Stats and ML for Persistence

Lecture 14 - CMSE 890

Prof. Elizabeth Munch

Michigan State University
::
Dept of Computational Mathematics, Science & Engineering

Thurs, Oct 16, 2025

Goals for today

Goals for today:

- Today: ML for Persistence
- Sorta follows Ch 13.1 but not entirely

Questions and tasks

Tasks

- Classification
- Regression

The Issue

- Most ML methods want vectors in $\mathbb{R}^n$.
- That implies some sorting or ordering, which we don't want for the persistence diagrams.
- Implies the same n for all data points, but we have a variable number of points in the diagrams.
- Usually, we need the data points to come from a vector space, but persistence diagrams don't.

It's even worse

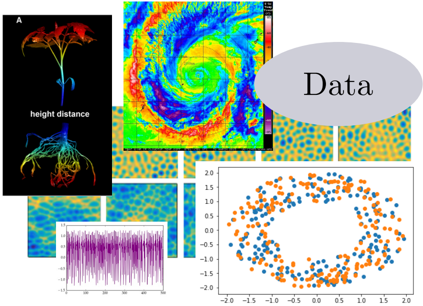
- Usually want ML inputs to come from a Banach space (complete normed vector space) or a Hilbert space (vector space with inner product and limits).
- Note all Hilbert spaces are Banach spaces, but not all Banach spaces are Hilbert spaces.

Theorem (Bubenik Wagner 2020)

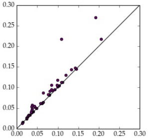
$(\mathcal{D}, W_p)$ does not admit an isometric embedding into a Hilbert space for any $1 \leq p \leq \infty$.

Featurization: the idea

Here be dragons.....

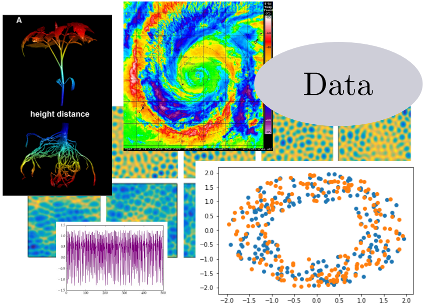


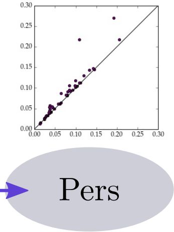
Pers



Featurization: the idea

Here be dragons.....

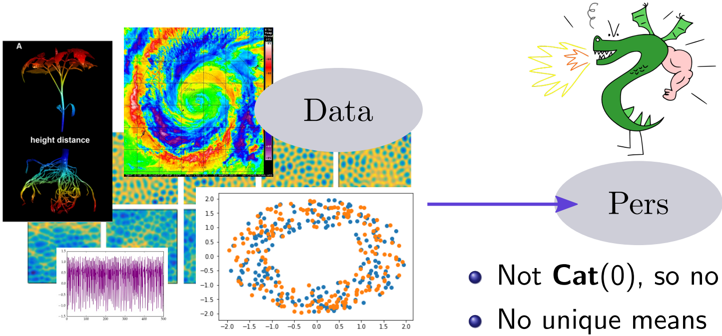




- Not **Cat**(0), so no unique geodesics
- No unique means
- No inner product

Featurization: the idea

Here be dragons.....



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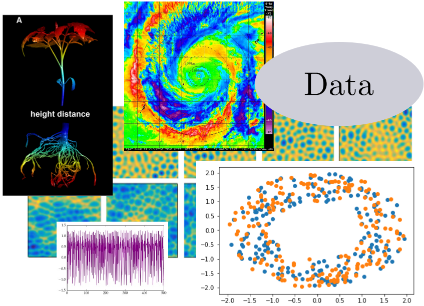
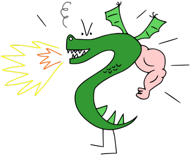
Featurization: the idea

Here be dragons.....





$\longrightarrow$ Pers $\longrightarrow \mathbb{R}^d$

- Not **Cat**(0), so no unique geodesics
- No unique means
- No inner product

Turning persistence diagrams into something else

Section 1

Algebraic structures

What if we just forget about the diagram?

