PERSISTENCE IMAGES AND CROCKER PLOTS AS TOPOLOGICAL FEATURE VECTORS

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Lori Ziegelmeier

TRIPODS Summer Bootcamp: Topology and Machine Learning
ICERM
INTRODUCTION
Goal:

Develop representations of persistent homology that ‘vectorize’ topological information in a way that is accessible to machine learning techniques.
PERSISTENT HOMOLOGY AND MACHINE LEARNING
1. Envision data as a point cloud

2. Create connections between proximate points
   - build simplicial complex

3. Determine topological structure of complex
   - compute homology

4. Vary proximity parameter to assess different scales
   - calculate persistent homology
COMPUTE PERSISTENT HOMOLOGY

$\varepsilon = 1.5$  
$\varepsilon = 5.0$  
$\varepsilon = 7.0$  
$\varepsilon = 9.5$

$b_0$

$b_1$

Proximity Parameter $\varepsilon$
Compute Persistent Homology

Proximity Parameter $\varepsilon$

$\varepsilon = 1.5$ $\varepsilon = 5.0$ $\varepsilon = 7.0$ $\varepsilon = 9.5$

$H_0$ $H_1$

dead birth

$0$ $4$ $8$ $12$
The space of Persistence Diagrams (PDs) can be endowed with a metric.

\[
W_p(B, B') = \inf_{\gamma: B \to B'} \left( \sum_{u \in B} ||u - \gamma(u)||_\infty^p \right)^{1/p},
\]

where \(1 \leq p < \infty\) and \(\gamma\) ranges over bijections between \(B\) and \(B'\).
The space of Persistence Diagrams (PDs) can be endowed with a metric.

**Definition**

The bottleneck distance between two PDs $B$ and $B'$ is given by

$$W_\infty(B, B') = \inf_{\gamma: B \to B'} \sup_{u \in B} \| u - \gamma(u) \|_\infty,$$

where ranges over bijections between $B$ and $B'$. 
OTHER APPROACHES

Rouse et al. (2015) create a vector representation by superimposing a grid over a PD and counting number of points in each bin.

Carriere et al. (2015) develop a stable vector representation by rearranging the entries of the distance matrix between points in a PD.

Reininghaus et al. (2015) produce a stable surface from a PD by taking sum of a positive Gaussian centered on each PD point together with a negative Gaussian centered on its reflection below the diagonal.
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- Reininghaus et al. (2015) produce a stable surface from a PD by taking sum of a positive Gaussian centered on each PD point together with a negative Gaussian centered on its reflection below the diagonal.
Bubenik (2015) develops persistence landscape (PL), a stable functional representation of a PD that lies in a Banach space.

A PL is a function $\lambda : \mathbb{N} \times \mathbb{R} \rightarrow [-\infty, \infty]$ (which can equivalently be thought of as a sequence of functions $\lambda_k : \mathbb{R} \rightarrow [-\infty, \infty]$)

$$\lambda_k(x) = k\text{-th largest value of } \min(x - b_i, d_i - x).$$
How can we represent a persistence diagram so that:

1. the output of the representation is a vector in $\mathbb{R}^n$, 
2. the representation is stable with respect to input noise, 
3. the representation is efficient to compute, 
4. the representation maintains an interpretable connection to the original PD, and 
5. the representation allows one to adjust the relative importance of points in different regions of the PD?
PERSISTENCE IMAGES
PERSISTENCE IMAGE PIPELINE

data__________  diagram $B$_________  diagram $T(B)$_________  surface_________  image_________

![Data Image](image1.png)

![Diagram B](image2.png)

![Diagram T(B)](image3.png)

![Surface Image](image4.png)

![Image Sequence](image5.png)
1. Transform the PD from birth-death coordinates to birth-persistence coordinates
   ○ via $T : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ the linear transformation $T(x, y) = (x, y - x)$
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   - via $T: \mathbb{R}^2 \to \mathbb{R}^2$ the linear transformation $T(x, y) = (x, y - x)$

