Statistical Shape Analysis using Topological Data Analysis

Part II: Representation and Modeling

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Outline

Various Representations of Persistence Diagrams

Although persistence diagrams include topological persistence signal information, it cannot be directly used as input in data analysis

- Euclidean space
  - Summary function (Adcock et al., 2016)
  - Binning (Bendich et al., 2016)
  - Persistence image (Adams et al., 2017)
- L^2-space
  - Persistence landscape (Bubenik, 2015)
  - Persistence intensity function (Chen et al., 2015)
- Reproducing kernel Hilbert space
  - Persistence scale-space kernel (Reininghaus et al., 2015)
  - Persistence weighted Gaussian kernel (Kusano et al., 2016)

Representation using Summary Functions

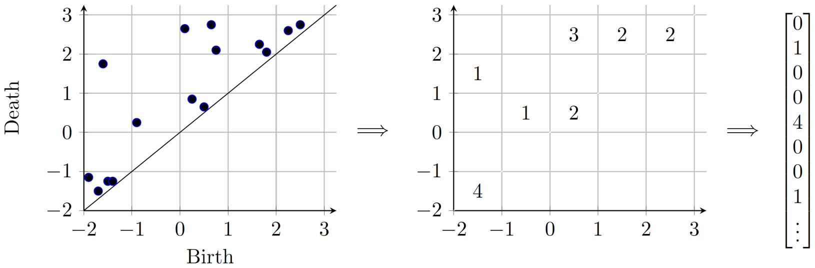
- Proposed by Adcock et al. (2016)
- Summarize birth, death, and persistence (death−birth)
  - Mean, median
  - Min, max
  - The n largest values
- Polynomials

$$\sum_i x_i(y_i - x_i),$$
$$\sum_i (y_{max} - y_i)(y_i - x_i),$$
$$\sum_i x_i^2(y_i - x_i)^4,$$
$$\sum_i (y_{max} - y_i)^2(y_i - x_i)^4,$$

- Easy to compute
- Difficult to interpret

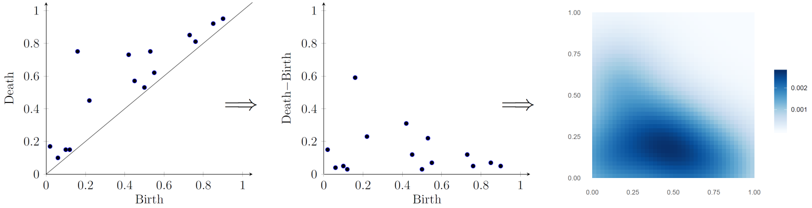
Vectorization by Binning

- Proposed by Bendich et al. (2016)
- Bin the persistence diagrams and count the number of points in each bin
- The representation by binning may not be stable



Persistence Image

- Proposed by Adams et al. (2017)
- Steps for generating persistence images
    1. Assigning weights to points
    2. Smoothing
    3. Converting to vector



Persistence Image

- Persistence diagram P is represented as persistence surface ρ_P

$$\rho_P(x,y) = \sum_{(b,d)\in P} g_{(b,d)}(x,y)\cdot w(b,d),$$

  where x and y are the (x,y)-coordinates of the persistence function, $g_{(b,d)}$ is a smoothing function for $(b,d) \in P$, and $w(b,d) \geq 0$ is a non-negative weight function
- The surface is discretized to a vector

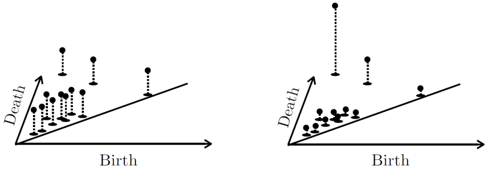
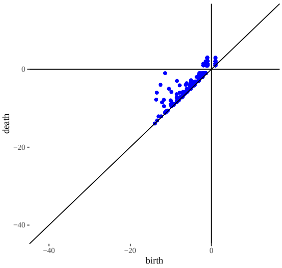
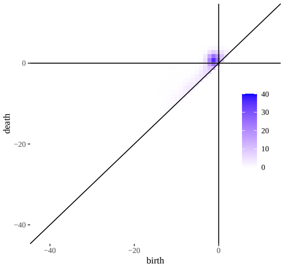


Figure: Unweighted vs. weighted persistence diagrams. Figure of Kusano et al. (2017).

