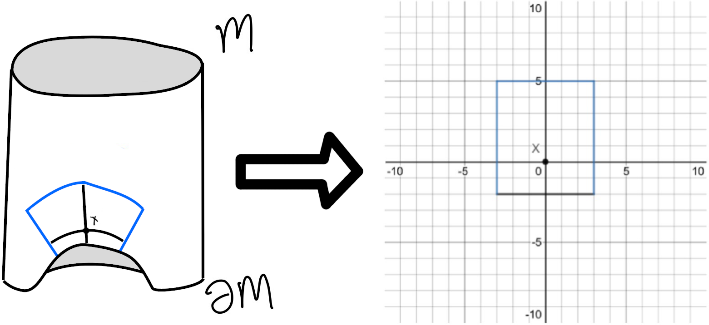
- Classical
- Less well-behaved
- Better for computations near hypersurfaces (∂M).

Semigeodesic Coordinates



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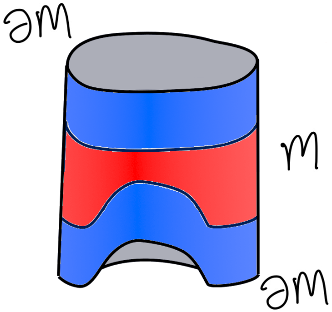
- The coordinate norm does not parameterize geodesic distance
(Different from normal coordinates)

Semigeodesic Coordinates

Generalization for manifolds with boundary:

$$M = \mathcal{M}_\epsilon \cup N_\epsilon$$



Semigeodesic Expansion

- Volume measure in normal coordinates:

$$
\begin{aligned}
d\mathrm{Vol} &= \sqrt{|\det g|}\; ds^1 \cdots ds^m \\
&= 1 - \frac{1}{6}\mathrm{Ric}(s,s) + \mathcal{O}(\|s\|_g^3) ds^1 \cdots ds^m .
\end{aligned}
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\end{aligned}
$$

- Volume measure in semigeodesic coordinates:

$$
d\mathrm{Vol}(u) = 1 + H(x)u^m + \mathcal{O}(\|u\|_{\mathrm{sem}}^2)
$$

Semigeodesic Expansion

- Distance comparison in normal coordinates (Smolyanov et al. [5] 2007)

$$\|x - y\|_{\mathbb{R}^d}^2 = \|s\|_g^2 - \frac{1}{12}\,\|\Pi(s,s)\|_g^2 + \mathcal{O}(\|s\|_g^5)$$

Semigeodesic Expansion

- Distance comparison in normal coordinates (Smolyanov et al. [5] 2007)

$$\|x-y\|^2_{\mathbb{R}^d} = \|s\|^2_g - \frac{1}{12}\|\Pi(s,s)\|^2_g + \mathcal{O}(\|s\|^5_g)$$

- Norm comparison in semigeodesic coordinates (V, 2020)

$$\|x-y\|^2_{\mathbb{R}^d} = \|u\|^2_{\text{sem}} - \left\langle \Pi_{\partial\mathcal{M}_{b_x}}(u^\top, u^\top), u^\perp \right\rangle_g + \mathcal{O}(\|u\|^4_{\text{sem}}).$$

Semigeodesic Expansion

Proposition (R. Vaughn, 2020)

For ϵ sufficiently small, let x be a point in N_ϵ. Then:

$$\frac{1}{\epsilon^m}\int_{y\in\mathcal{M}} k(\epsilon,x,y)f(y)\,d\mathrm{Vol} = m_0^\partial(x)f(x) + \epsilon m_1^\partial(x)\left(\langle\nabla f,\eta_x\rangle_g - \frac{m-1}{2}H(x)f(x)\right) + \mathcal{O}(\epsilon^2)$$

where $m_0^\partial(x)$ and $m_2^\partial(x)$ are functions of the distance to the boundary and $H(x)$ is the mean curvature of the hypersurface parallel to ∂M intersecting x.

The long-standing mystery...

$$\frac{1}{m_2\epsilon^2}\mathcal{L}_\epsilon f(x) \equiv \frac{\epsilon^{-m}}{m_2\epsilon^2}\int_{\mathcal{M}} k_\epsilon(x,y)f(y) - k_\epsilon(x,y)f(x)\,dy$$

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$$= \Delta f(x) - \frac{c\nabla f(x)\cdot\eta}{\epsilon} + \mathcal{O}(\epsilon)$$

Solution: Analyze $\mathcal{L}_\epsilon$ in the weak-sense

Main Result

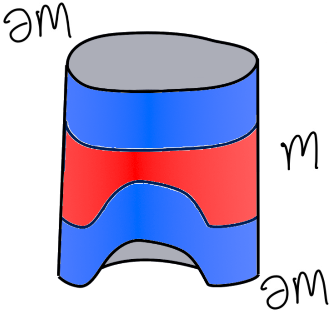
Theorem (R. Vaughn, [8])