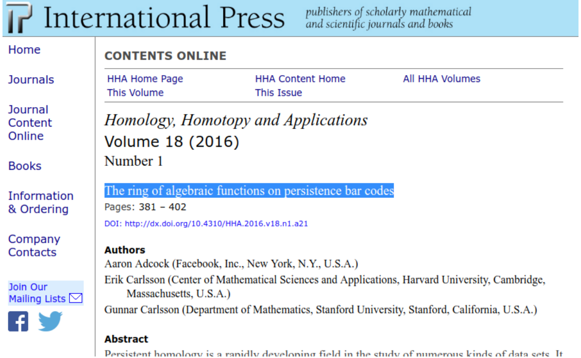
- Just treat a persistence diagram as a set of points in $\mathbb{R}^2$

$$\{(x_1, y_1), \cdots, (x_n, y_n)\} \rightsquigarrow (x_1, y_1, x_2, y_2, \cdots, x_n, y_n) \in \mathbb{R}^{2n}$$

- Problems:
  - Order shouldn't matter
  - n isn't fixed

Algebraic geometry to the rescue!

- Associate persistence diagrams to $k[x_1, y_1, x_2, y_2, \cdots]/\sim$
- Come up with functions on the points that don't care about order



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Homology, Homotopy and Applications
Volume 18 (2016)
Number 1

The ring of algebraic functions on persistence bar codes

Pages: 381 – 402

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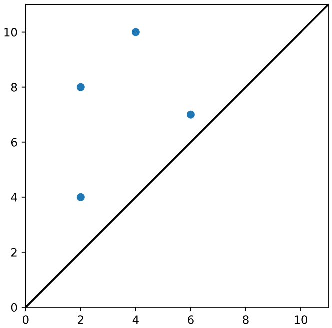
Abstract

Persistent homology is a rapidly developing field in the study of numerous kinds of data sets. It

Example



$$\{(2,4),(2,8),(4,10),(6,7)\}$$

- Ex. $\displaystyle\sum_i (x_i)(y_i - x_i)$

- Ex. $\displaystyle\sum_i (y_{\text{max}} - y_i)(y_i - x_i)$

Mnist Data

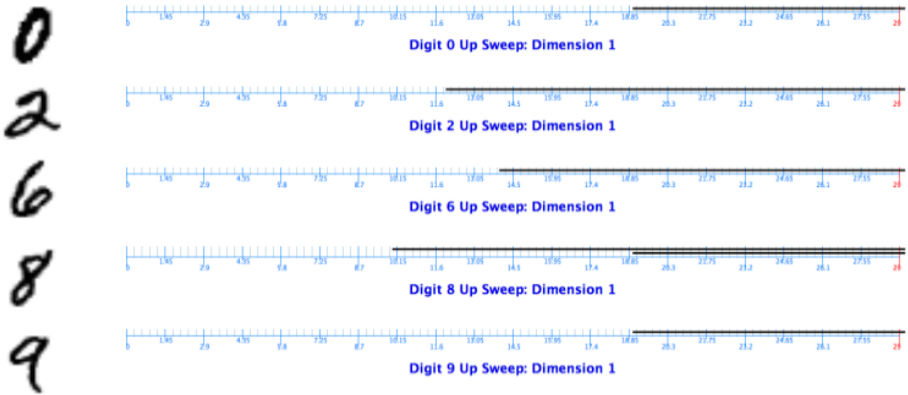
Build complex:

- Put vertex at each white pixel
- Connect vertices if their pixels touch.
- My assumption: clique complex after that