Persistence Image Example

- Persistence image representation using the Gaussian smoothing function $g_{(b,d)}(x,y) = \frac{\exp\left[-\left((x-b)^2+(y-d)^2\right)\right]}{\sigma^2}$ with $\sigma = 1$ and the linear weight $w(b,d) = d - b$





Properties of Persistence Image

- Persistence image is a stable representation of persistence diagram with respect to 1-Wasserstein distance (Adams et al., 2017)

$$\|\rho_B - \rho_{B'}\|_\infty \leq \sqrt{10}\big(\|f\|_\infty |\nabla\phi| + \|\phi\|_\infty |\nabla f|\big) W_1(B, B').$$

- The persistence image can be used as an input of statistical models or ML algorithms
- Due to the high-dimensionality of persistence image, dimension reduction or feature selection is often required

Outline

Idea of Persistence Landscape

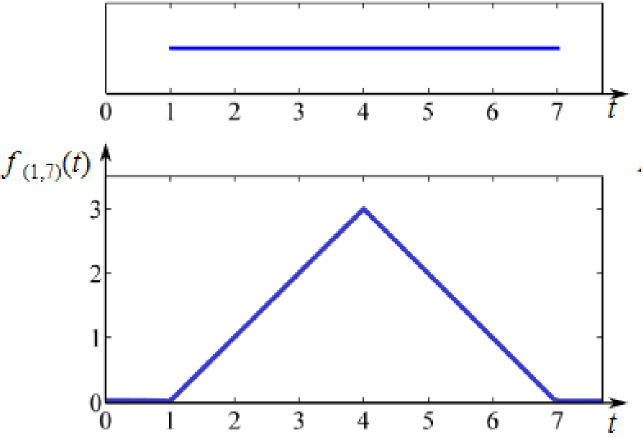


Figure: Figure from Kovacev-Nikolic et al. (2016)

Persistence Diagram

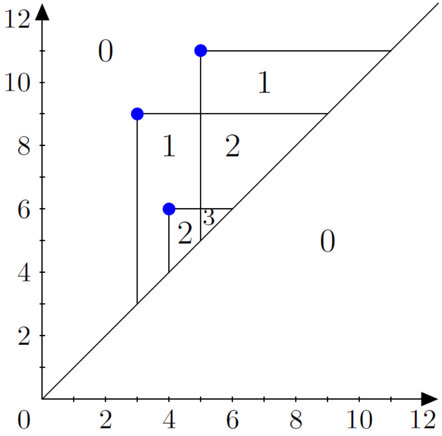


Figure: Figure from Bubenik (2015)

Persistence Landscape

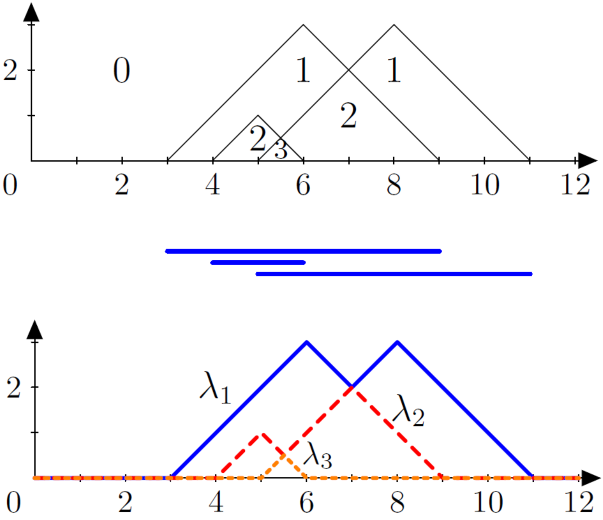


Figure: Figure from Bubenik (2015)

