Geometric Flows and Dimension Reduction

Aneesh Malhotra

George Mason University

Introduction

Given a Riemannian manifold $(\mathcal{M}, g)$ with a specified metric g the goal of minimal embedding is to find a smooth map $F : \mathcal{M} \to \mathbb{R}^m$ such that:

1. $F(\mathcal{M})$ Isometric
2. Has Minimal Extrinsic Curvature, i.e. to find:

$$F' = \underset{F}{\text{argmin}} \underbrace{\int_{\mathcal{M}} || \det HF(x)^{\perp} || \, d\text{vol}}_{\text{Extrinsic Curvature}} \text{ subject to } \underbrace{DF(x)^{\top} DF(x) = g_x}_{\text{Preserve the geometry}}.$$

We can solve this analytically for simple cases. Consider the circle S^1 embedded into $\mathbb{R}^4$ via

$$\mathbf{F} = \frac{1}{\sqrt{1+k^2}} (\cos\theta, \sin\theta, \cos k\theta, \sin k\theta)$$

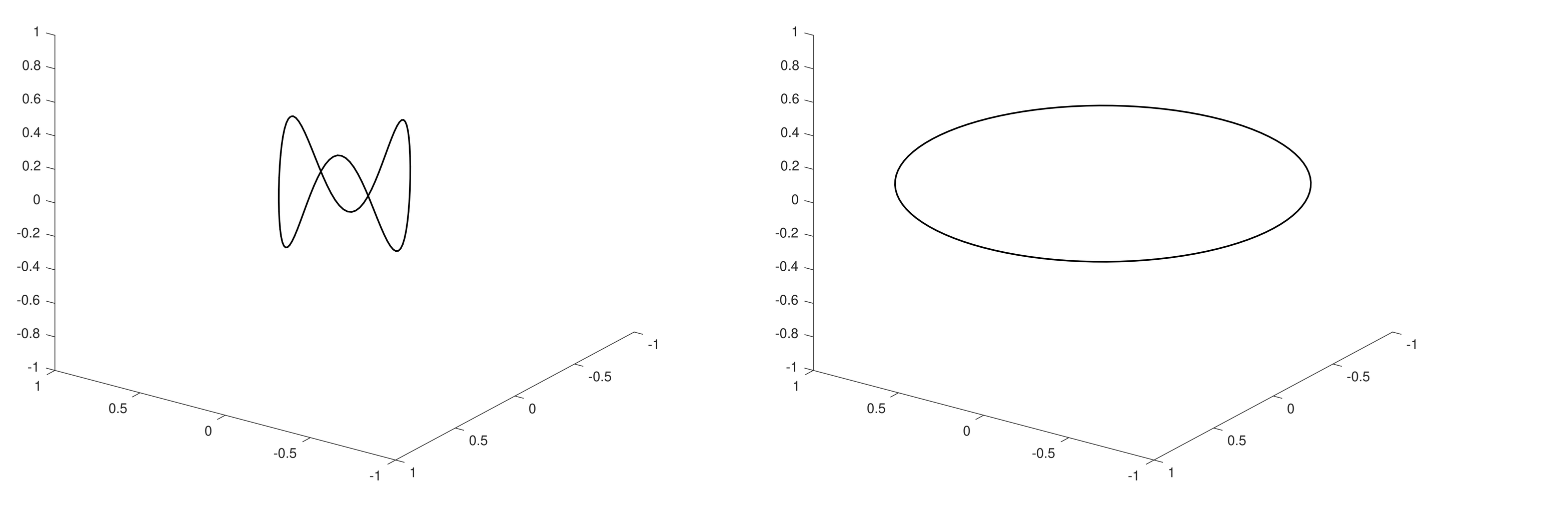

Figure 1:[First 3 coordinates] Our initial embedding of S^1 (left) and its solution, a 2D embedding (right)

Goal

Consider a data set of N points sampled from $\mathcal{M}$ given by $X = \{x_i\}_{i=1}^N$. We seek to perform a similar minimization on the extrinsic curvature of the data while preserving the geometry. The example we will work with is a discretization of the earlier example.

$$x_i = \frac{1}{\sqrt{1+k^2}} (\cos(\theta_i), \sin(\theta_i), \cos(k\theta_i), \sin(k\theta_i))$$

