Statistical Inference for Topological Data Analysis

Jisu KIM

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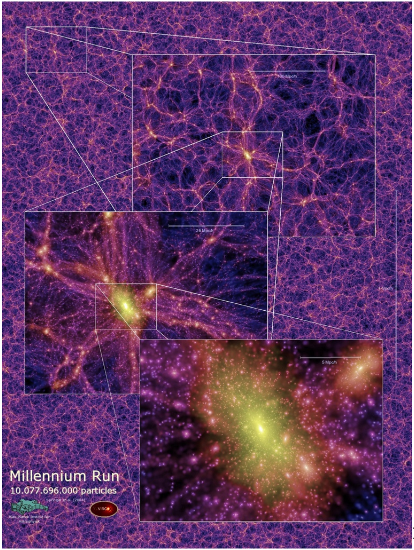
Topological structures in the data provide information.



[1]

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

Persistent Homology: observe topological structure with multi resolutions.

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- Georges Seurat, A Sunday afternoon on the island of La Grande Jatte (Un dimanche après-midi à l'Île de la Grande Jatte)

Statistic Inference for Topological Data Analysis is explored.

- 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, 2021)
- Statistical Inference for Persistent Homology
  - Confidence sets for persistence diagrams (Fasy, Lecci, Rinaldo, Wasserman, Balakrishnan, Singh, 2014)

The number of holes is used to summarize topological features.

- Geometrical objects:
  - A, B, C, D, E, F, G, H, I, J, K, L, M, O, P, Q, R, S, T, U, V, W, X, Y, Z, IJ
- 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) 

Example : Objects are classified by homologies.

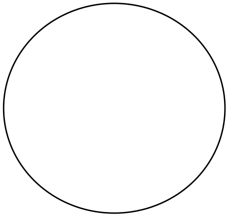
1. β_0 =# of connected components 
2. β_1 =# of loops (holes inside 1-dim sphere) 

$\beta_0 \setminus \beta_1$	0	1	2
1	C, E, F, G, H, I, J, K, L, M, N, S, T, U, V, W, X, Y, Z	A, D, O, P, Q, R	B
2	IJ		

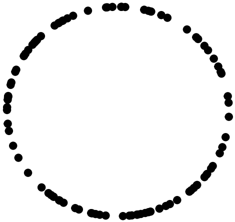
Homology of finite sample is different from homology of underlying manifold, hence it cannot be directly used for the inference.

- 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:

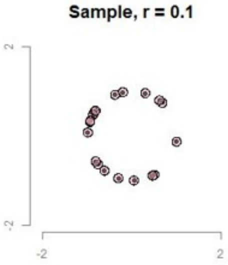
Underlying circle: $\beta_0 = 1$, $\beta_1 = 1$



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.



Augmented Set

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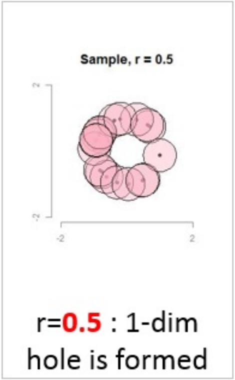

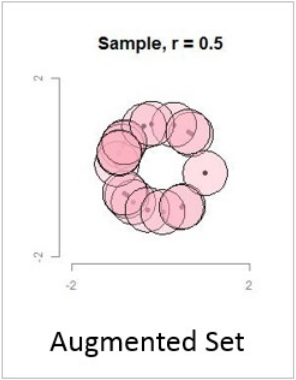

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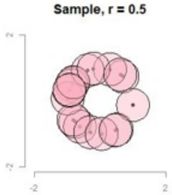
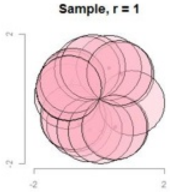
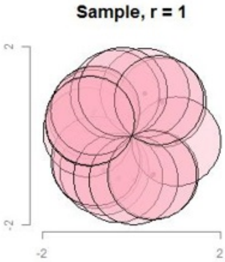