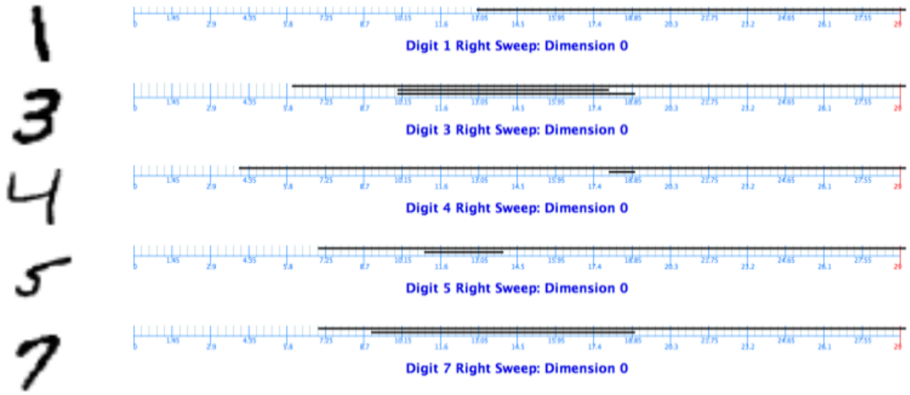
Filtration:

- Pick cardinal direction
- Add vertices in order in that direction
- Gives 4 each 0- and 1-dimensional diagrams

Results - Loops



Results - Non-loops



Features - Digits example

For each digit

Diagrams:

- 4 directions
- 0- and 1-dimensional diagrams for each direction
- $=8$ diagrams each

Features:

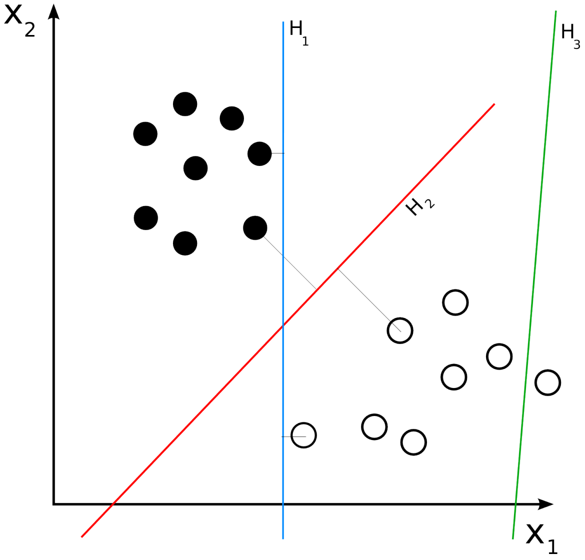
- Each Diagram has 4 features
- $=32$ features total

Features

$y_{\max} =$ max death for all diagrams
Diagrams $X = \{(x_i, y_i)\}$.

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

Support Vector Machine (SVM)



Results

Table 1: Classification Accuracy of two SVM Kernels

SVM	1000 Digits	5000 Digits	10000 Digits
Gaussian	87.70%	91.54%	92.04%
Polynomial	88.00%	91.62%	92.10%

(a) Stylistic Problems

(b) Spurious Topological Changes

Figure 5: Common Misclassifications

Pros & Cons

Pros

- Incredibly simple to explain
- Works well in lots of simple cases
- Fast to compute

Cons

- Not stable with respect to distances

Section 2

Landscapes

Paper

Journal of Machine Learning Research 16 (2015) 77-102 Submitted 7/14; Published 1/15

Statistical Topological Data Analysis using Persistence Landscapes

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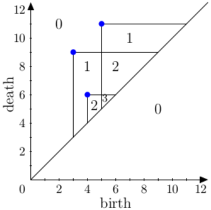
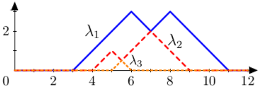
Editor: David Dunson

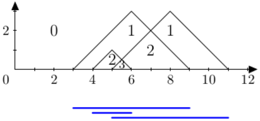
Abstract

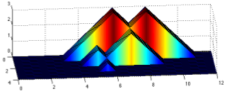
We define a new topological summary for data that we call the persistence landscape. Since this summary lies in a vector space, it is easy to combine with tools from statistics and machine learning, in contrast to the standard topological summaries. Viewed as a random variable with values in a Banach space, this summary obeys a strong law of large numbers and a central limit theorem. We show how a number of standard statistical tests can be used for statistical inference using this summary. We also prove that this summary is