Persistence Landscape

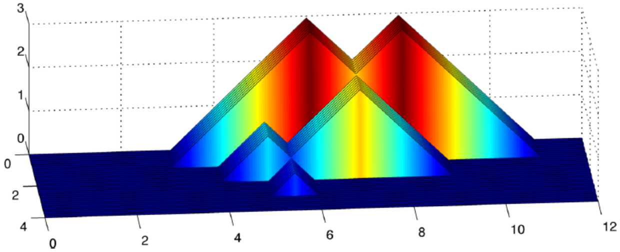


Figure: Figure from Bubenik (2015)

Persistence Landscape Example

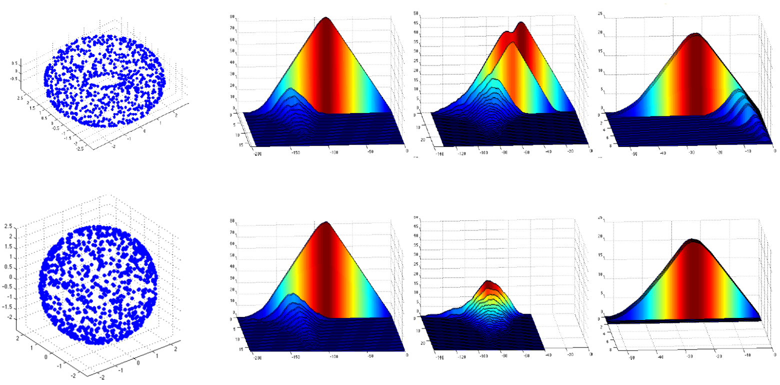


Figure: Figure from Bubenik (2015)

Properties of Persistence Landscape

- Persistence landscape is stable

Theorem 5.1 (∞-Landscape Stability Theorem). *Let $f, g : X \to \mathbb{R}$. Then*

$$\Lambda_\infty(M(f), M(g)) \leq \|f - g\|_\infty.$$

Theorem 5.5 (p-Landscape stability theorem). *Let X be a triangulable, compact metric space that implies bounded degree-k total persistence for some real number $k \geq 1$, and let f and g be two tame Lipschitz functions. Then*

$$\Lambda_p(D(f), D(g))^p \leq C\|f - g\|_\infty^{p-k},$$

for all $p \geq k$, where $C = C_X \max\{\mathrm{Lip}(f)^k, \mathrm{Lip}(g)^k, \mathrm{Lip}(f)^{k+1}, \mathrm{Lip}(g)^{k+1}\}(W_\infty(D, \emptyset) + \frac{1}{p+1})$.

Properties of Persistence Landscape

- Mean persistence landscape exists: pointwise average
- SLLN and CLT holds for persistence landscape

mean landscape $\overline{\lambda(X)}_n$ is given by the pointwise mean.

$$\overline{\lambda(X)}_n(x,y) = \frac{1}{n}\sum_{i=1}^{n} \lambda(X_i)(x,y)$$

Theorem 3.4 (Strong Law of Large Numbers for persistence landscapes). $\overline{\lambda(X)}_n \to E(\lambda(X))$ *almost surely if and only if* $E\|\lambda(X)\| < \infty$.

Theorem 3.5 (Central Limit Theorem for peristence landscapes). *Assume* $\lambda(X) \in L^p(\mathcal{S})$ *with* $2 \leq p < \infty$. *If* $E\|\lambda(X)\| < \infty$ *and* $E(\|\lambda(X)\|^2) < \infty$ *then* $\sqrt{n}[\overline{\lambda(X)}_n - E(\lambda(X))]$ *converges weakly to a Gaussian random variable with the same covariance structure as* $\lambda(X)$.

