Statistical Inference and application to Machine Learning
For Geometric and Topological Data

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Introduction

Minimax Rates for Geometric Parameters of a Manifold

- Minimax Rates for Estimating the Dimension of a Manifold
- The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

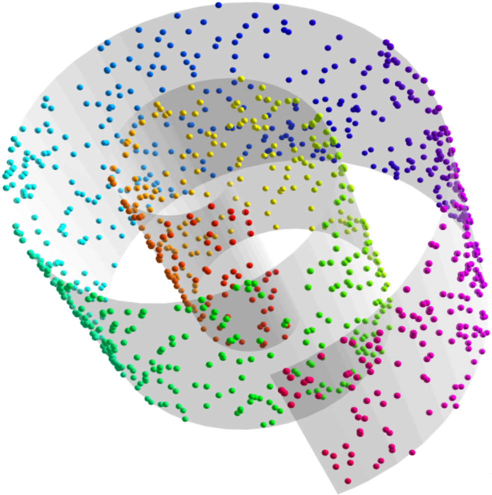
Topological Data Analysis: Persistent Homology

Statistical Inference for Persistent Homology

Application of Topological Data Analysis to Machine Learning

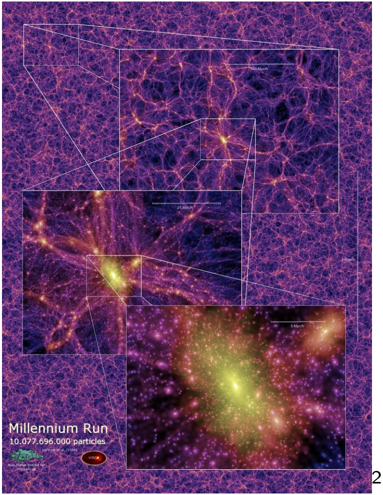
- Featurization of Topological Data Analysis using Persistence Landscapes

The curse of dimensionality from the high dimensional data is mitigated when there is a low dimensional geometric and topological structure.

 [1]

[1] http://www.skybluetrades.net/blog/posts/2011/10/30/machine-learning/

Geometric and topological structures in the data provide information.



[2]

[2] http://www.mpa-garching.mpg.de/galform/virgo/millennium/poster_half.jpg

Statistical Inference and application to Machine Learning For Geometric and Topological Data are explored.

- Minimax Rates for Geometric Parameters of a Manifold
  - Minimax Rates for Estimating the Dimension of a Manifold (Kim, Rinaldo, Wasserman, 2019)
  - The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory (Aamari, Kim, Chazal, Michel, Rinaldo, Wasserman, 2019)
- General Introduction to Topological Data Analysis
  - Computational Topology: An Introduction (Edelsbrunner, Harer, 2010)
  - Topological Data Analysis (Wasserman, 2016)
  - An introduction to Topological Data Analysis: fundamental and practical aspects for data scientists (Chazal, Michel, 2017)
- Statistical Inference for Persistent Homology
  - Confidence sets for persistence diagrams (Fasy, Lecci, Rinaldo, Wasserman, Balakrishnan, Singh, 2014)
- Application of Topological Data Analysis to Machine Learning
  - Time Series Featurization via Topological Data Analysis (Kim, Kim, Rinaldo, Chazal, 2020)
  - Efficient Topological Layer based on Persistence Landscapes (Kim, Kim, Zaheer, Kim, Chazal, Wasserman, 2020)

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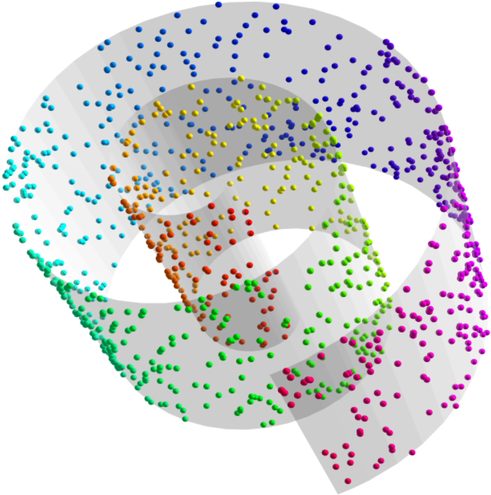
A manifold is a low dimensional geometric structure that locally resembles Euclidean space.



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[3] http://www.skybluetrades.net/blog/posts/2011/10/30/machine-learning/

The maximum risk of an estimator is its worst expected error.

- the maximum risk of an estimator $\hat{\theta}_n$ is the worst expected error that the estimator $\hat{\theta}_n$ can make.
- $$\sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[\ell \left(\hat{\theta}_n(X),\ \theta(P) \right) \right]$$
  - $X = (X_1, \cdots, X_n)$ is drawn from a fixed distribution P, where P is contained in set of distributions $\mathcal{P}$.
  - estimator $\hat{\theta}_n$ is any function of data X.
  - The loss function $\ell(\cdot, \cdot)$ measures the error of the estimator $\hat{\theta}_n$.

The minimax rate describes the statistical difficulty of estimating a parameter.

- The minimax rate R_n is the risk of an estimator that performs best in the worst case, as a function of sample size.
- $$R_n = \inf_{\hat{\theta}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[\ell \left(\hat{\theta}_n(X),\ \theta(P) \right) \right]$$
  - $X = (X_1, \cdots, X_n)$ is drawn from a fixed distribution P, where P is contained in set of distributions $\mathcal{P}$.
  - estimator $\hat{\theta}_n$ is any function of data X.
  - The loss function $\ell(\cdot, \cdot)$ measures the error of the estimator $\hat{\theta}_n$.

We measure the statistical difficulty of estimating geometric parameters of a manifold by their minimax rate.

- Minimax Rates for Estimating the Dimension of a Manifold (Kim, Rinaldo, Wasserman, 2019)
- The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory (Aamari, Kim, Chazal, Michel, Rinaldo, Wasserman, 2019)

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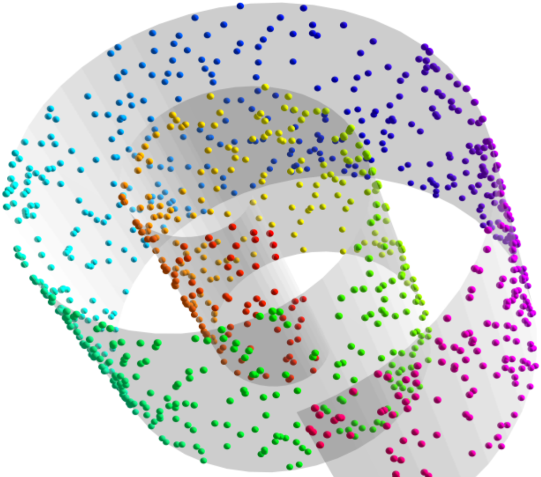
The intrinsic dimension of a manifold needs to be estimated a prior to the manifold learning.

- Most manifold learning algorithms require the intrinsic dimension of the manifold as input.
- The intrinsic dimension is rarely known in advance and therefore has to be estimated.



Minimax rate for estimating the dimension

- $$R_n = \inf_{\hat{\dim}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[1 \left(\hat{\dim}_n(X) \neq \dim(P) \right) \right]$$
  - $X = (X_1, \cdots, X_n)$ is drawn from a fixed distribution P, where P is contained in set of distributions $\mathcal{P}$.
  - estimator $\hat{\dim}_n$ is any function of data X.
  - $0 - 1$ loss function is considered, so for all $x, y \in \mathbb{R}$, $\ell(x, y) = 1(x \neq y)$.

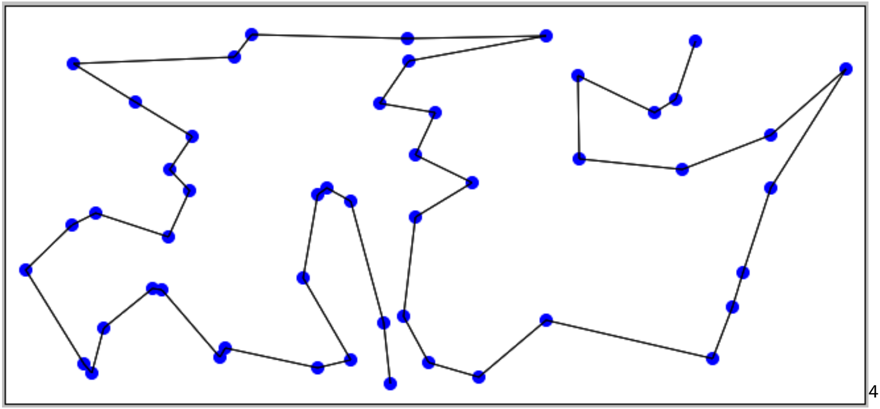
Minimax rate for estimating the dimension: we first consider dimension d_1 vs d_2.