Definition by picture



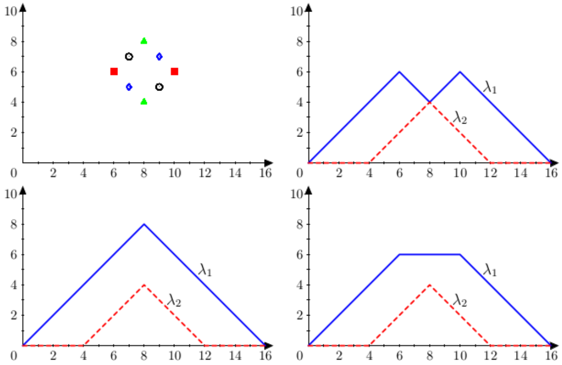




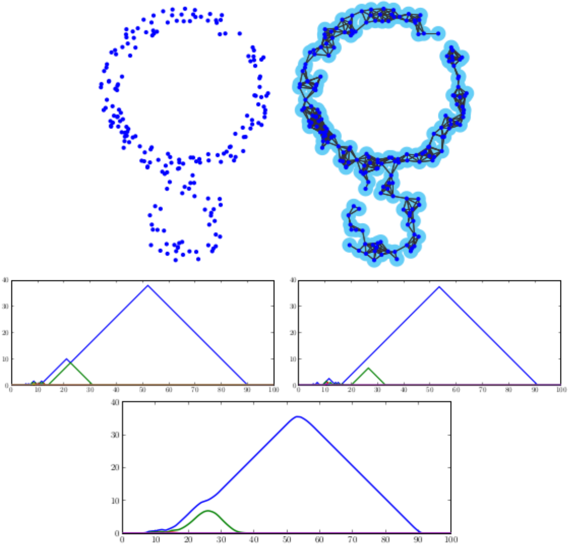


- Take diagram
- Rank function:
  $\beta^{a,b} = \dim(\mathrm{Im}\ (H_k(X_a) \to H_k(X_b)))$
- Rotate $(x, y) \mapsto \left(\frac{x+y}{2}, \frac{y-x}{2}\right)$
- $\lambda : \mathbb{N} \times \mathbb{R} \to \mathbb{R}$, $(k, t) \to \lambda_k(t)$
- $\lambda_k(t) = \sup(m \geq 0 \mid \beta^{t-m,t+m} \geq k)$

Everyone's favorite example

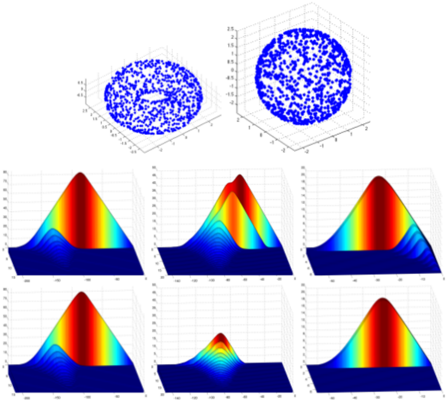


200 points, repeated 100 times



- Top two are example landscapes
- Bottom is average over all landscapes

Torus and Sphere



Average landscapes:

- Row 1: torus; Row 2: Sphere
- Col: 0-, 1-, and 2-dimensional diagram

Stability

Define

$$\|\lambda^D\|_p = \left(\sum_{k=1}^{\infty} \|\lambda_k^D\|_p^p \right)^{1/p}$$

Then

$$\|\lambda^{D_1} - \lambda^{D_2}\|_\infty \leq d_B(D_1, D_2).$$

Pros & Cons

Pros

- Can take averages, do ML etc
- Probably the #1 used ML featurization approach
- Stability

Cons

- Average might not be something that comes from a diagram

Section 3

Persistence Images

Images paper

Journal of Machine Learning Research 18 (2017) 1-35 Submitted 7/16; Published 2/17