Outline

Representation in Reproducing Kernel Hilbert Space

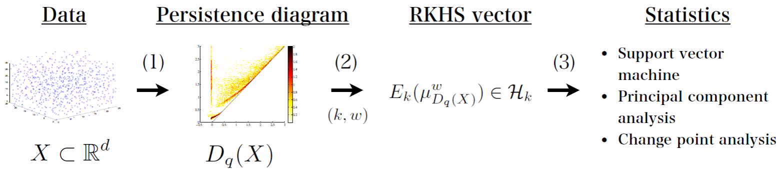


Figure: Figure from Kusano (2018)

- Persistence scale-space kernel (Reininghaus et al., 2015)
- Persistence weighted Gaussian kernel (PWGK) (Kusano, 2018)

Kernel Trick

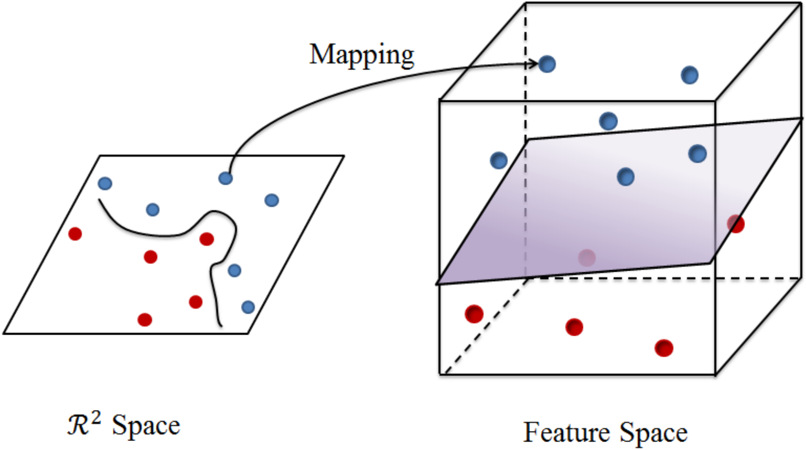


Figure: Figure from
`http://songcy.net/posts/story-of-basis-and-kernel-part-2/`

Kernel Trick

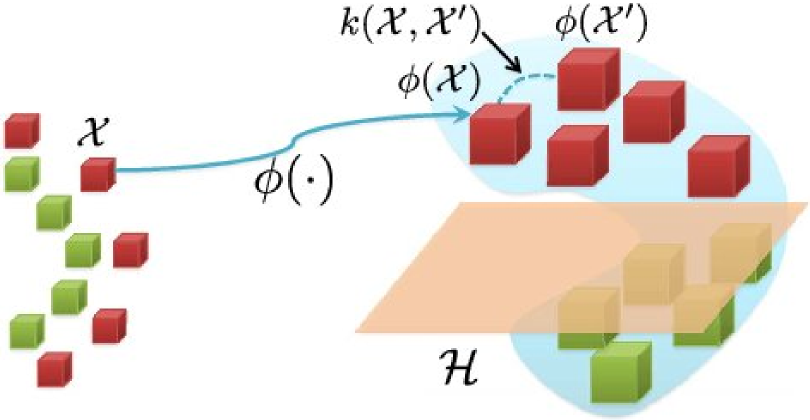


Figure: Figure from Zhao et al. (2013)

Kernel Methods

- Support vector machine
- Kernel ridge regression
- Kernel principal component analysis
- Gaussian process

Outline

Motivation

- How can we identify a signal from persistence homology results?