- $$R_n = \inf_{\hat{\dim}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[1 \left(\hat{\dim}_n(X) \neq \dim(P) \right) \right]$$
  - $X = (X_1, \cdots, X_n)$ is drawn from a fixed distribution P, where P is contained in set of distributions $\mathcal{P} = \mathcal{P}^{d_1} \cup \mathcal{P}^{d_2}$, where $\mathcal{P}^d$ is a set of d-dimensional distributions..
  - estimator $\hat{\dim}_n$ is any function of data X.
  - $0 - 1$ loss function is considered, so for all $x, y \in \mathbb{R}$, $\ell(x, y) = 1(x \neq y)$.

The Maximum Risk of any chosen Estimator Provides an Upper Bound on the Minimax Rate.

$$
\begin{aligned}
R_n &= \inf_{\hat{\mathrm{dim}}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[1 \left(\hat{\mathrm{dim}}_n(X) \neq \mathrm{dim}(P) \right) \right] \\
&\leq \underbrace{\sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[1 \left(\hat{\mathrm{dim}}_n(X) \neq \mathrm{dim}(P) \right) \right]}_{\text{the maximum risk of any chosen estimator}}
\end{aligned}
$$

TSP(Travelling Salesman Problem) Path Finds Shortest Path that Visits Each Points exactly Once.



[4]

[4] http://www.heatonresearch.com/fun/tsp/anneal

Our Estimator estimates Dimension to be d_2 if d_1-squared Length of TSP Generated by the Data is Long.

- When intrinsic dimesion is higher, length of TSP path is likely to be longer.
- $$\hat{\dim}_n(X) = d_1 \iff$$
$$\min_{\sigma \in S_n} \sum_{i=1}^{n-1} \|X_{\sigma(i+1)} - X_{\sigma(i)}\|_{\mathbb{R}^m}^{\boldsymbol{d_1}} \leq C,$$

  where C is some constant.

Mimimax rate is upper bounded by $O\left(n^{-\left(\frac{d_2}{d_1}-1\right)n}\right)$.

Proposition

(Proposition 9) Let $1 \leq d_1 < d_2 \leq m$. Then

$$\inf_{\hat{\dim}_n} \sup_{P \in \mathcal{P}^{d_1} \cup \mathcal{P}^{d_2}} \mathbb{E}_{P^{(n)}} \left[1 \left(\hat{\dim}_n(X) \neq \dim(P) \right) \right] \lesssim n^{-\left(\frac{d_2}{d_1}-1\right)n}.$$

Le Cam's Lemma provides lower bounds for estimating the dimension.

Lemma

(Lemma 10, Le Cam's Lemma) Let $\mathcal{P}$ be a set of probability measures, and $\mathcal{P}^{\mathbf{d_1}}, \mathcal{P}^{\mathbf{d_2}} \subset \mathcal{P}$ be such that for all $P \in \mathcal{P}^{\mathbf{d}_i}$, $\theta(P) = \theta_i$ for $i = 1, 2$. For any $Q_i \in co(\mathcal{P}_i)$, let q_i be density of Q_i with respect to measure ν. Then

$$\begin{aligned}&\inf_{\hat{\theta}} \sup_{P \in \mathcal{P}} \mathbb{E}_P \left[1 \left(\hat{\dim}_n(X) \neq \dim(P) \right) \right] \\ &\geq \frac{1(\theta_1 \neq \theta_2)}{4} \sup_{Q_i \in co(\mathcal{P}^{d_i})} \int [q_1(x) \wedge q_2(x)] d\nu(x).\end{aligned}$$

Mimimax rate is lower bounded by $\Omega\left(n^{-2(d_2-d_1)n}\right)$.

Proposition

(Proposition 14)

$$\inf_{\hat{\dim}} \sup_{P\in\mathcal{P}^{d_1}\cup\mathcal{P}^{d_2}} \mathbb{E}_{P^{(n)}}\left[1\left(\hat{\dim}_n(X)\neq\dim(P)\right)\right] \gtrsim n^{-2(d_2-d_1)n}.$$

Minimax rate for estimating the dimension

Theorem

(Proposition 16 and 17)

$$n^{-2n} \lesssim \inf_{\hat{\dim}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[1 \left(\hat{\dim}_n(X) \neq \dim(P) \right) \right] \lesssim n^{-\frac{\mathbf{1}}{m-\mathbf{1}} n}.$$

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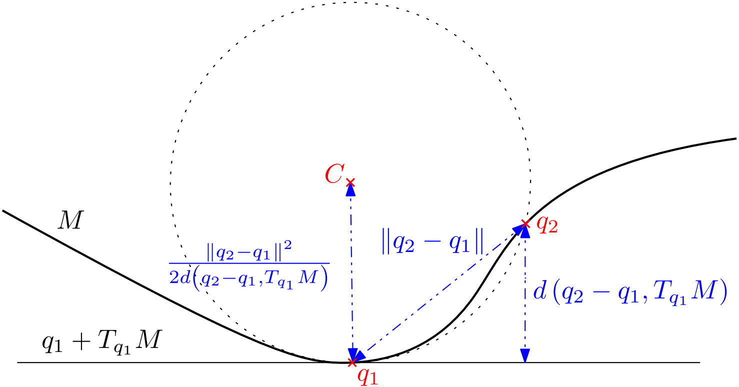
The reach is the maximum radius of a ball that can roll over the manifold.

Definition

When $M \subset \mathbb{R}^m$ is a manifold, the reach of M, denoted by $\tau(M)$, can be defined as

$$\tau(M) = \inf_{q_2 \neq q_1 \in M} \frac{\|q_2 - q_1\|_2^2}{2d(q_2 - q_1,\ T_{q_1}M)},$$

where $T_a M$ is the tangent space of M at a.



The reach is a regularity parameter in many geometrical inference problem.

- The reach is a key paramter in:
  - Dimension estimation
  - Homology inference
  - Volume estimation
  - Manifold clustering
  - Diffusion maps

Minimax rate for estimating the reach

- $$R_n = \inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[\left| \frac{1}{\tau(P)} - \frac{1}{\hat{\tau}_n(X)} \right|^q \right]$$

    - $X = (X_1, \cdots, X_n)$ is drawn from a fixed distribution P, where P is contained in set of distributions $\mathcal{P}$.
    - estimator $\hat{\tau}_n$ is any function of data X.
    - inverse l_q loss function is considered, so for all $x, y \in \mathbb{R}$, $\ell(x, y) = \left| \frac{1}{x} - \frac{1}{y} \right|^q$.

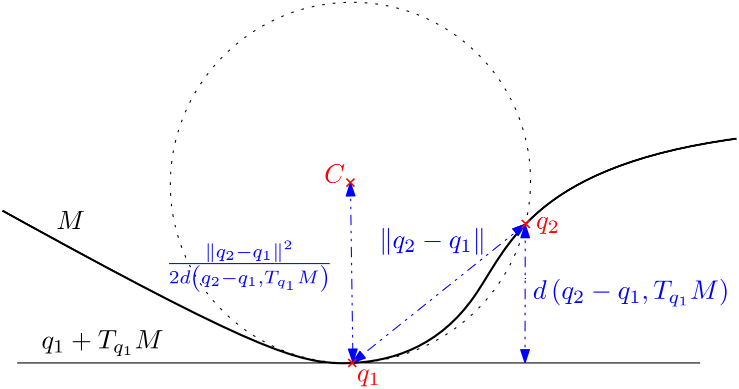
The maximum risk of our estimator provides an upper bound on the minimax rate.

$$
\begin{aligned}
R_n &= \inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^n} \left[\left| \frac{1}{\tau(P)} - \frac{1}{\hat{\tau}_n(X)} \right|^q \right] \\
&\leq \underbrace{\sup_{P \in \mathcal{P}} \mathbb{E}_{P^n} \left[\left| \frac{1}{\tau(P)} - \frac{1}{\hat{\tau}(X)} \right|^q \right]}_{\text{the maximum risk of our estimator}}
\end{aligned}
$$

We define the reach estimator $\hat{\tau}_n$ as the maximum radius of a ball that you can roll over the point cloud.

- Given observation $X = (X_1, \ldots, X_n)$, then the reach estimator $\hat{\tau}_n$ is a plugin estimator as

$$\hat{\tau}_n(X) = \inf_{1 \leq i \neq j \leq n} \frac{\|X_j - X_i\|_2^2}{2d(X_j - X_i,\ T_{X_i}M)}.$$


C
M
$\frac{\|q_2 - q_1\|^2}{2d\left(q_2 - q_1, T_{q_1}M\right)}$
$\|q_2 - q_1\|$
q_2
$d\left(q_2 - q_1, T_{q_1}M\right)$
$q_1 + T_{q_1}M$
q_1

Minimax rate is upper bounded by $O\left(n^{-\frac{2q}{3d-1}}\right)$.