r=**0.5** : 1-dim hole is formed



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



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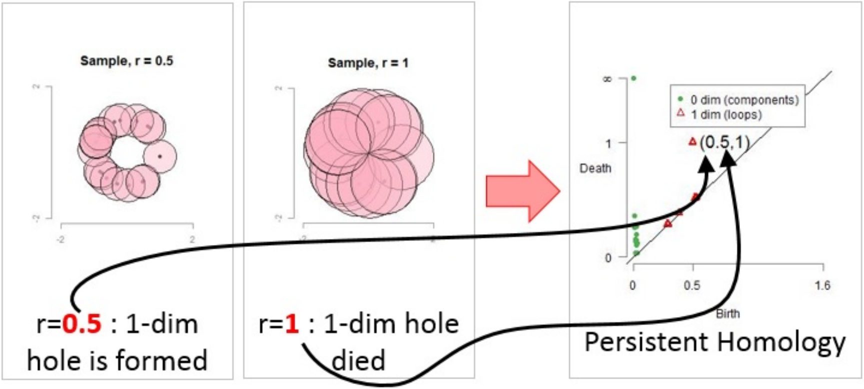

We rely on the superlevel sets of the kernel density estimator to extract topological information of the underlying distribution.

- The kernel density estimator is

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

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

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

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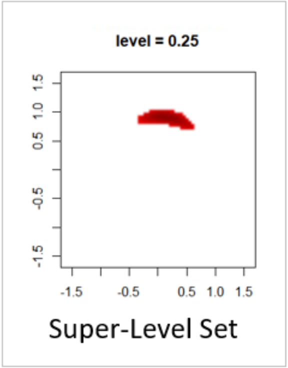

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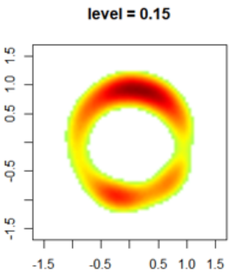
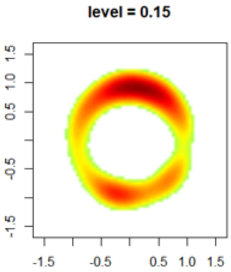
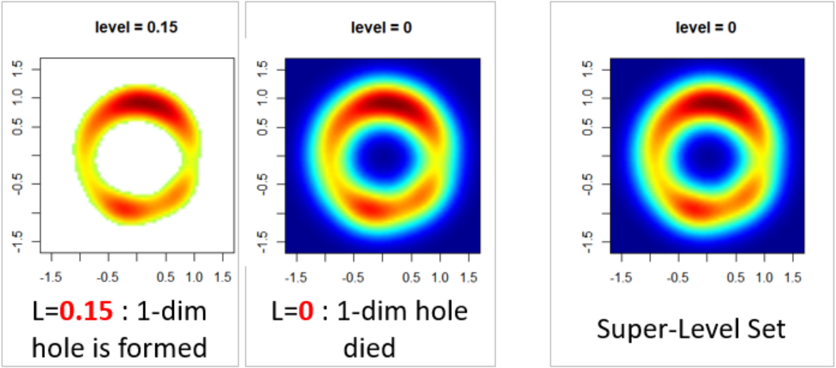