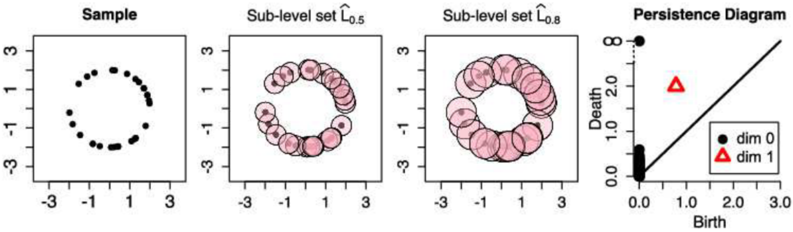


Figure: Figure from Fasy et al. (2014)

Confidence Sets for Persistence Diagram

- Proposed by Fasy et al. (2014)

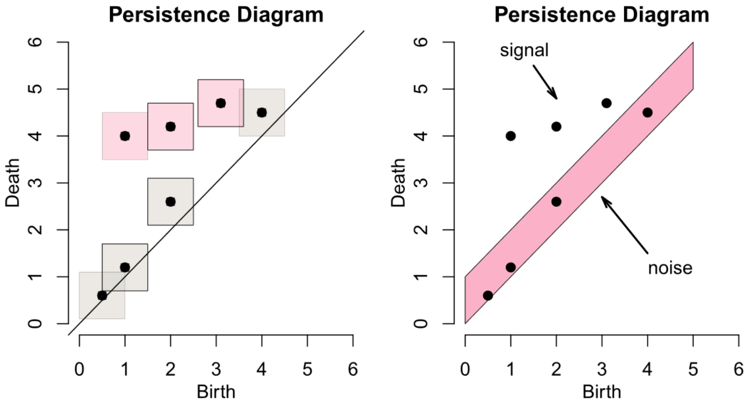


Figure: Figure from Fasy et al. (2014)

Confidence Set Example

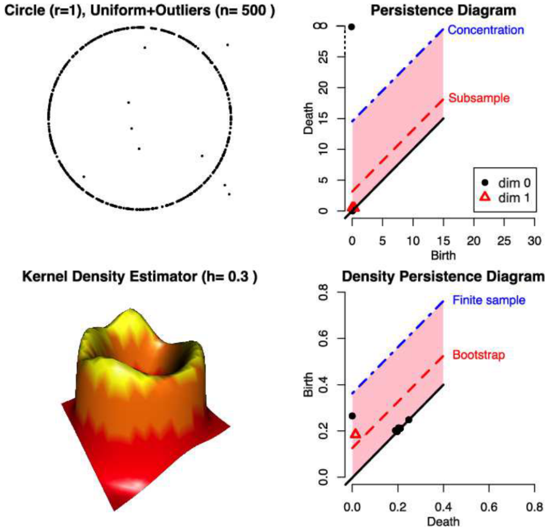


Figure: Figure from Fasy et al. (2014)

Bootstrap Band for Persistence Landscape

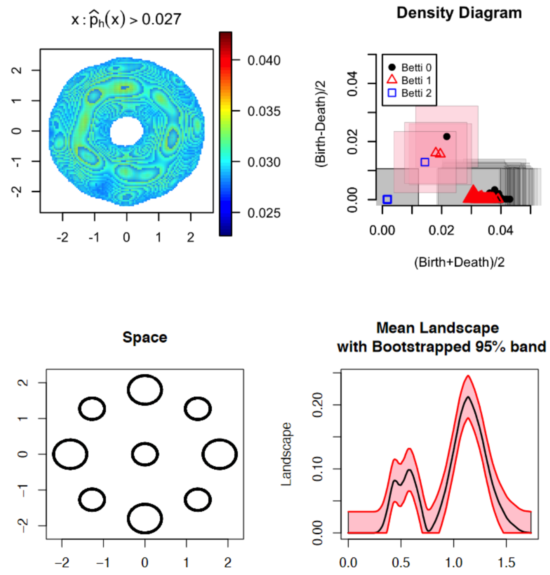
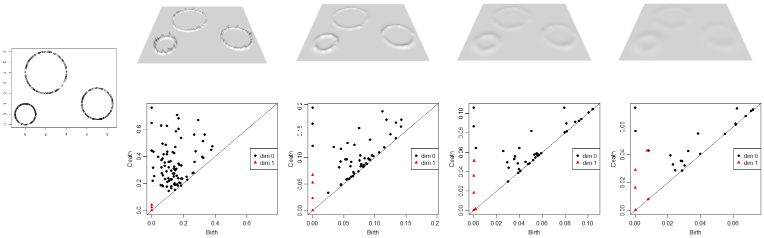