Theorem

(Theorem 5.1)

$$\inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^n}\left[\left|\frac{1}{\tau(P)} - \frac{1}{\hat{\tau}_n(X)}\right|^q\right] \lesssim n^{-\frac{2q}{3d-1}}.$$

Le Cam's lemma provides a lower bound based on the reach difference and the statistical difference of two distributions.

- Total variance distance between two distributions is defined as

$$TV(P, P') = \sup_{A \in \mathcal{B}(\mathbb{R}^D)} |P(A) - P'(A)| .$$

Lemma

(Lemma 5.2) Let $P, P' \in \mathcal{P}$ with respective supports M and M'. Then

$$\inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^n} \left[\left| \frac{1}{\tau(P)} - \frac{1}{\hat{\tau}_n(X)} \right|^q \right] \gtrsim \left| \frac{1}{\tau(M)} - \frac{1}{\tau(M')} \right|^q (1 - TV(P, P'))^{2n} .$$

Mimimax rate is lower bounded by $\Omega\left(n^{-\frac{q}{d}}\right)$.

Proposition

(Proposition 5.6)

$$\inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^n}\left[\left|\frac{1}{\tau(P)} - \frac{1}{\hat{\tau}_n(X)}\right|^q\right] \gtrsim n^{-\frac{q}{d}}.$$

Minimax rate for estimating the reach

Theorem

(Theorem 5.1 and Proposition 5.6)

$$n^{-\frac{q}{d}} \lesssim \inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[\left| \frac{1}{\tau(P)} - \frac{1}{\hat{\tau}_n(X)} \right|^q \right] \lesssim n^{-\frac{\mathbf{2}q}{\mathbf{3}d-\mathbf{1}}}.$$

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The number of holes is used to summarize topological features.

- Geometrical objects :
  - ㄱ, ㄴ, ㄷ, ㄹ, ㅁ, ㅂ, ㅅ, ㅇ, ㅈ, ㅊ, ㅋ, ㅌ, ㅍ, ㅎ
  - A, 字, あ
- The number of holes of different dimensions is considered.
  1. $\beta_0 = \#$ of connected components
  2. $\beta_1 = \#$ of loops (holes inside 1-dim sphere)
  3. $\beta_2 = \#$ of voids (holes inside 2-dim sphere) : if $dim \geq 3$

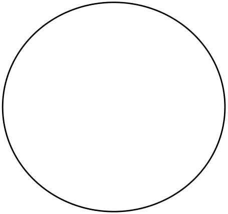
Example : Objects are classified by homologies.

1. $\beta_0 =\#$ of connected components ●
2. $\beta_1 =\#$ of loops ○

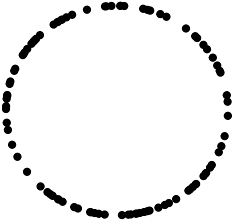
$\beta_0 \setminus \beta_1$	0	1	2
1	ㄱ, ㄴ, ㄷ, ㄹ, ㅅ, ㅈ, ㅋ, ㅌ	ㅁ, ㅇ, ㅂ, ㅍ, A	あ
2	ㅊ, 字		
3		ㅎ	

Homology of finite sample is different from homology of underlying manifold, hence it cannot be directly used for the inference.

- When analyzing data, we prefer robust features where features of the underlying manifold can be inferred from features of finite samples.
- Homology is not robust:

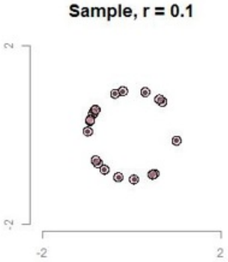


Underlying circle: $\beta_0 = 1$, $\beta_1 = 1$



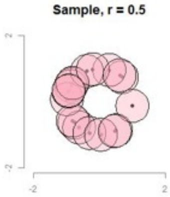
100 samples: $\beta_0 = 100$, $\beta_1 = 0$

Persistent homology computes homologies on collection of sets, and tracks when topological features are born and when they die.

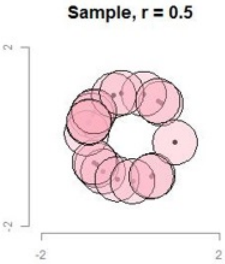

Sample, r = 0.1

Augmented Set

Persistent homology computes homologies on collection of sets, and tracks when topological features are born and when they die.



r=**0.5** : 1-dim hole is formed



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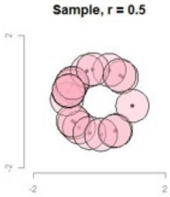
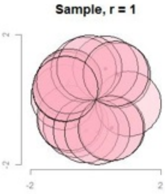
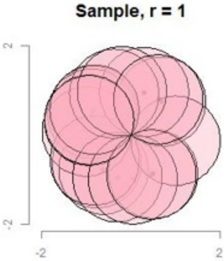


r=**0.5** : 1-dim hole is formed



r=**1** : 1-dim hole died



Augmented Set

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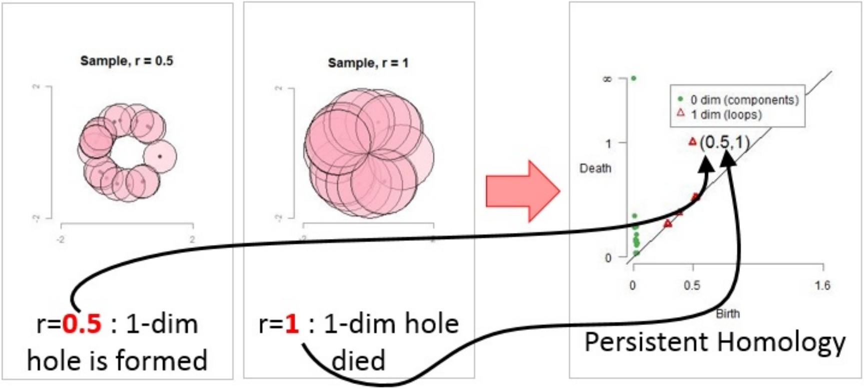


r=**0.5** : 1-dim hole is formed

r=**1** : 1-dim hole died

Persistent Homology

We rely on the superlevel sets of the kernel density estimator to extract topological information of the underlying distribution.

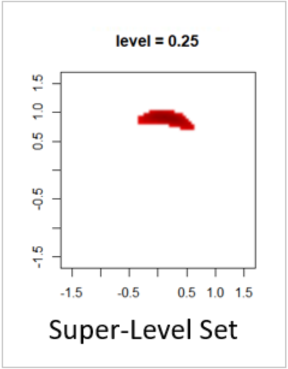
- The kernel density estimator is

$$\hat{p}_h(x) = \frac{1}{nh^m} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right).$$

- We look at superlevel sets of the kernel density estimator as

$$\left\{x \in \mathbb{R}^m : \hat{p}_h(x) \geq L\right\}_{L>0}.$$

Persistent homology computes homologies on collection of sets, and tracks when topological features are born and when they die.



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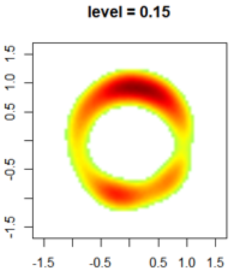
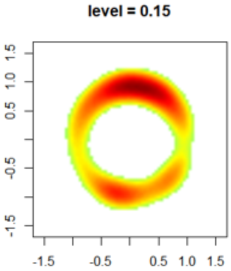
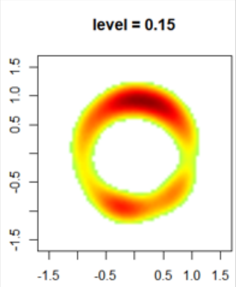


L=0.15 : 1-dim hole is formed

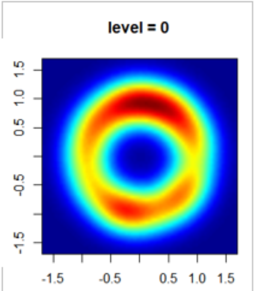


Super-Level Set

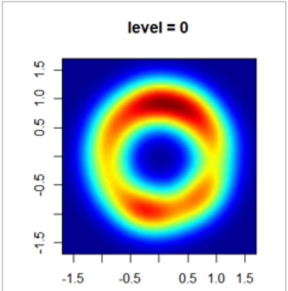
Persistent homology computes homologies on collection of sets, and tracks when topological features are born and when they die.