L=**0.15** : 1-dim hole is formed



Super-Level Set

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



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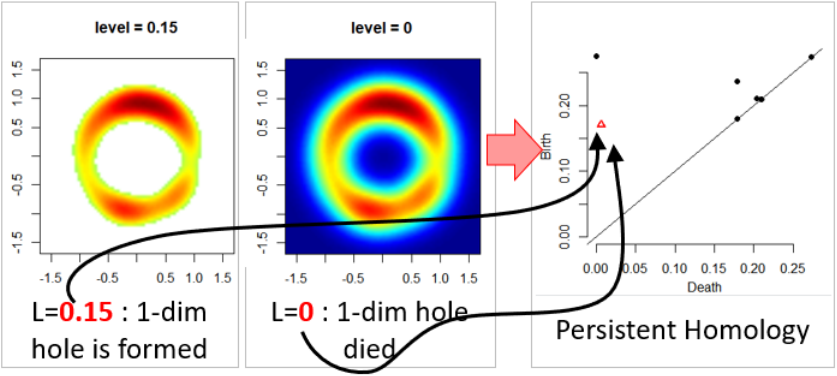
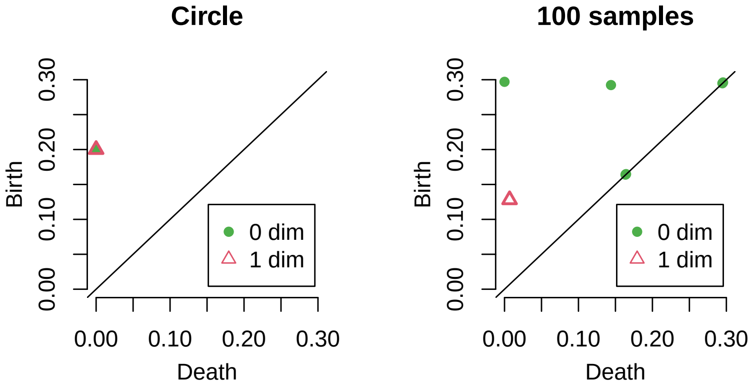


Persistent homology of the underlying manifold can be inferred from persistent homology of finite samples.



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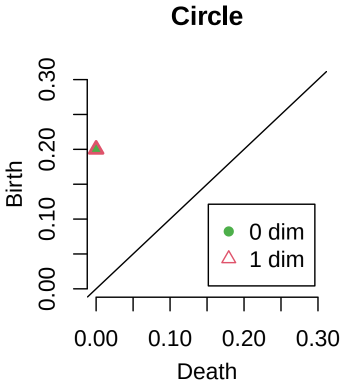

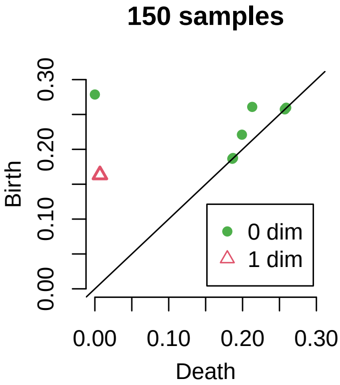

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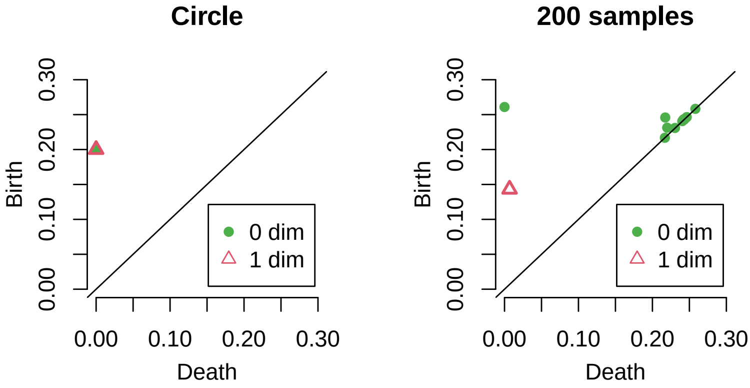

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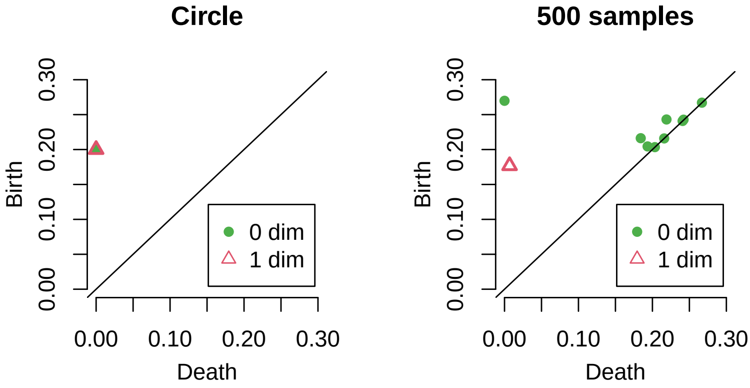
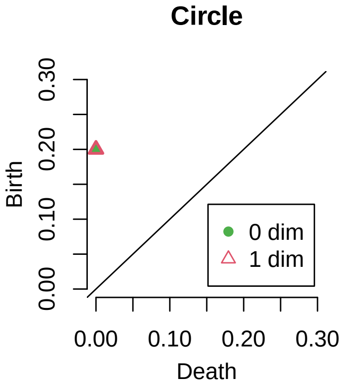
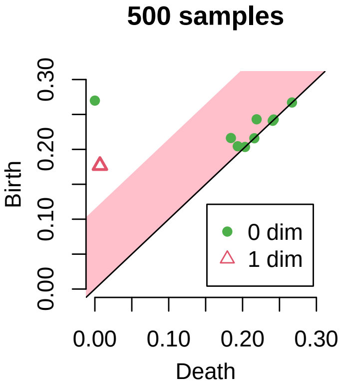