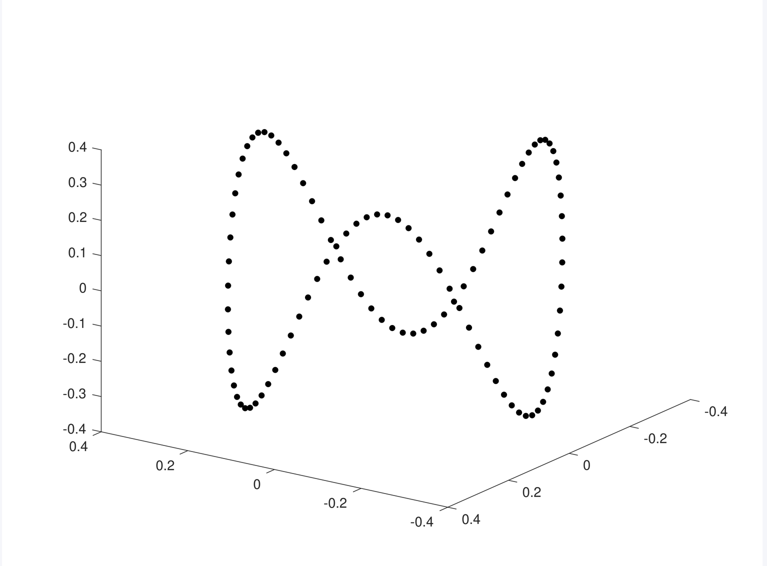

Figure 2:First three coordinates of our discretized data-set

Diffusion Maps

Our method relies on being able to *parameterize* our data. In order to do this we will use the diffusion maps algorithm [1] to approximate eigenfunctions of the Laplacian $\{\phi_k\}_{k\in\mathbb{Z}^+}$ which form a basis for $L^2(\mathcal{M})$ i.e. in the continuous case we would rewrite each coordinate of the embedding function as

$$f_j(z) = \sum_{k=1}^{\infty} C_{kj} U_k(z) \text{ with } z \in \mathcal{M}$$

Theorem

Following Coifman and Lafon, let $k(x,y) = \exp\left(-\frac{\|x-y\|^2}{\epsilon^2}\right)$ *so that* $L_{ij} = \frac{k(x_i,x_j)}{\sum_j k(x_i,x_j)}$. *Then* $L\vec{f} \to \Delta f$ *as* $N \to \infty$ *and* $\epsilon \to 0$, *where* Δ *denotes the Laplace operator. The eigenfunctions of the Laplacian* Δ *can be approximated in the discrete case by the eigenvectors of the graph Laplacian* L.

Approximating Eigenfunctions

Find the matrix of eigenvectors, U such that $L = UVU^T$. This allows us to write our data as $X_i = \sum_k U_{ik} C_{k*}$ so $X = UC$.

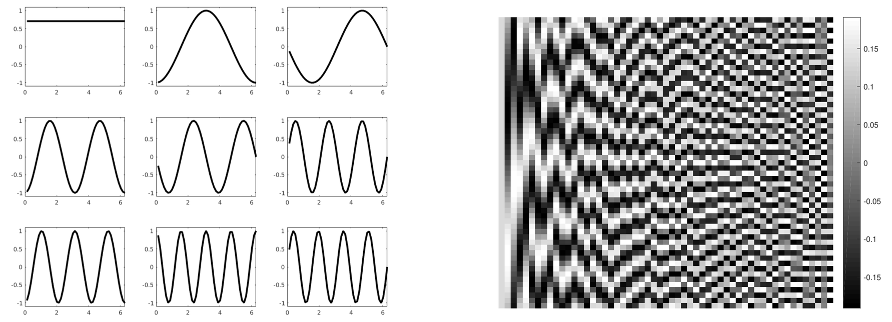

Figure 3:Eigenvectors of L approximate the eigenfunction of Δ on S^1

Curvature Estimate

Let X be a dataset of N points embedded in $\mathbb{R}^n$ sampled from a manifold $\mathcal{M}$ of dimension d, and define the kernel matrix $K_{ij} = k_\epsilon(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{\epsilon^2}\right)$. Let $f\colon \mathbb{R}^n \to \mathbb{R}$ be continuous. We can evaluate f at the data points in X by letting $\mathbf{f} = \left(f(x_1),\ f(x_2),\ \ldots,\ f(x_N)\right)^T$. Then

$$\frac{\epsilon^{-d}}{N}(K\mathbf{f})_i \approx m_0 f(x_i)\rho(x_i) + \epsilon^2 m_2 \left(f(x_i)\rho(x_i)\omega(x_i) + \Delta(f(x_i)\rho(x_i)) + \mathcal{O}(\epsilon^4)\right)$$

- m_i denotes the i_{th} moment of the kernel. $m_0 = \sqrt{2\pi}$ and $m_2 = \frac{\sqrt{2\pi}}{2}$.
- ρ is the sampling density and ω is the second fundamental form of $\mathcal{M}$

In order to separate the the second fundamental form from the sampling density we used a Richardson extrapolation where we compute a second kernel $K_{a\epsilon}$ for $a = 1.05$.

$$\hat{\mathbf{p}} = \frac{a^2 K_\epsilon \mathbf{1} - a^{-d} K_{a\epsilon}\mathbf{1}}{a^2 - 1}$$

The curvature is then given by

$$\omega = \frac{16}{\epsilon^2}\left(K_\epsilon \frac{1}{\hat{\mathbf{p}}} - 1\right)$$

*The curvature estimate extends a result of Hein et al.

Curvature Estimate

We varied ϵ between 0.02 and 0.5 and see that our curvature estimate is robust to these variations.