L=**0.15** : 1-dim hole is formed

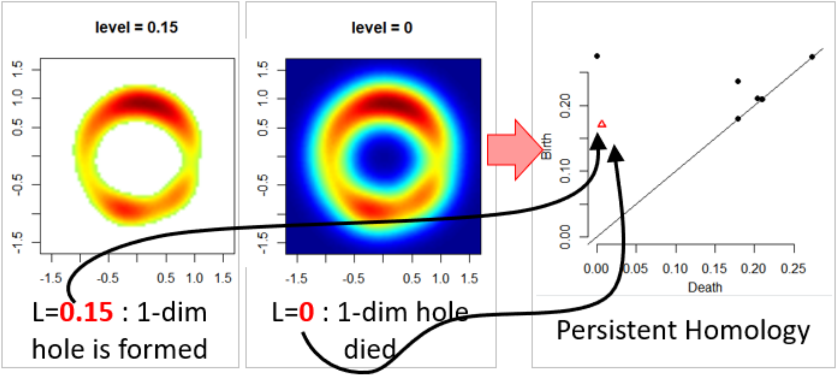


L=**0** : 1-dim hole died



Super-Level Set

Persistent homology computes homologies on collection of sets, and tracks when topological features are born and when they die.

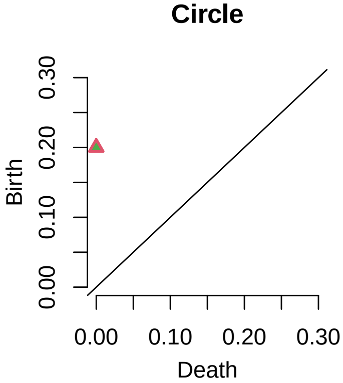


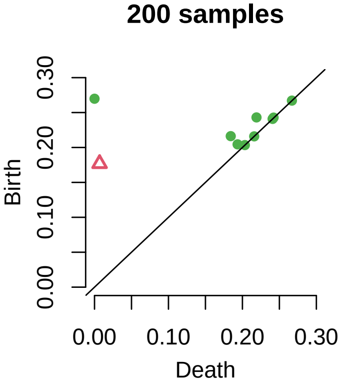
L=0.15 : 1-dim hole is formed

L=0 : 1-dim hole died

Persistent Homology

Persistent homology of the underlying manifold can be inferred from persistent homology of finite samples.





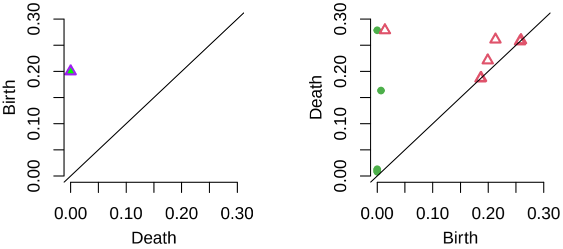
Bottleneck distance gives a metric on the space of persistent homology.

Definition

Let $D_1,\, D_2$ be multiset of points. Bottleneck distance is defined as

$$d_B(D_1,\, D_2) = \inf_{\gamma} \sup_{x \in D_\mathbf{1}} \|x - \gamma(x)\|_\infty,$$

where γ ranges over all bijections from D_1 to D_2.



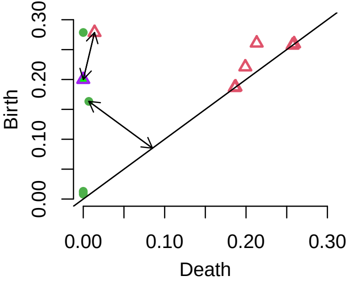
Bottleneck distance gives a metric on the space of persistent homology.

Definition

Let D_1, D_2 be multiset of points. Bottleneck distance is defined as

$$d_B(D_1,\, D_2) = \inf_{\gamma} \sup_{x \in D_\mathbf{1}} \|x - \gamma(x)\|_\infty,$$

where γ ranges over all bijections from D_1 to D_2.



Bottleneck distance can be controlled by the corresponding distance on functions: Stability Theorem.

Theorem

[Edelsbrunner and Harer, 2010][Chazal, de Silva, Glisse, and Oudot, 2012] Let $\mathbb{X}$ be finitely triangulable space and $f,\ g : \mathbb{X} \to \mathbb{R}$ be two continuous functions. Let $Dgm(f)$ and $Dgm(g)$ be corresponding persistence diagrams. Then

$$d_B(Dgm(f), Dgm(g)) \leq \|f - g\|_\infty.$$

Introduction

Minimax Rates for Geometric Parameters of a Manifold

- Minimax Rates for Estimating the Dimension of a Manifold
- The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

Topological Data Analysis: Persistent Homology

Statistical Inference for Persistent Homology

Application of Topological Data Analysis to Machine Learning

- Featurization of Topological Data Analysis using Persistence Landscapes

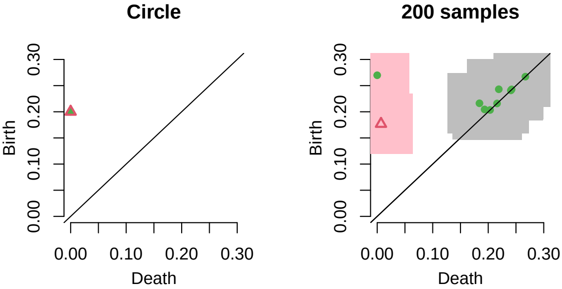
Statistical inference for persistent homology.

- Confidence sets for persistence diagrams (Fasy, Lecci, Rinaldo, Wasserman, Balakrishnan, Singh, 2014)

Confidence set for the persistent homology is a random set containing the persistent homology with high probability.

Let M be a compact manifold, and $X = \{X_1, \cdots, X_n\}$ be n samples. Let f_M and f_X be corresponding functions whose persistent homology is of interest. Given the significance level $\alpha \in (0,1)$, $(1-\alpha)$ confidence band $c_n = c_n(X)$ is a random variable satisfying

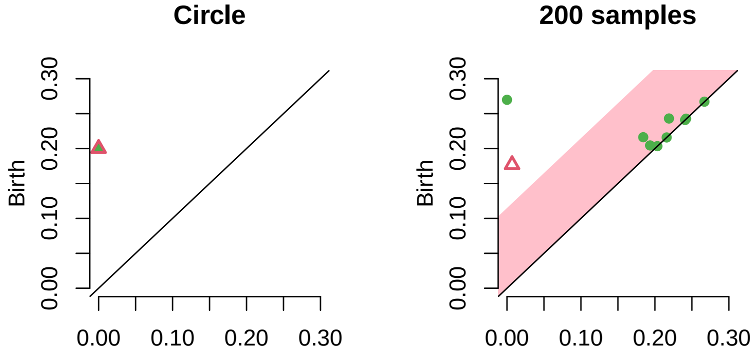
$$\mathbb{P}\left(Dgm(f_M) \in \{\mathcal{D} : d_B(\mathcal{D}, Dgm(f_X)) \leq c_n\}\right) \geq 1 - \alpha.$$



Confidence band for persistent homology separates homological signal from homological noise.

Let M be a compact manifold, and $X = \{X_1, \cdots, X_n\}$ be n samples. Let f_M and f_X be corresponding functions whose persistent homology is of interest. Given the significance level $\alpha \in (0,1)$, $(1-\alpha)$ confidence band $c_n = c_n(X)$ is a random variable satisfying

$$\mathbb{P}\left(d_B(Dgm(f_M),\, Dgm(f_X)) \le c_n\right) \ge 1 - \alpha.$$



Confidence band for the persistent homology can be obtained by the corresponding confidence band for functions.

From Stability Theorem, $\mathbb{P}\left(||f_M - f_X|| \leq c_n\right) \geq 1 - \alpha$ implies

$$\mathbb{P}\left(d_B(Dgm(f_M),\, Dgm(f_X)) \leq c_n\right) \geq \mathbb{P}\left(||f_M - f_X||_\infty \leq c_n\right) \geq 1 - \alpha,$$

so the confidence band of corresponding functions f_M can be used for confidene band of persistent homologies $Dgm(f_M)$.

Confidence band for the persistent homology can be computed using the bootstrap algorithm.