Persistence Images: A Stable Vector Representation of Persistent Homology

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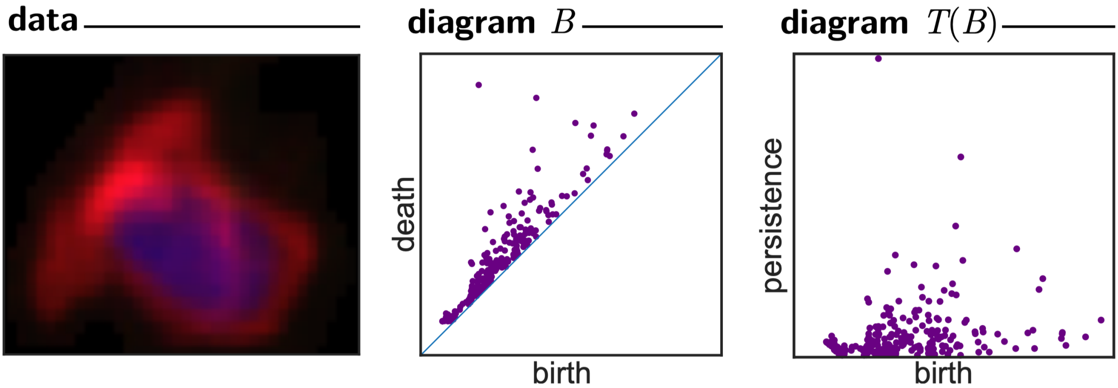
Editor: Michael Mahoney

Their view on the problem

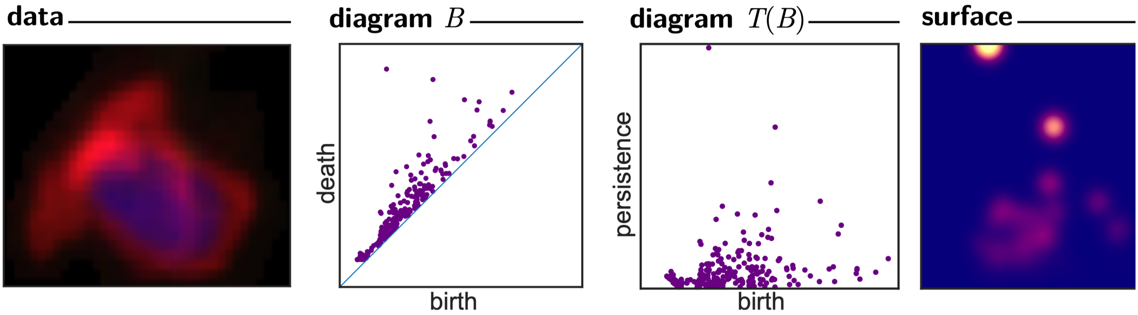
Problem Statement: How can we represent a persistence diagram so that

- the output of the representation is a vector in $\mathbb{R}^n$,
- the representation is stable with respect to input noise,
- the representation is efficient to compute,
- the representation maintains an interpretable connection to the original PD, and
- the representation allows one to adjust the relative importance of points in different regions of the PD?



- Transform: $T(X) = \{(x, y - x) \mid (x, y) \in X\}$

Persistence surface

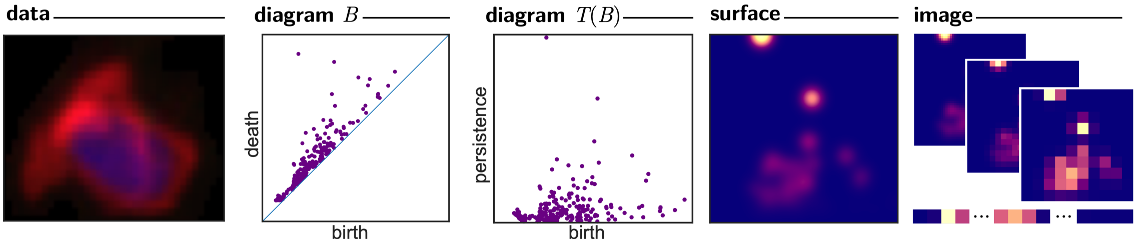


- Weight function e.g., $f(u) = u_y/\text{maxPers}$
- Gaussian: $\varphi_u(z) = \frac{1}{2\pi\sigma^2}\exp(-[(x-u_x)^2 + (y-u_y)^2]/(2\sigma^2))$