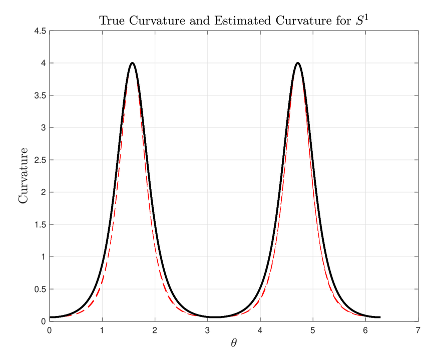

Figure 4:The true curvature is well approximated by our method for various ϵ

Gradient Descent

In order to minimize curvature, we found an analytic expression for the gradient of the Fourier coefficients with respect to the curvature. In order to enforce the isometry constraint we also found the gradient of C with with respect to the norm of the kernel difference $\|K_X - K_{UC}\|_{fro}$.

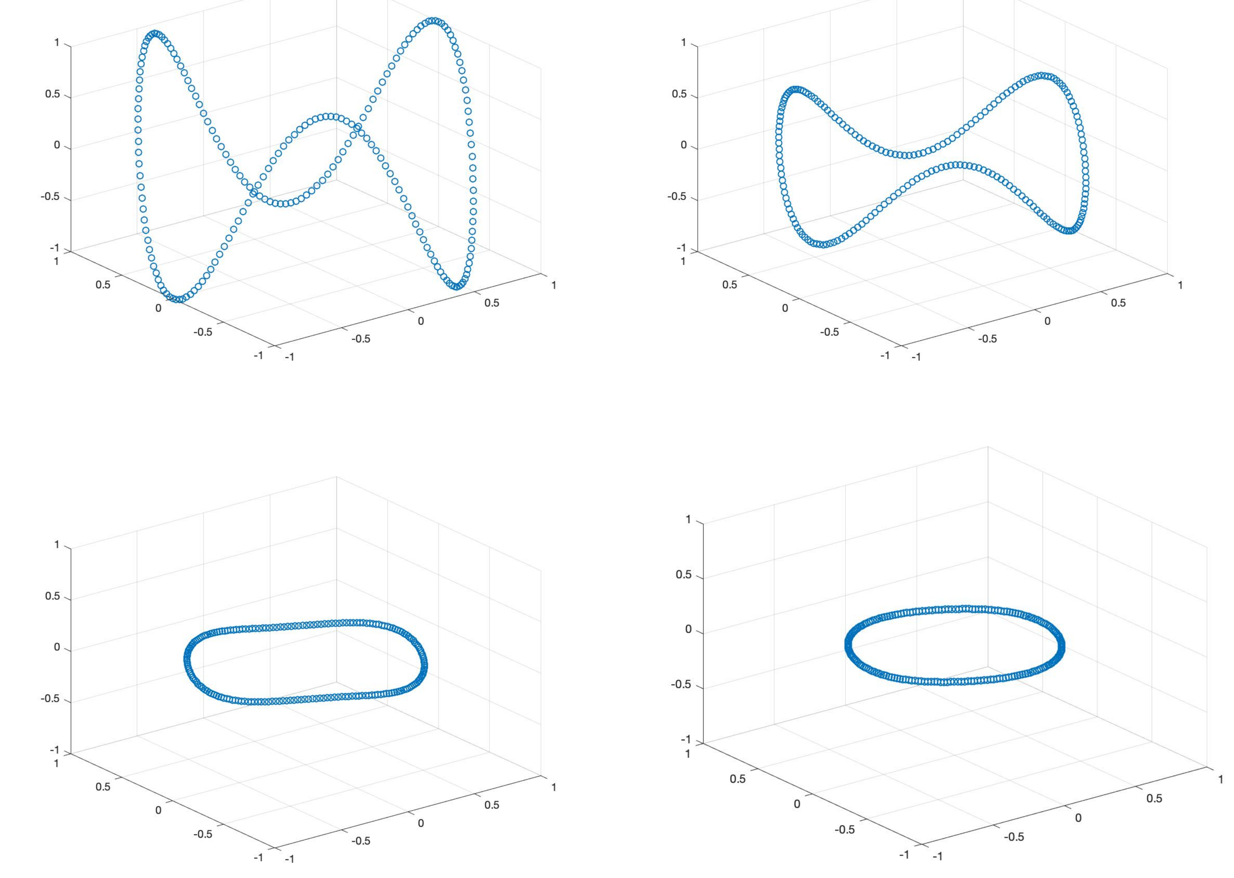

Figure 5:Gradient descent reduces extrinsic curvature

References

[1] Ronald R Coifman and Stéphane Lafon.
Diffusion maps.
Applied and Computational Harmonic Analysis, 21(1):5--30, 2006.

[2] Matthias Hein, Jean-Yves Audibert, and Ulrike von Luxburg.
From Graphs to Manifolds -- Weak and Strong Pointwise Consistency of Graph Laplacians.
In Peter Auer and Ron Meir, editors, *Learning Theory*, pages 470--485, Berlin, Heidelberg, 2005. Springer.

Acknowledgements

We would like to thank the Mason Experimental Geometry Lab and Tyrus Berry for supporting this project.