Figure: Figure from Chazal et al. (2013)

Significance for Point Cloud Data?

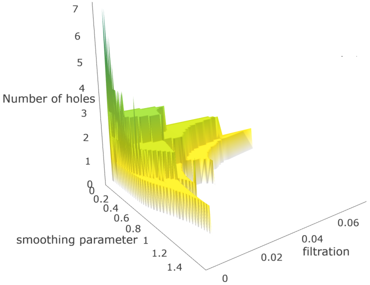
	Direct Estimation	Density Estimator
Pros	Fast and simple	Robust
Cons	Sensitive	Smoothing parameter selection
Significance	Size	Point density

- Use a range of smoothing parameters instead of a single smoothing parameter

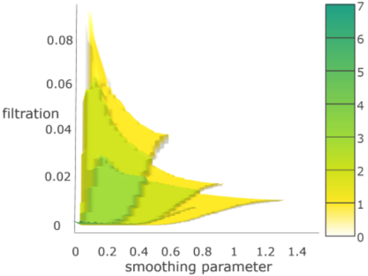


Persistence Terrace

- Persistence terrace is a 3D summary plot where features are represented as terrace layers (Moon et al., 2018)



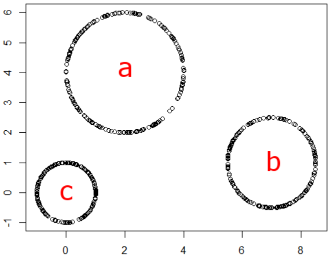
(a) Overall view

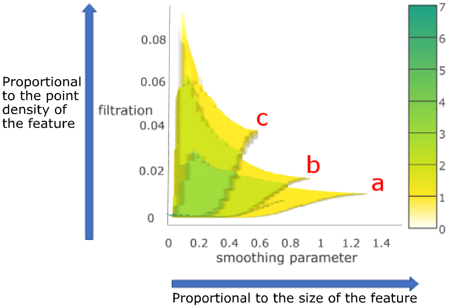


(b) Satellite view

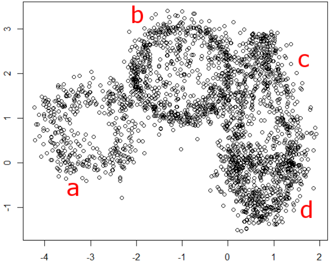
Interpretation of Persistence Terrace

- Robust inference of topological features while capturing both size point density information

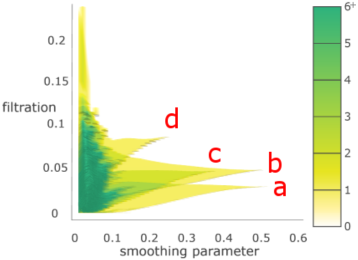




Persistence Terrace Example



(a) Scatterplot of noisy loops



(b) Dimension 1 persistence terrace

- Persistence terrace identifies four noisy loops
- The two large loops (square a and circle b) with different point density
- One slightly smaller loop (triangle c) and one smaller and denser loop (triangle d)

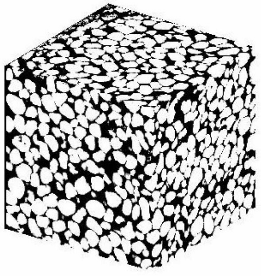
Additional Notes

- These approaches are based on the idea that the longer-surviving topological features are a signal and shorter-surviving topological features are noise
- However, short-surviving topological features may contain valuable information