For a Pers Dgm X, the persistence surface is

$$\begin{aligned} \mu_X : \quad \mathbb{R}^2 &\to \mathbb{R} \\ x &\mapsto \sum_{u \in T(X)} f(u)\varphi_u(z) \end{aligned}$$

Persistence Images



- Grid up box
- Integrate the function in each box
- Treat the outputs as a vector

Example: linked twist map

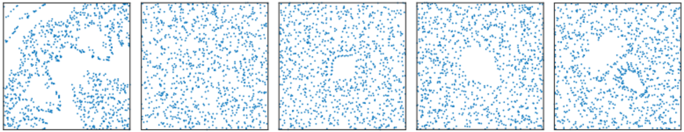


Figure 4: Examples of the first 1000 iterations, $\{(x_n, y_n) \; : \; n = 0, \ldots, 1000\}$, of the linked twist map with parameter values $r = 2$, 3.5, 4.0, 4.1 and 4.3, respectively.

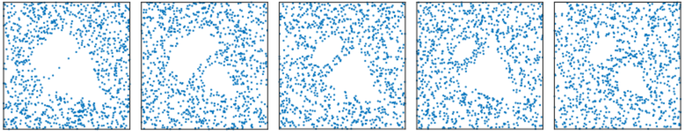


Figure 5: Truncated orbits, $\{(x_n, y_n) \; : \; n = 0, \ldots, 1000\}$, of the linked twist map with fixed $r = 4.3$ for different initial conditions (x_0, y_0).

- Generate point clouds from a discrete dynamical system

$$x_{n+1} = x_n + r y_n (1 - y_n) \quad \bmod 1$$
$$y_{n+1} = y_n + r x_n (1 - x_n) \quad \bmod 1$$

- Goal: Classify trials by r
- Scores
    - Both H_0 and H_1: 82.5%
    - H_0: 49.8%
    - H_1: 65.7%

Stability

Theorem 13.3. *Suppose persistence images are computed with the normalized Gaussian distribution with variance σ^2 and weight function $\omega : \mathbb{R}^2 \to \mathbb{R}$. Then the persistence images are stable w.r.t. the* 1*-Wasserstein distance between persistence diagrams. More precisely, given two finite and bounded persistence diagrams D and E, we have:*

$$\| \mathrm{I}_D - \mathrm{I}_E \|_1 \leq \left(\sqrt{5}|\nabla\omega| + \sqrt{\frac{10}{\pi}} \frac{\|\omega\|_\infty}{\sigma} \right) \cdot \mathsf{d}_{W,1}(D, E).$$

Here, $\nabla\omega$ stands for the gradient of ω, and $|\nabla\omega| = \sup_{z\in\mathbb{R}^2} \|\nabla\omega\|_2$ is the maximum norm of the gradient vector of ω at any point in $\mathbb{R}^2$. The same upper bound holds for $\| \mathrm{I}_D - \mathrm{I}_E \|_2$ and $\| \mathrm{I}_D - \mathrm{I}_E \|_\infty$ as well.

Section 4

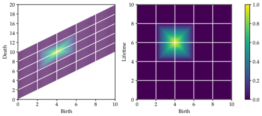
Tent Functions

Paper

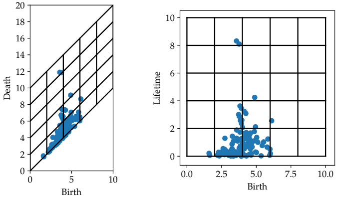
Template functions

Step 1: Choose collection of functions: $\{f_i\}$

- f_i :  $\to \mathbb{R}$
- compact support



Step 2: Evaluate each function f at each point in each diagram: $f(p)$ for $p \in D$.