Statistically significant homological features can be distinguished from statistically insignificant ones.

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





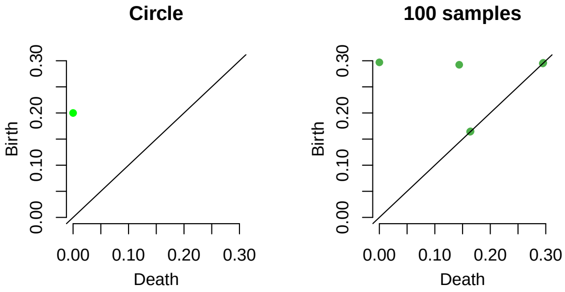
Bottleneck distance gives a metric on the space of persistent homology.

Definition

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

$$W_\infty(D_1, D_2) = \inf_{\gamma} \sup_{x \in D_1} \|x - \gamma(x)\|_\infty,$$

where γ ranges over all bijections from D_1 to D_2.



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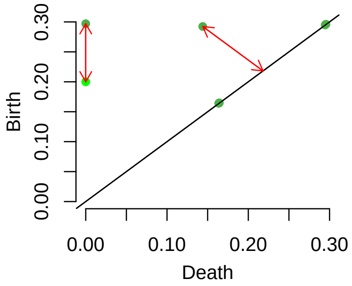

$$\sup_{x \in D_1} \|x - \gamma_1(x)\|_\infty = 0.1$$

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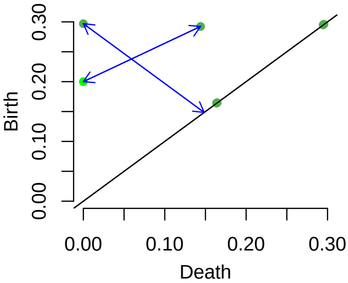

$$\sup_{x \in D_1} \|x - \gamma_2(x)\|_\infty = 0.15$$

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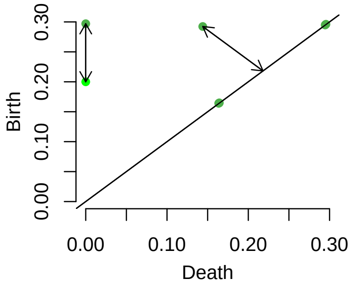
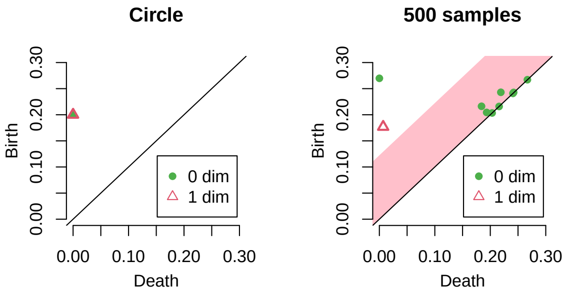


$$\inf_\gamma \sup_{x \in D_1} \|x - \gamma(x)\|_\infty = 0.1$$

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

Let $Dgm(M)$ and $Dgm(X)$ be persistent homologies of the manifold M and the data X, respectively. Given the significance level $\alpha \in (0,1)$, $(1-\alpha)$ confidence band $c_n = c_n(X)$ is a random variable satisfying