1. Given a sample $X = \{x_1, \dots, x_n\}$, compute the kernel density estimator $\hat{p}_h$.
2. Draw $X^* = \{x_1^*, \dots, x_n^*\}$ from $X = \{x_1, \dots, x_n\}$ (with replacement), and compute $\theta^* = \sqrt{nh^m}||\hat{p}_h^*(x) - \hat{p}_h(x)||_\infty$, where $\hat{p}_h^*$ is the density estimator computed using X^*.
3. Repeat the previous step B times to obtain $\theta_1^*, \dots, \theta_B^*$
4. Compute $\hat{z}_\alpha = \inf \left\{ q : \frac{1}{B} \sum_{j=1}^{B} I(\theta_j^* \geq q) \leq \alpha \right\}$
5. The $(1-\alpha)$ confidence band for $\mathbb{E}[p_h]$ is $\left[\hat{p}_h - \frac{\hat{z}_\alpha}{\sqrt{nh^m}} \, , \, \hat{p}_h + \frac{\hat{z}_\alpha}{\sqrt{nh^m}} \right]$.

Introduction

Minimax Rates for Geometric Parameters of a Manifold

- Minimax Rates for Estimating the Dimension of a Manifold
- The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

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Statistical Inference for Persistent Homology

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(Very rough) sketch to Machine Learning

- For a given task and data, Machine Learning / Deep Learning fits a parametrized model.
  - Given data X,
  - Parametrized model f_θ,
  - Loss function $\mathcal{L}$ tailored to the task,
  - Machine Learning minimizes $\arg\min_\theta \mathcal{L}(f_\theta, \mathcal{X})$.
- Many cases, getting explicit formula for $\arg\min_\theta \mathcal{L}(f_\theta, \mathcal{X})$ is impossible or too costly (e.g., inverting a large scale matrix). So, gradient descent is used with the $\nabla_\theta \mathcal{L}(f_\theta, \mathcal{X})$:

$$\theta_{n+1} = \theta_n - \lambda \nabla_\theta \mathcal{L}(f_\theta, \mathcal{X}).$$

Application of Topological Data Analysis to Machine Learning

- Application of Topological Data Analysis to Machine Learning is usually in two directions:
  - using TDA as features, so that the data X is augmented with extra TDA features : more common
  - Loss function $\mathcal{L}$ is accompanied with topological loss terms : recently received attentions

Introduction

Minimax Rates for Geometric Parameters of a Manifold

- Minimax Rates for Estimating the Dimension of a Manifold
- The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

Topological Data Analysis: Persistent Homology

Statistical Inference for Persistent Homology

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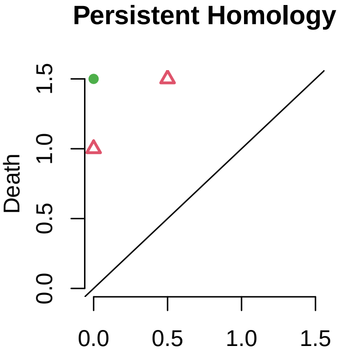
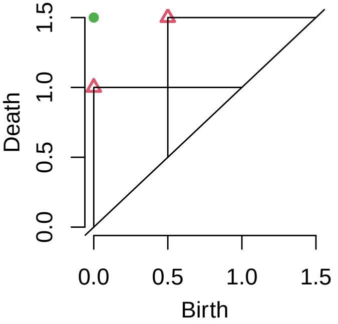
Persistent homology is further summarized and embedded into a Euclidean space or a functional space.

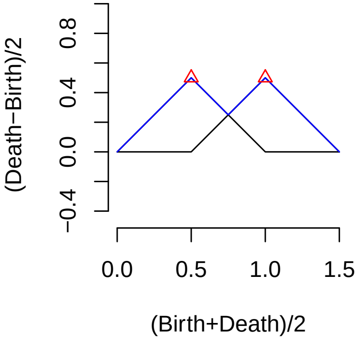
- The space of the persistent homology is complex, so directly applying in machine learning is difficult.
- If the persistent homology is further summarized and embedded into a Euclidean space or a functional space, then applying in machine learning becomes much more convenient.
    - e.g., Persistence Landscape, Persistence Silhouette, Persistence Image



Persistence Landscape is a functional summary of the persistent homology.



Persistent Homology



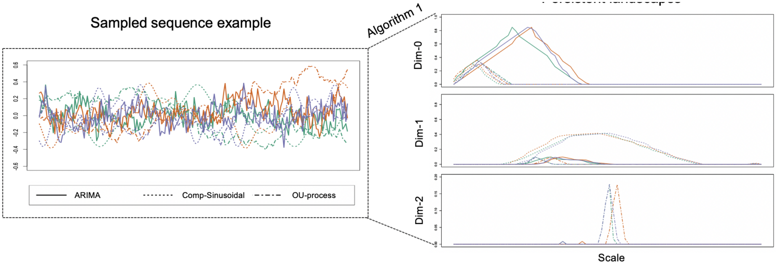
Landscape

Featurizing using Persistence Landscape

- Featurization using time-delayed embedding and Persistence Landscape
    - Time Series Featurization via Topological Data Analysis (Kim, Kim, Rinaldo, Chazal, 2020)
- Build topological layer using Persistence Landscape
    - PLLay: Efficient Topological Layer based on Persistence Landscapes (Kim, Kim, Zaheer, Kim, Chazal, Wasserman, 2020)

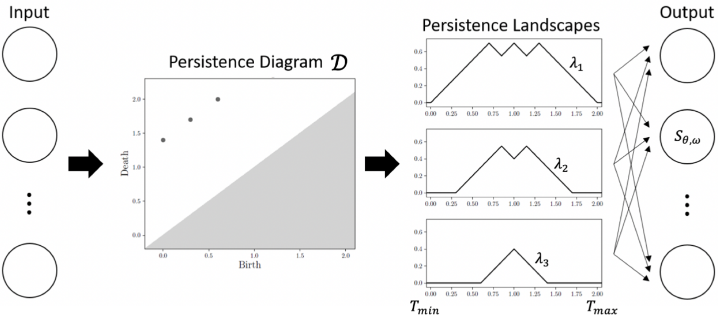
Featurization using time-delayed embedding and Persistence Landscape

1. From time series data $x = \{x_0, \cdots, x_N\} \subset \mathbb{R}$, construct the point cloud $X \subset \mathbb{R}^m$ using the time-delayed embedding.
2. Perform PCA(Principal Component Analysis) on X and obtain $X^\ell \subset \mathbb{R}^l$.
3. Construct the Vietoris-Rips filtration R_{X^l} and compute the persistence diagram $Dgm(X^l)$.
4. From $Dgm(X^l)$, compute the persistence landscape $\lambda : \mathbb{N} \times \mathbb{R} \to \mathbb{R}$, and vectorize to get $\lambda^K \in \mathbb{R}^K$.
5. Perform PCA on λ^K and get $\lambda^k \in \mathbb{R}^k$.

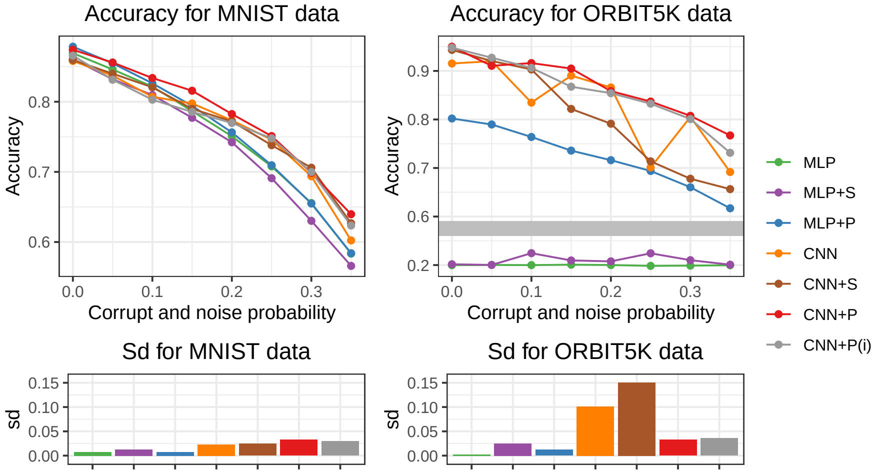


Build topological layer using Persistence Landscape

1. From data X, choose an appropriate simplicial complex K and a function f to compute the Persistece diagram $\mathcal{D}$.
2. From the persistence diagram $\mathcal{D}$, compute the persistence landscape $\lambda : \mathbb{N} \times \mathbb{R} \to \mathbb{R}$.
3. Compute the weighted average function $\bar{\lambda}_\omega(t) := \sum_{k=1}^{K_{\max}} \omega_k \lambda_k(t)$, and vectorize to get $\bar{\Lambda}_\omega \in \mathbb{R}^m$.
4. For a parametrized differentiable map $g_\theta : \mathbb{R}^m \to \mathbb{R}$, compute $S_{\theta,\omega}(\mathcal{D}) := g_\theta(\bar{\Lambda}_\omega)$.



Build topological layer using Persistence Landscape



Thank you!

