Geometric Flows and Dimension Reduction

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Fall 2018

Goal

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:

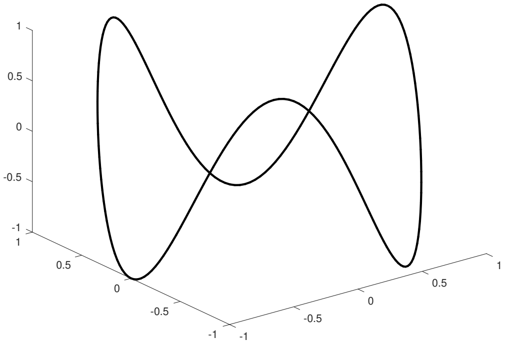
1. $F(\mathcal{M})$ Isometric
2. Has Minimal Extrinsic Curvature

Definition. Minimal Embedding of a Riemannian Manifold

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

Example: Initial Embedding for S^1

The Pringle Chip!

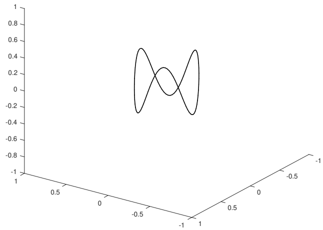
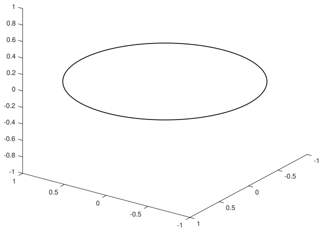


$$x = F(\theta) = [cos(\theta), sin(\theta), cos(k\theta), sin(k\theta)]/\sqrt{1+k^2} \text{ for } k = 3$$

Example: Initial Embedding for S^1

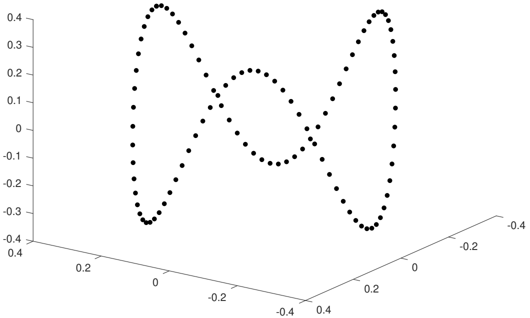
Let $F = (f_1, f_2, f_3, f_4)$. We can solve the constrained problem using the method of Lagrange multipliers:

$$\min_{\lambda, f_1, \ldots, f_4} \left\{ \int_0^{2\pi} \sum_{i=1}^{4} f_i''(\theta)^2 + \lambda(\theta) \left(\sum_{i=1}^{4} f_i'(\theta)^2 - 1 \right) \, d\theta \right\}$$

Initial Embedding	Expected Fixed Point
	

Discrete case

The Pringle Chip Redux!



$$x_i = F(\theta_i) = [cos(\theta_i), sin(\theta_i), cos(k\theta_i), sin(k\theta_i)]/\sqrt{1+k^2} \text{ for } k = 3$$

Key idea from the continuous case: Parametrize F!

- Eigenfunctions ϕ_k of the Laplacian, $\Delta_{\mathcal{M}}$, form a basis for $L^2(\mathcal{M})$
- We can write f_j in terms of them $f_j(z) = \sum_{k=1}^{\infty} (\hat{f}_j)_k \phi_k(z)$

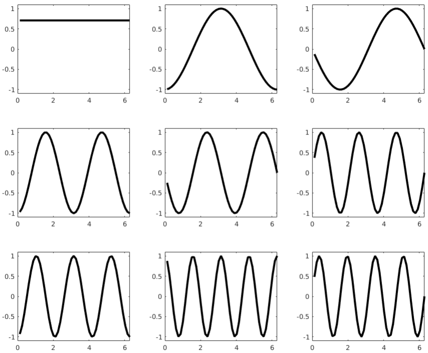
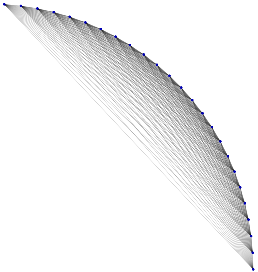


Figure: First 9 eigenfunctions of Δ_{S^1}

Recovering the Graph Laplacian from data

Theorem. (Due to Coifman and Lafon)

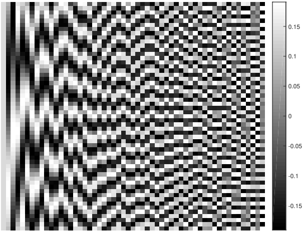
Let $k(x,y) = exp\{-\frac{\|x-y\|^2}{\epsilon^2}\}$ so that $L_{ij} = \frac{k(x_i,x_j)}{\sum_j k(x_i,x_j)}$.
Then, $L\bar{f} \to \overline{\Delta f}$ as $N \to \infty$ and $\epsilon \to 0$



(Connected Graph over the Data)

Approximating the eigenfunctions

- Since we only have data, we can only approximate these eigenfunctions (as eigenvectors) by finding U, V such that $K_X = UVU^t$ where K_X approximates this Laplacian operator
- We can find $\hat{f}_j$ such that $\bar{f}_j = U\hat{f}_j$.
- More generally, we can define a matrix $Cz = [\hat{f}_1|...|\hat{f_m}]$ so that $X = UC = U[\hat{f}_1|...|\hat{f_m}]$



(The matrix, U)

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 $f : \mathbb{R}^n \to \mathbb{R}$ be continuous. We can evaluate f at the data points in X by letting $\mathbf{f} = \Big(f(x_1), \quad f(x_2), \quad \dots, \quad f(x_N)\Big)^T$. Then

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

- 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 $\mathcal{M}$
- Our goal is to isolate ω.

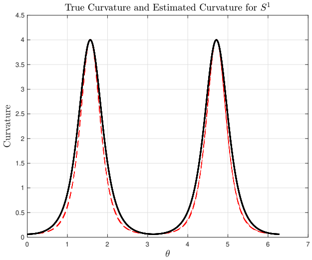
Curvature Estimate

To do this we used a Richardson Extrapolation, requiring us to compute $K_{a\epsilon}$, for $a \approx 1.05$. Let

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

. The curvature estimate is given by

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



Gradient Descent

Now we will consider data sets that were generated using Fourier coefficients C using the eigenvectors of the Laplacian U.

- We computed two gradients:

$$\frac{\partial \omega}{C_{uv}}$$
$$\frac{\partial}{C_{uv}} \|K_X - K_{UC}\|$$

- Our gradient descent algorithm will be to move C in the direction of steepest descent in both directions

Minimization by Gradient Descent

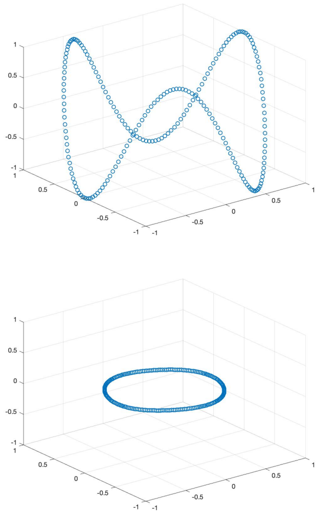


Figure: Dimensionality Reduction

References I

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