$$\mathbb{P}\left(W_\infty(Dgm(M),\, Dgm(X)) \leq c_n\right) \geq 1 - \alpha.$$



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

1. Given a sample $X = \{x_1, \ldots, x_n\}$, compute the kernel density estimator $\hat{p}_h$.
2. Draw $X^* = \{x_1^*, \ldots, x_n^*\}$ from $X = \{x_1, \ldots, x_n\}$ (with replacement), and compute $\theta^* = \sqrt{nh^d}||\hat{p}_h^*(x) - \hat{p}_h(x)||_\infty$, where $\hat{p}_h^*$ is the density estimator computed using X^*.
3. Repeat the previous step B times to obtain $\theta_1^*, \ldots, \theta_B^*$
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 $\mathbb{E}[\hat{p}_h]$ is $\left[\hat{p}_h - \frac{\hat{z}_\alpha}{\sqrt{nh^d}}\ ,\ \hat{p}_h + \frac{\hat{z}_\alpha}{\sqrt{nh^d}}\right]$.

Reference I

Frédéric Chazal and Bertrand Michel. An introduction to topological data analysis: Fundamental and practical aspects for data scientists. *Frontiers Artif. Intell.*, 4:667963, 2021. doi: 10.3389/frai.2021.667963. URL `https://doi.org/10.3389/frai.2021.667963`.

Frédéric Chazal, Vin de Silva, Marc Glisse, and Steve Oudot. The structure and stability of persistence modules. *arXiv preprint arXiv:1207.3674*, 2012.

Frédéric Chazal, Brittany Terese Fasy, Fabrizio Lecci, Bertrand Michel, Alessandro Rinaldo, and Larry Wasserman. Robust topological inference: Distance-to-a-measure and kernel distance. *Technical Report*, 2014.

Herbert Edelsbrunner and John L. Harer. *Computational topology*. American Mathematical Society, Providence, RI, 2010. ISBN 978-0-8218-4925-5. doi: 10.1090/mbk/069. URL `https://doi.org/10.1090/mbk/069`. An introduction.

Reference II

Brittany Terese Fasy, Fabrizio Lecci, Alessandro Rinaldo, Larry Wasserman, Sivaraman Balakrishnan, and Aarti Singh. Confidence sets for persistence diagrams. *Ann. Statist.*, 42(6):2301–2339, 2014. ISSN 0090-5364. doi: 10.1214/14-AOS1252. URL `https://doi.org/10.1214/14-AOS1252`.

Larry Wasserman. Topological data analysis, 2016.

Thank you!

Persistent Homology

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

Theorem

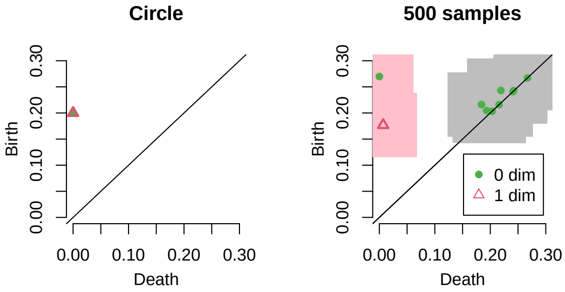
[Edelsbrunner and Harer, 2010][Chazal, de Silva, Glisse, and Oudot, 2012] Let $\mathbb{X}$ be finitely triangulable space and $f,\ g : \mathbb{X} \to \mathbb{R}$ be two continuous functions. Let $Dgm(f)$ and $Dgm(g)$ be corresponding persistence diagrams. Then

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

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

Let $Dgm(M)$ and $Dgm(X)$ be persistent homologies of the manifold M and the data X, respectively. Given the significance level $\alpha \in (0, 1)$, $(1 - \alpha)$ confidence set $\{D \in Dgm : \; W_\infty(Dgm(X), \, D) \leq c_n\}$ is a random set satisfying

$$\mathbb{P}\left(Dgm(M) \in \{D \in Dgm : \; W_\infty(Dgm(X), \, D) \leq c_n\}\right) \geq 1 - \alpha.$$



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

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

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

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.

Bootstrap algorithm can be applied to peristent homology.

- for the case of kernel density estimator in Fasy et al. [2014],
- for the case of distance to measure and kernel distance in Chazal et al. [2014].