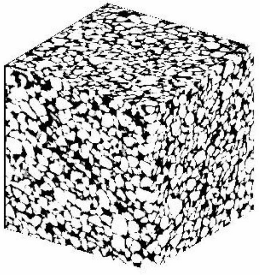
Outline

Motivating Example: Rock Comparison

- Data: three-dimensional rock images
- Scanned by a focus ion beam scanning electron microscopes



(a) Unground silica

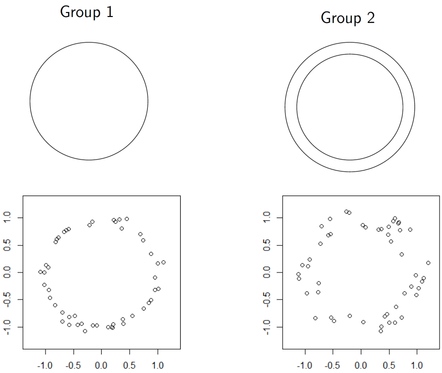


(b) Leavenseat sand

Figure: Figures of Talabi et al. (2009)

- We can summarize structure/connectivity information of rocks using topological data analysis
  - How can we compare based on topological characteristics?
  - Which topological features differ the most?

Toy Example



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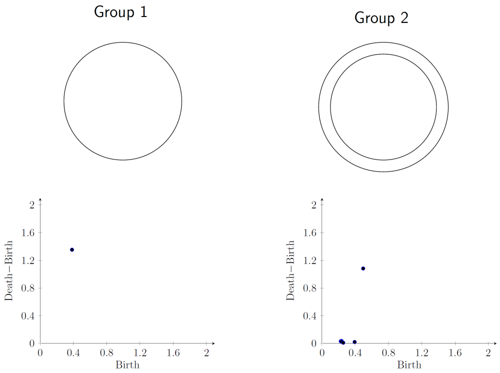

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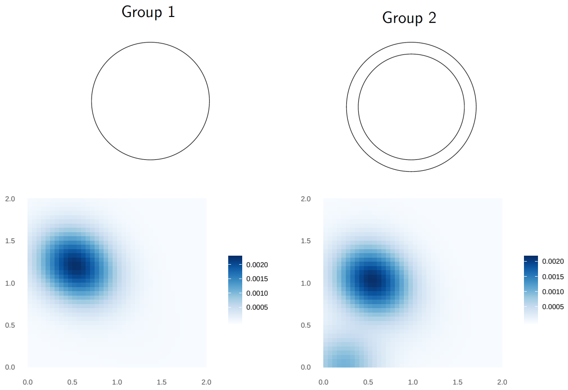
Toy Example



- How can we compare based on topological characteristics?
- Which topological features differ the most?

Permutation-based Hypothesis Test

Permutation test using Bottleneck/Wasserstein distances

- Two labels by Robinson and Turner (2017)
- Multiple labels using ANOVA by Cericola et al. (2018)
- Implementing multiple testing by Vejdemo-Johansson and Mukherjee (2018)

Algorithm S1 Permutation test (Robinson and Turner, 2017)

Input: Persistence diagrams, given group label $G_{\text{unshuffled}}$, number of repetitions N, joint loss function L

Output: Permutation p-value Z

Compute $L(G_{\text{unshuffled}})$

Create an empty vector L of size N

for $i = 1 \to N$ **do**

  Randomly generate shuffled group label G^i_{shuffled}

  $L[i] \leftarrow L(G^i_{\text{shuffled}})$

end for

$Z \leftarrow \text{sum}(L < L(G_{\text{unshuffled}}))/N$

Kernel Test

Kernel test using maximum mean discrepancy

- Kernel two-sample test of Gretton et al. (2006) is applied to TDA literature by Kusano (2018)