Step 3: For fixed diagram D and function f, sum up for all points in diagram: $\nu_f(D) = \sum_{p \in D} f(p)$

Result: $\{f_i\}_{i=1}^k \quad \rightsquigarrow \quad D \mapsto (\nu_{f_1}(D), \nu_{f_2}(D), \cdots, \nu_{f_k}(D))$

Template function definition

- $\mathcal{D}$: Space of persistence diagrams
- $C_c(\mathbb{W})$: functions from $\mathbb{W} =$  to $\mathbb{R}$ with compact support

Definition

A **coordinate system** for $\mathcal{D}$ is a collection $\mathcal{F} \subset C(\mathcal{D}, \mathbb{R})$ which *separates points*.

$D \neq D' \in \mathcal{D}$, then there exists $F \in \mathcal{F}$ for which $F(D) \neq F(D')$.

Definition

A **template system** for $\mathcal{D}$ is a collection $\mathcal{T} \subset C_c(\mathbb{W})$ so that

$$\mathcal{F}_{\mathcal{T}} = \{\nu_f : f \in \mathcal{T}\}$$

is a coordinate system for $\mathcal{D}$.

The elements of $\mathcal{T}$ are called **template functions**.

$$\nu_f(D) = \sum_{p \in D} f(p)$$

In theory, it works...

Theorem (Perea, Munch, Khasawneh, 2019)

- *Let* $\mathcal{T} \subset C_c(\mathbb{W})$ *be a template system for* $\mathcal{D}$,
- $\mathcal{C} \subset \mathcal{D}$ *compact, and*
- $F : \mathcal{C} \longrightarrow \mathbb{R}$ *be continuous.*

Then for every $\varepsilon > 0$ *there exist*

- $N \in \mathbb{N}$,
- *a polynomial* $p \in \mathbb{R}[x_1, \ldots, x_N]$ *and*
- *template functions* $f_1, \ldots, f_N \in \mathcal{T}$

so that

$$\left| p(\nu_{f_1}(D), \nu_{f_2}(D), \cdots, \nu_{f_k}(D)) - F(D) \right| < \varepsilon$$

for every $D \in \mathcal{C}$.

... what about in practice?

Questions

- What choice of template functions?
- What polynomial?

Unsatisfying answers

- Any collection of functions on $\mathbb{W}$ with compact support that separate points should work.
- Machine learning to the rescue!

Tent functions

Parameters

- d: number of subdivisions
- δ: partition scale
- ε: shift away from the diagonal

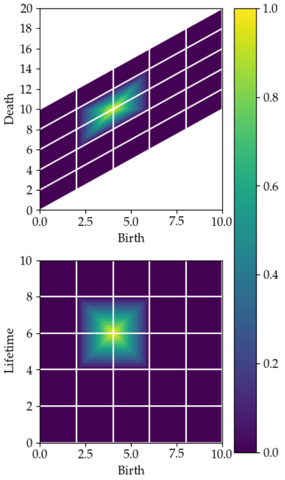
Tent function (i, j) in the birth-lifetime plane

$$i \in 0, \cdots, d; \; j \in 1, \cdots, d$$

$$\tilde{g}_{i,j}(x, \tilde{y}) = \left|1 - \frac{1}{\delta} \max\left\{|x - \delta i|, |\tilde{y} - (\delta j + \varepsilon)|\right\}\right|_+$$

Given a persistence diagram $D = (S, \mu)$,

$$G_{i,j}(D) = \sum_{\tilde{\mathbf{x}} \in S} \mu(\tilde{\mathbf{x}}) \cdot \tilde{g}_{i,j}(\tilde{\mathbf{x}})$$



Parameters

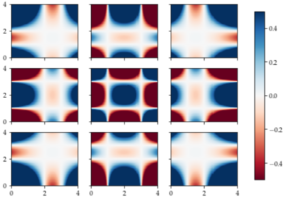
- $\mathcal{A} = \{a_1 < a_2 < \cdots < a_n\}$: partition of x-axis
- $\mathcal{B} = \{b_1 < b_2 < \cdots < b_n\}$: partition of y-axis