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- Regularity conditions
- Upper Bound
- Lower Bound
- Upper Bound and Lower Bound for General Case

The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

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- Reach estimator and its analysis
- Minimax Estimates

References

Minimax Rates for Estimating the Dimension of a Manifold

- Regularity conditions
- Upper Bound
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The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

- Reach and its Geometry
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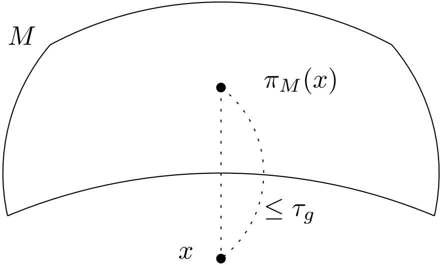
References

The supporting manifold M is assumed to be bounded.

$$M \subset I := [-K_I, K_I]^m \subset \mathbb{R}^m \text{ with } K_I \in (0, \infty)$$

The reach is assumed to be lower bounded to avoid an arbitrarily complicated manifold.

- $\mathcal{P}$ is a set of distributions P that is supported on a bounded manifold M, with its reach $\tau(M) \geq \tau_g$, and with other regularity assumptions.



The reach is assumed to be lower bounded to avoid an arbitrarily complicated manifold.

- M is of local reach $\geq \tau_\ell$, if for all points $p \in M$, there exists a neighborhood $U_p \subset M$ such that U_p is of reach $\geq \tau_\ell$.

Density is bounded away from ∞ with respect to the uniform measure.

- Distribution P is absolutely continuous to induced Lebesgue measure vol_M, and $\frac{dP}{dvol_M} \leq K_p$ for fixed K_p.
- This implies that the distribution on the manifold is of essential dimension d.
- $\mathcal{P}^d_{\kappa_l,\kappa_g,K_p}$ denotes set of distributions P that is supported on d-dimensional manifold of (global) reach $\geq \tau_g$, local reach $\geq \tau_\ell$, and density is bounded by K_p.

Minimax Rates for Estimating the Dimension of a Manifold

- Regularity conditions
- Upper Bound
- Lower Bound
- Upper Bound and Lower Bound for General Case

The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

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Our Estimator has Maximum Risk of $O\left(n^{-\left(\frac{d_2}{d_1}-1\right)n}\right)$.

- Our estimator makes error with probability at most $O\left(n^{-\left(\frac{d_2}{d_1}-1\right)n}\right)$ if intrinsic dimension is d_2.
- Our estimator is always correct when the intrinsic dimension is d_1.

Our Estimator makes Error with Probability at most $O\left(n^{-\left(\frac{d_2}{d_1}-1\right)n}\right)$ if Intrinsic Dimension is d_2.

- Based on the following lemma:

Lemma

(Lemma 6) Let $X_1, \cdots, X_n \sim P \in \mathcal{P}^{\boldsymbol{d_2}}_{\kappa_l, \kappa_g, K_p}$, then

$$P^{(n)}\left[\sum_{i=1}^{n-1} \|X_{i+1} - X_i\|^{\boldsymbol{d_1}} \leq L\right] \lesssim n^{-\frac{\boldsymbol{d_2}}{\boldsymbol{d_1}} n}.$$

Our Estimator is always Correct when the Intrinsic Dimension is d_1.

- Based on following lemma:

Lemma

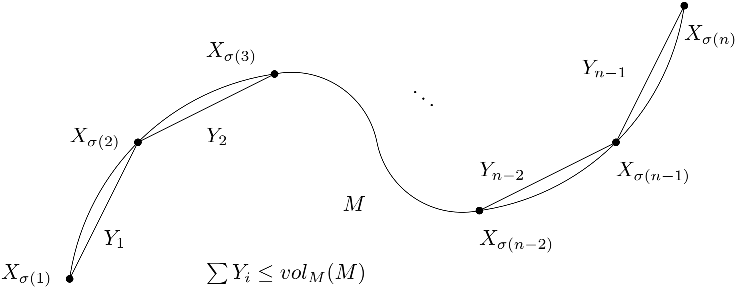
(Lemma 7) Let M be a d_1-dimensional manifold with global reach $\geq \tau_g$ and local reach $\geq \tau_\ell$, and $X_1, \cdots, X_n \in M$. Then there exists C which depends only on m, d_1 and K_l, and there exists $\sigma \in S_n$ such that

$$\sum_{i=1}^{n-1} \|X_{\sigma(i+1)} - X_{\sigma(i)}\|_{\mathbb{R}^m}^{d_1} \leq C.$$

Our estimator is always correct when the intrinsic dimension is d_1.

$$\sum_{i=1}^{n-1} \|X_{\sigma(i+1)} - X_{\sigma(i)}\|_{\mathbb{R}^m}^{\boldsymbol{d_1}} \leq C.$$

- When $d_1 = 1$ so that the manifold is a curve, length of TSP path is bounded by length of curve $vol_M(M)$.

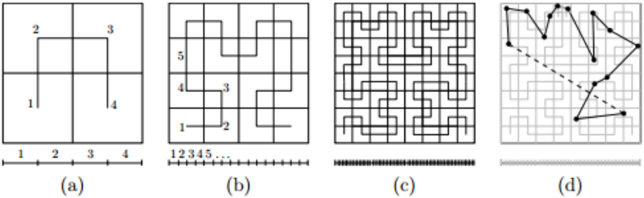


- Global reach$\geq \tau_g$ implies $vol_M(M)$ is bounded.

Our estimator is always correct when the intrinsic dimension is d_1.

$$\sum_{i=1}^{n-1} \|X_{\sigma(i+1)} - X_{\sigma(i)}\|_{\mathbb{R}^m}^{d_1} \leq C.$$

- When $d_1 > 1$, Several conditions implied by regularity conditions combined with Hölder continuity of d_1-dimensional space-filling curve is used.



Our estimator is always correct when the intrinsic dimension is d_1.

$$\sum_{i=1}^{n-1} \|X_{\sigma(i+1)} - X_{\sigma(i)}\|_{\mathbb{R}^m}^{d_1} \leq C.$$

- When $d_1 > 1$, Several conditions implied by regularity conditions combined with Hölder continuity of d_1-dimensional space-filling curve is used.

Lemma

(Lemma 22, Space-filling curve) There exists surjective map $\psi_d : \mathbb{R} \to \mathbb{R}^d$ which is Hölder continuous of order $1/d$, i.e.

$$0 \leq \forall s, t \leq 1, \ \|\psi_d(s) - \psi_d(t)\|_{\mathbb{R}^d} \leq 2\sqrt{d+3}|s-t|^{1/d}.$$

Minimax Rates for Estimating the Dimension of a Manifold

- Regularity conditions
- Upper Bound
- Lower Bound
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The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

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- Reach estimator and its analysis
- Minimax Estimates

References

A subset $T \subset [-K_I, K_I]^n$ and set of distributions $\mathcal{P}_1^{d_1}$, $\mathcal{P}_2^{d_2}$ are found so that, whenever $X = (X_1, \cdots, X_n) \in T$, we cannot distinguish two models.

- The lower bound measures how hard it is to tell whether the data come from a d_1 or d_2 -dimensional manifold.
- T, $\mathcal{P}_1^{\boldsymbol{d_1}}$ and $\mathcal{P}_2^{\boldsymbol{d_2}}$ are linked to the lower bound by using Le Cam's lemma.

Le Cam's Lemma provides lower bounds based on the minimum of two densities $q_1 \wedge q_2$, where q_1, q_2 are in convex hull of $\mathcal{P}_1^{d_1}$ and convex hull of $\mathcal{P}_2^{d_2}$, respectively.