Definition 2 *Let $\mathcal{F}$ be a class of functions $f : \mathcal{X} \to \mathbb{R}$ and let p,q,x,y,X,Y be defined as above. We define the maximum mean discrepancy (MMD) as*

$$\mathrm{MMD}[\mathcal{F},p,q] := \sup_{f\in\mathcal{F}} \left(\mathbf{E}_x[f(x)] - \mathbf{E}_y[f(y)]\right). \tag{1}$$

In the statistics literature, this is known as an integral probability metric (Müller, 1997). A biased[2] *empirical estimate of the MMD is obtained by replacing the population expectations with empirical expectations computed on the samples X and Y,*

$$\mathrm{MMD}_b[\mathcal{F},X,Y] := \sup_{f\in\mathcal{F}} \left(\frac{1}{m}\sum_{i=1}^{m} f(x_i) - \frac{1}{n}\sum_{i=1}^{n} f(y_i)\right). \tag{2}$$

Some Limitations

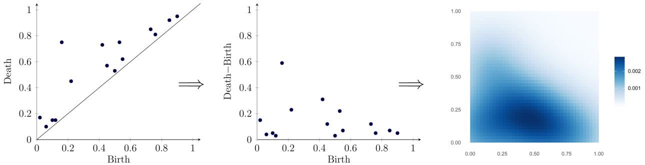
Permutation test using Bottleneck/Wasserstein distances

- High computation cost
- No information on which topological features contribute how much to the differences

Kernel test using maximum mean discrepancy

- No information on which topological features contribute how much to the differences

Two-stage Test using Persistence Image



Two-stage hypothesis test by Moon and Lazar (2020)

1. Filtering
   - Filter statistic: T^{I}
   - Filter pixels in the sparse region
   - Remove the pixel i if $\bar{X}^{i} < C^{th}$ percentile of $\bar{X}'s$
2. Testing
   - Test statistics: T^{II}
   - Control the false discovery rate using the q-value procedure by Storey (2002)

Hypothesis Test Example

- Generate two-dimensional pseudo-rock images using algorithm of Obayashi et al. (2018) using three sets of parameters: (M=180, S=80), (M=190, S=75), (M=200, S=70)
- 50 images for each parameter set

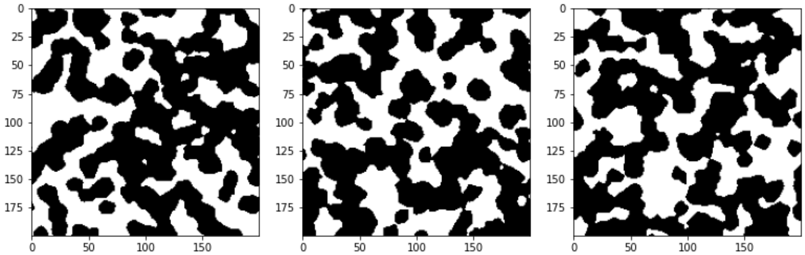


Figure: Examples of two-dimensional pseudo-rock images with parameters $(M = 180, S = 80)$ (left), $(M = 190, S = 75)$ (center), and $(M = 200, S = 70)$ (right).

Hypothesis Test Example

- Scenario 1 examines two groups of $(M = 180, S = 80)$ images
- Scenario 2 compares $(M = 180, S = 80)$ and $(M = 190, S = 75)$ groups
- Scenario 3 tests $(M = 180, S = 80)$ and $(M = 200, S = 70)$ groups

	Scenario 1		Scenario 2		Scenario 3	
	Dim 0	Dim 1	Dim 0	Dim 1	Dim 0	Dim 1
Two-stage test	0.763	0.798	0.121	0.792	0.003	0.019
Permutation test	0.520	0.700	0.090	0.475	0.000	0.000

Table: Minimum q-values of two-stage tests and p-values of permutation tests.

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