Assume q is a uniform distribution for simplicity. Then for any smooth function f and any smooth test function ϕ, we have:

$$\mathcal{L}_\epsilon \equiv \frac{\epsilon^{-m-2}}{m_2} \int_{\mathcal{M}} \phi \cdot (\mathcal{K}_\epsilon f - f \mathcal{K}_\epsilon 1) \ d\text{Vol}$$

$$= - \int_{\mathcal{M}} \langle \nabla \phi, \nabla f \rangle_g \ d\text{Vol} + \mathcal{O}(\epsilon).$$

Elements of Proof



- $\mathcal{M}_\epsilon$ grows as $\epsilon \to 0$
- N_ϵ shrinks as $\epsilon \to 0$

The additional integral allows us to subdivide $\mathcal{M}$ into two regions for every ϵ.

Elements of Proof

$$\int_{\mathcal{M}} \phi \mathcal{L}_\epsilon f \; d\mathrm{Vol} = \int_{\mathcal{M}_\epsilon \cup N_\epsilon} \phi \mathcal{L}_\epsilon f \; d\mathrm{Vol}$$

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$$= \int_{\mathcal{M}_\epsilon} \phi \mathcal{L}_\epsilon f \; d\mathrm{Vol} + \int_{N_\epsilon} \phi \mathcal{L}_\epsilon f \; d\mathrm{Vol}$$

Elements of Proof

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$$= \int_{\mathcal{M}_\epsilon} \phi \mathcal{L}_\epsilon f \; d\text{Vol} - \int_{\partial \mathcal{M}} \langle \phi \; \nabla f, \eta \rangle_g \; d\text{Vol} + \mathcal{O}(\epsilon)$$

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Elements of Proof

Hence,

$$\vec{\phi}^{\top} L_{\epsilon} \vec{f} \approx \int_{\mathcal{M}} \phi \mathcal{L}_{\epsilon} f \ d\text{Vol} = -\int_{\mathcal{M}} \langle \nabla \phi, \nabla f \rangle_{g} \ d\text{Vol} + \mathcal{O}(\epsilon)$$

Elements of Proof

Hence,

$$\vec{\phi}^\top L_\epsilon \vec{f} \approx \int_{\mathcal{M}} \phi \mathcal{L}_\epsilon f \; d\mathrm{Vol} = -\int_{\mathcal{M}} \langle \nabla \phi, \nabla f \rangle_g \; d\mathrm{Vol} + \mathcal{O}(\epsilon)$$

- The kernel based estimator does not converge pointwise
- **But** it converges to the variational form of Δ with Neumann B.C. in the weak sense.

Boundary Integrals

Use distance-to-boundary function to estimate boundary integrals:

Theorem (R. Vaughn, [8])

For $f : \mathcal{M} \to \mathbb{R}$, $d_{\mathcal{M}}$ the intrinsic distance, and h with fast decay we have,

$$\frac{1}{\epsilon} \int_{x \in N_\epsilon} h\left(\frac{d_{\mathcal{M}}(x, \partial M)^2}{\epsilon^2}\right) f(x)\, d\mathrm{Vol} = \overline{m}_0 \int_{x \in \partial\mathcal{M}} f(x)\, d\mathrm{Vol}_\partial + \mathcal{O}(\epsilon)$$

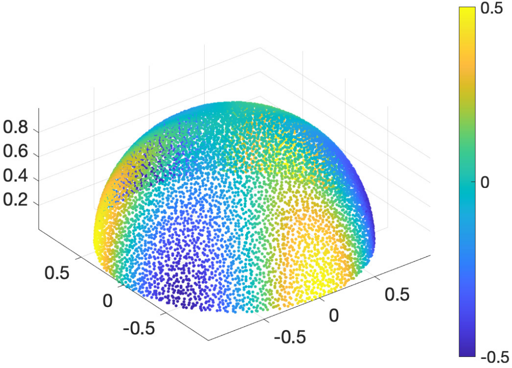
where $\overline{m}_0 = \int_0^\infty h(u)\, du$.

Mesh-free solver for BVPs on Embedded Manifolds

Weak-sense formulation:

$$\int_{\mathcal{M}} \nabla u \cdot \nabla v \, dx + \int_{\mathcal{M}} uv \, dx = \int_{\mathcal{M}} fv \, dx + \int_{\partial \mathcal{M}} gv \, ds$$

Dirichlet Energy   Volume Integral   Boundary Integral



Consequences

Manifold Learning:

- Diffusion Maps returns Neumann eigenfunctions [2]
- Our result rigorously explains this empirical phenomenon
- Eigenproblem, $\vec{v}^\top L_\epsilon \vec{v} \approx \int_{\mathcal{M}} \nabla\phi \cdot \nabla\phi \, dx$
- Natural boundary condition is Neumann

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Density Estimation, Volume Integrals [1]:

`http://math.gmu.edu/~tberry/`

Dirichlet energy & boundary integrals [8]:

`http://math.gmu.edu/~rvaughn5/`