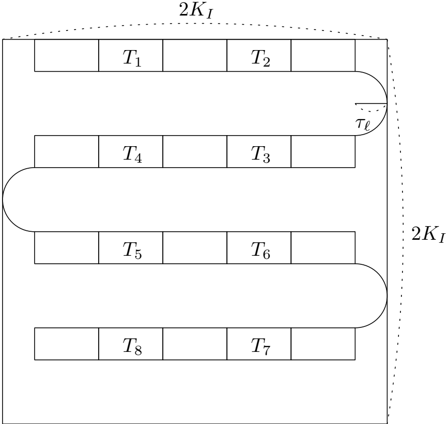
Lemma

(Lemma 10, Le Cam's Lemma) Let $\mathcal{P}$ be a set of probability measures, and $\mathcal{P}^{\mathbf{d_1}}, \mathcal{P}^{\mathbf{d_2}} \subset \mathcal{P}$ be such that for all $P \in \mathcal{P}^{d_i}$, $\theta(P) = \theta_i$ for $i = 1, 2$. For any $Q_i \in co(\mathcal{P}_i)$, let q_i be density of Q_i with respect to measure ν. Then

$$\inf_{\hat{\theta}} \sup_{P \in \mathcal{P}} \mathbb{E}_P \left[1 \left(\hat{\dim}_n(X) \neq \dim(P) \right) \right] \geq \frac{1(\theta_1 \neq \theta_2)}{4} \sup_{Q_i \in co(\mathcal{P}^{d_i})} \int [q_1(x) \wedge q_2(x)] d\nu(x$$

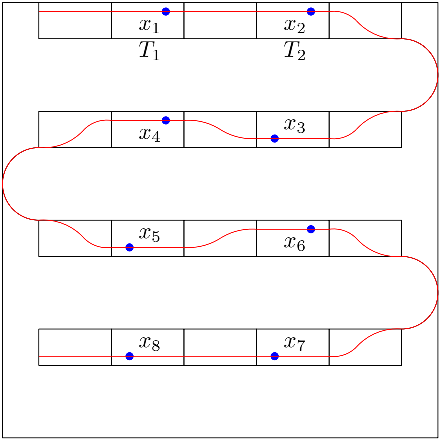
T is constructed so that for any $x = (x_1, \cdots, x_n) \in T$, there exists a d_1-dimensional manifold that satisfies regularity conditions and passes through $x_1, \cdots, x_n$.

- T_i's are cylinder sets in $[-K_I, K_I]^{d_2}$, and then T is constructed as $T = S_n \prod_{i=1}^{n} T_i$, where the permutation group S_n acts on $\prod_{i=1}^{n} T_i$ as a coordinate change.



T is constructed so that for any $x = (x_1, \cdots, x_n) \in T$, there exists a d_1-dimensional manifold that satisfies regularity conditions and passes through $x_1, \cdots, x_n$.

- Given $x_1, \cdots, x_n \in T$ (blue points), manifold of global reach $\geq \tau_g$ and local reach $\geq \tau_\ell$ (red line) passes through $x_1, \cdots, x_n$.



$\mathcal{P}_1^{d_1}$ is constructed as set of distributions that are supported on manifolds that passes through $x_1, \cdots, x_n$ for $x = (x_1, \cdots, x_n) \in T$, and $\mathcal{P}_2^{d_2}$ is a singleton set consisting of the uniform distirbution on $[-K_I, K_I]^{d_2}$.

If $X \in T$, it is hard to determine whether X is sampled from distribution P in either $\mathcal{P}_1^{d_1}$ or $\mathcal{P}_2^{d_2}$.

- There exists $Q_1 \in co(\mathcal{P}_1^{d_1})$ and $Q_2 \in co(\mathcal{P}_2^{d_2})$ such that $q_1(x) \geq Cq_2(x)$ for every $x \in T$ with $C < 1$.
- Then $q_1(x) \wedge q_2(x) \geq Cq_2(x)$ if $x \in T$, so $C \int_T q_2(x)dx$ can serve as lower bound of minimax rate.
- Based on following claim:

Claim

(Claim 25) Let $T = S_n \prod_{i=1}^{n} T_i$. Then for all $x \in \operatorname{int} T$, there exists $C > 0$ that depends only on κ_I, K_I, and $r_x > 0$ such that for all $r < r_x$,

$$Q_1\left(B(x_i, r)\right) \geq CQ_2\left(B(x_i, r)\right).$$

Minimax Rates for Estimating the Dimension of a Manifold

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- Upper Bound
- Lower Bound
- Upper Bound and Lower Bound for General Case

The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

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References

Multinary Classification and $0 - 1$ Loss are Considered.

- $$R_n = \inf_{\hat{\dim}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[1 \left(\hat{\dim}_n(X) \neq \dim(P) \right) \right]$$
- Now the manifolds are of any dimensions between 1 and m, so considered distribution set is $\mathcal{P} = \bigcup_{d=1}^{m} \mathcal{P}^d$.
- $0 - 1$ loss function is considered, so for all $x, y \in \mathbb{R}$, $\ell(x, y) = I(x = y)$.

Mimimax Rate is Upper Bounded by $O\left(n^{-\frac{1}{m-1}n}\right)$, and Lower Bounded by $\Omega\left(n^{-2n}\right)$.

Proposition

(Proposition 16 and 17)

$$n^{-2n} \lesssim \inf_{\hat{\dim}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^{(n)}} \left[1 \left(\hat{\dim}_n \neq \dim(P) \right) \right] \lesssim n^{-\frac{\mathbf{1}}{m-\mathbf{1}}n}.$$

Minimax Rates for Estimating the Dimension of a Manifold

- Regularity conditions
- Upper Bound
- Lower Bound
- Upper Bound and Lower Bound for General Case

The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

- Reach and its Geometry
- Reach estimator and its analysis
- Minimax Estimates

References

Minimax Rates for Estimating the Dimension of a Manifold

- Regularity conditions
- Upper Bound
- Lower Bound
- Upper Bound and Lower Bound for General Case

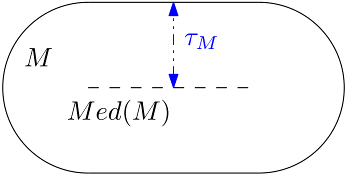
The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

- Reach and its Geometry
- Reach estimator and its analysis
- Minimax Estimates

References

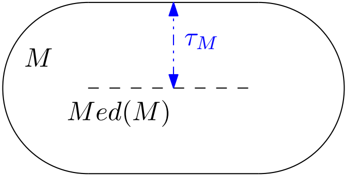
The medial axis of a set M is the set of points that have at least two nearest neighbors on the set M.

- $$Med(M) = \{z \in \mathbb{R}^m : \text{ there exists } p \neq q \in M \text{ with } \|p - z\| = \|q - z\| = d(z, M)\}.$$



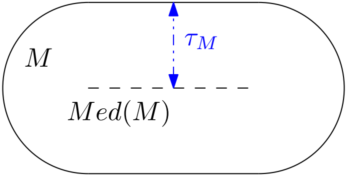
The reach of M, denoted by τ_M, is the minimum distance from $Med(M)$ to M.

- $$\tau_M = \inf_{x \in Med(M), y \in M} \|x - y\| .$$



The reach τ_M gives the maximum offset size of M on which the projection is well defined.

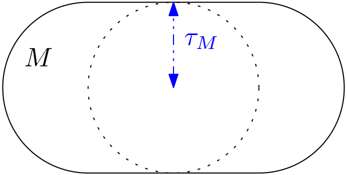
- $$\tau_M = \inf_{x \in Med(M), y \in M} \|x - y\|.$$



The reach τ_M gives the maximum radius of a ball that you can roll over M.

- When $M \subset \mathbb{R}^m$ is a manifold,

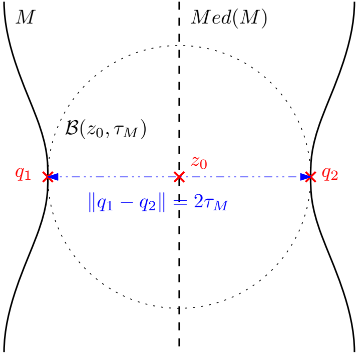
$$\tau_M = \inf_{q_2 \neq q_1 \in M} \frac{\|q_2 - q_1\|^2}{2d(q_2 - q_1, T_{q_1}M)}.$$



The bottleneck is a geometric structure where the manifold is nearly self-intersecting.

Definition

(Definition 3.1) A pair of points (q_1, q_2) in M is said to be a bottleneck of M if there exists $z_0 \in Med(M)$ such that $q_1, q_2 \in \mathcal{B}(z_0, \tau_M)$ and $\|q_1 - q_2\| = 2\tau_M$.

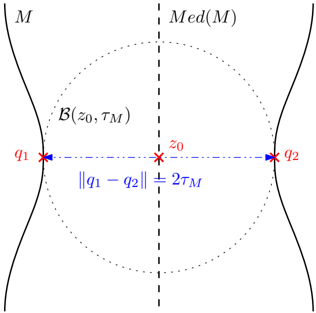


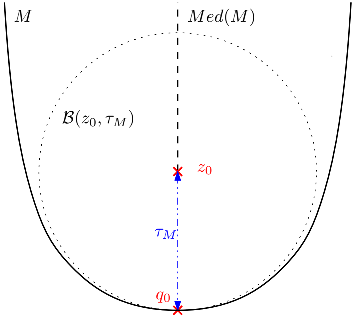
The reach is attained either from the bottleneck (global case) or the area of high curvature (local case).