Interplating polynomial (i, j) in the birth-lifetime plane

$$f(x, y) = \ell_i^{\mathcal{A}}(x) \cdot \ell_j^{\mathcal{B}}(y)$$

where

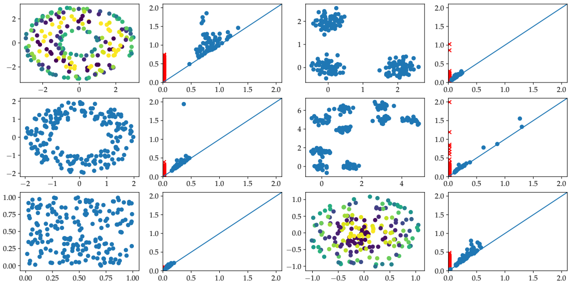
$$\ell_j^{\mathcal{A}}(x) = \prod_{i \neq j} \frac{x - a_i}{a_j - a_i} \qquad \ell_j^{\mathcal{B}}(x) = \prod_{i \neq j} \frac{x - b_i}{b_j - b_i}$$

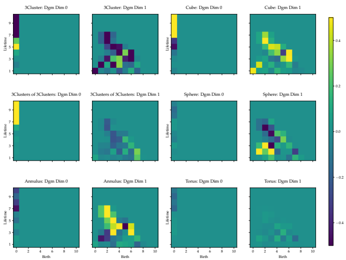


Given a persistence diagram $D = (S, \mu)$,

$$F_{i,j}^{\mathcal{A},\mathcal{B},K,\varepsilon}(D) := \sum_{\tilde{\mathbf{x}} \in \tilde{S}} \mu(\tilde{\mathbf{x}}) \cdot f_{i,j}^{\mathcal{A},\mathcal{B}}(\tilde{\mathbf{x}}) \cdot h_{K,\varepsilon}(\tilde{\mathbf{x}}).$$

Manifold experiment

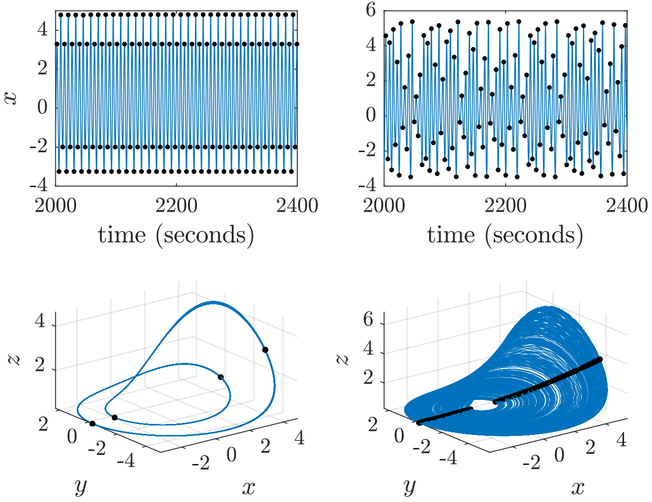




	Tents		Polynomials	
No. Dgms	Train	Test	Train	Test
10	$99.8\% \pm 0.9$	$96.5\% \pm 3.2$	$99.8\% \pm 0.9$	$95.0\% \pm 3.9$
25	$99.9\% \pm 0.3$	$99.0\% \pm 1.0$	$99.7\% \pm 0.5$	$97.6\% \pm 1.5$
50	$99.9\% \pm 0.2$	$99.9\% \pm 0.3$	$100\% \pm 0$	$99.2\% \pm 0.9$
100	$99.8\% \pm 0.1$	$99.7\% \pm 0.4$	$99.6\% \pm 0.2$	$99.3\% \pm 0.5$
200	$99.5\% \pm 0.1$	$99.5\% \pm 0.3$	$99.2\% \pm 0.2$	$98.9\% \pm 0.5$

Rössler

Classification of chaotic vs periodic



Section 5

The point

The point

- Can either work with persistence diagrams directly, or map somewhere else
- Working with persistence diagrams directly is hard
- Mapping somewhere else means you need to decide on that map.