Theorem

(Theorem 3.4) At least one of the following two assertions holds:

- *(Global Case) M has a bottleneck $(q_1, q_2) \in M^2$.*
- *(Local case) There exists $q_0 \in M$ and an arc-length parametrized γ_0 such that $\gamma_0(0) = q_0$ and $\|\gamma_0''(0)\| = \frac{1}{\tau_M}$.*





Minimax Rates for Estimating the Dimension of a Manifold

Regularity conditions

Upper Bound

Lower Bound

Upper Bound and Lower Bound for General Case

The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

Reach and its Geometry

Reach estimator and its analysis

Minimax Estimates

References

The statistical efficiency of the reach estimator $\hat{\tau}$ is analyzed through its risk.

- The risk of the estimator $\hat{\tau}$ is the expected loss the estimator.

$$\mathbb{E}_{P^{(n)}}\left[\ell\left(\hat{\tau}(\mathcal{X}),\ \tau_M\right)\right].$$

  - $\mathcal{X} = \{X_1, \ldots, X_n\}$ is drawn from a fixed distribution P with its support M.
  - The loss function used is $\ell(\tau, \tau') = \left|\frac{1}{\tau} - \frac{1}{\tau'}\right|^p$, $p \geq 1$.

The risk of the reach estimator $\hat{\tau}$ is analyzed.

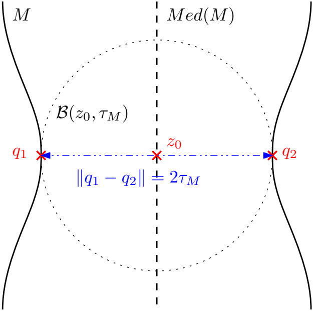
- The risk of the estimator $\hat{\tau}$ is the expected loss the estimator

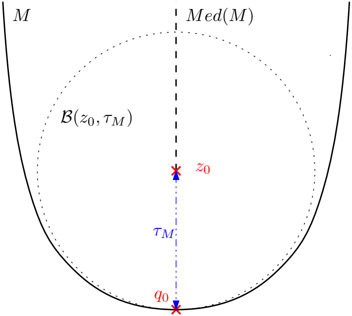
$$\mathbb{E}_{P^{(n)}}\left[\left|\frac{1}{\tau_M} - \frac{1}{\hat{\tau}(\mathcal{X})}\right|^q\right].$$

  - $\mathcal{X} = \{X_1, \ldots, X_n\}$ is drawn from a fixed distribution P with its support M.
  - The loss function used is $\ell(\tau, \tau') = \left|\frac{1}{\tau} - \frac{1}{\tau'}\right|^q$, $q \geq 1$.

The reach estimator has the risk of $O\left(n^{-\frac{2q}{3d-1}}\right)$.

- The reach estimator has the risk of $O\left(n^{-\frac{q}{d}}\right)$ for the global case.
- The reach estimator has the risk of $O\left(n^{-\frac{\mathbf{2q}}{\mathbf{3d-1}}}\right)$ for the local case.



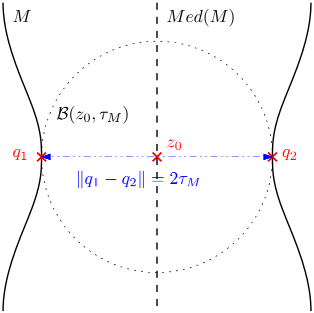


The reach estimator has the maximum risk of $O\left(n^{-\frac{q}{d}}\right)$ for the global case.

Proposition

(Proposition 4.3) Assume that the support M has a bottleneck. Then,

$$\mathbb{E}_{P^n}\left[\left|\frac{1}{\tau_M} - \frac{1}{\hat{\tau}(\mathcal{X})}\right|^q\right] \lesssim n^{-\frac{q}{d}}.$$

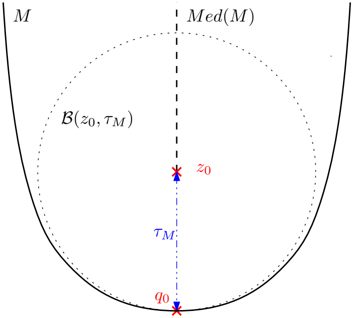


The reach estimator has the maximum risk of $O\left(n^{-\frac{2q}{3d-1}}\right)$ for the local case.

Proposition

(Proposition 4.7) Suppose there exists $q_0 \in M$ and a geodesic γ_0 with $\gamma_0(0) = q_0$ and $\|\gamma_0''(0)\| = \frac{1}{\tau_M}$. Then,

$$\mathbb{E}_{P^n}\left[\left|\frac{1}{\tau_M} - \frac{1}{\hat{\tau}(\mathcal{X})}\right|^q\right] \lesssim n^{-\frac{2q}{3d-1}}.$$



Minimax Rates for Estimating the Dimension of a Manifold

- Regularity conditions
- Upper Bound
- Lower Bound
- Upper Bound and Lower Bound for General Case

The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

- Reach and its Geometry
- Reach estimator and its analysis
- Minimax Estimates

References

The statistical difficulty of the reach estimation problem is analyzed by the minimax rate.

- Minimax rate is the risk of an estimator that performs best in the worst case, as a function of sample size.
- $$R_n = \inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^n} \left[\ell \left(\hat{\tau}_n(\mathcal{X}),\ \tau_M \right) \right].$$
  - $\mathcal{X} = \{X_1, \ldots, X_n\}$ is drawn from a fixed distribution P with its support M, where P is contained in set of distributions $\mathcal{P}$.
  - An estimator $\hat{\tau}_n$ is any function of data $\mathcal{X}$.
  - The loss function used is $\ell(\tau, \tau') = \left| \frac{1}{\tau} - \frac{1}{\tau'} \right|^q$, $q \geq 1$.

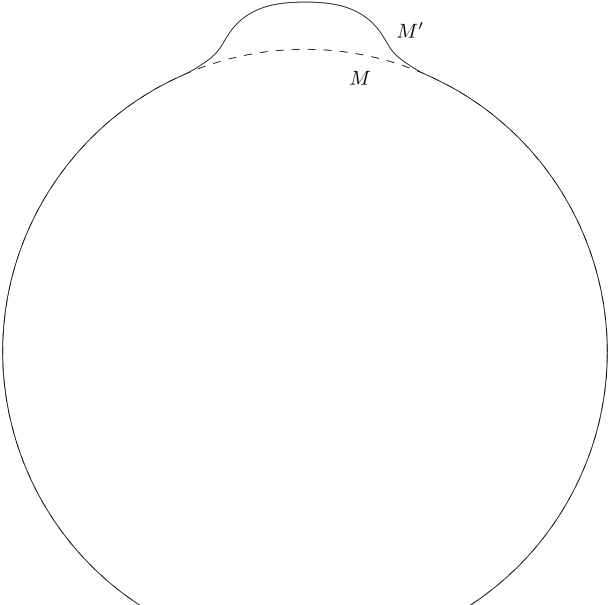
The statistical difficulty of the reach estimation problem is analyzed by the minimax rate.

- Minimax rate is the risk of an estimator that performs best in the worst case, as a function of sample size.
- $$R_n = \inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^n} \left[\left| \frac{1}{\tau_M} - \frac{1}{\hat{\tau}_n(\mathcal{X})} \right|^q \right].$$
  - $\mathcal{X} = \{X_1, \ldots, X_n\}$ is drawn from a fixed distribution P with its support M, where P is contained in set of distributions $\mathcal{P}$.
  - An estimator $\hat{\tau}_n$ is any function of data $\mathcal{X}$.
  - The loss function used is $\ell(\tau, \tau') = \left| \frac{1}{\tau} - \frac{1}{\tau'} \right|^q$, $q \geq 1$.

Two distributions P, P' are found so that their reaches differ but they are statistically difficult to distinguish.

- $$\inf_{\hat{\tau}_n} \sup_{P \in \mathcal{P}} \mathbb{E}_{P^n} \left[\left| \frac{1}{\tau_M} - \frac{1}{\hat{\tau}_n} \right|^q \right] \gtrsim \left| \frac{1}{\tau_M} - \frac{1}{\tau_{M'}} \right|^q (1 - TV(P, P'))^{2n} .$$
- The lower bound measures how hard it is to tell whether the data is from distributions with different reaches.
- P and P' are found so that $\left| \frac{1}{\tau_M} - \frac{1}{\tau_{M'}} \right|^q$ is large while $(1 - TV(P, P'))^{2n}$ is small.

P is a distribution supported on a sphere while P' is a distribution supported on a bumped sphere.



Minimax Rates for Estimating the Dimension of a Manifold

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- Upper Bound
- Lower Bound
- Upper Bound and Lower Bound for General Case

The Origin of the Reach: Better Understanding Regularity Through Minimax Estimation Theory

- Reach and its Geometry
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- Minimax Estimates

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