2. For each point $u = (u_x, u_y)$ in PD $T(B)$, center a probability distribution $\phi_u$
   - In our applications, $\phi_u = g_u$ a normalized Gaussian distribution:
     $$g_u(x, y) = \frac{1}{2\pi \sigma^2} e^{-\frac{(x-u_x)^2 + (y-u_y)^2}{2\sigma^2}}$$
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     $$g_u(x, y) = \frac{1}{2\pi \sigma^2} e^{-\left[(x-u_x)^2+(y-u_y)^2\right]/2\sigma^2}$$

3. Produce a persistence surface as a weighted sum of these distributions
   - $\rho_B(x, y) = \sum_{u \in T(B)} f(u)g_u(x, y)$

4. Overlay a grid onto the PD

5. The image value at pixel $p$, a square in the grid, is the integral of the persistence surface over that pixel
   - $I(\rho_B)_p = \iint_p \rho_B(x, y) \, dy \, dx$
PERSISTENCE IMAGE (PI)

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   ○ via \( T: \mathbb{R}^2 \rightarrow \mathbb{R}^2 \) the linear transformation \( T(x, y) = (x, y - x) \)
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   - \( I(\rho_B)_p = \iint_p \rho_B(x, y) \, dydx \)
THE WEIGHTING FUNCTION

Define a weighting function \( f : \mathbb{R}^2 \rightarrow \mathbb{R} \) that is

- zero along the horizontal axis,
- continuous, and
- piecewise differentiable.
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Convenient choice depends only on the vertical persistence coordinate $y$. 
THE WEIGHTING FUNCTION

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- zero along the horizontal axis,
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- piecewise differentiable.

Convenient choice depends only on the vertical persistence coordinate $y$.

For example:

$$f(x, y) = w_b(y) = \begin{cases} 
0 & y \leq 0 \\
\frac{y}{b} & 0 < y < b \\
1 & y \geq b 
\end{cases}$$

where $b$ is the persistence value of the most persistent feature in all trials.
Figure: $H_1$ PIs of a noisy circle. The first row has resolution $5 \times 5$ while the second has $50 \times 50$. The columns have variance $\sigma = 0.2$, $\sigma = 0.01$, and $\sigma = 0.0001$, respectively.
Figure: $H_1$ PIs of a noisy torus. The first row has resolution $5 \times 5$ while the second has $50 \times 50$. The columns have variance $\sigma = 0.2$, $\sigma = 0.01$, and $\sigma = 0.0001$, respectively.
Persistence diagrams are stable (Lipschitz) with respect to the bottleneck metric (Cohen-Steiner, Edelsbrunner, Harer 2007)

\[ W_{\infty}(B(f), B(g)) \leq ||f - g||_{\infty} \]

Want: \[ ||\rho_B - \rho_{B'}||_p \leq C \cdot W_{p'}(B, B') \]
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Want: \[ ||\rho_B - \rho_{B'}||_p \leq C \cdot W_p(B, B') \]

**Theorem**

The persistence surface \( \rho \) is stable with respect to the 1-Wasserstein distance between two diagrams \( B, B' \). That is,

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

The persistence image $I(\rho_B)$ is stable with respect to the 1-Wasserstein distance between diagrams. More precisely, if $A$ is the maximum area of any pixel in the image, $A'$ is the total area of the image, and $n$ is the number of pixels in the image, then

\[
\|I(\rho_B) - I(\rho_{B'})\|_\infty \leq \sqrt{10A}(\|f\|_\infty |\nabla \phi| + \|\phi\|_\infty |\nabla f|)W_1(B, B')
\]
\[
\|I(\rho_B) - I(\rho_{B'})\|_1 \leq \sqrt{10A'}(\|f\|_\infty |\nabla \phi| + \|\phi\|_\infty |\nabla f|)W_1(B, B')
\]
\[
\|I(\rho_B) - I(\rho_{B'})\|_2 \leq \sqrt{10nA}(\|f\|_\infty |\nabla \phi| + \|\phi\|_\infty |\nabla f|)W_1(B, B').
\]
Theorem

The persistence surface \( \rho \) with Gaussian distributions is stable with respect to the 1-Wasserstein distance between two diagrams \( B, B' \). That is,

\[
\| \rho_B - \rho_{B'} \|_1 \leq \left( \sqrt{5} |\nabla f| + \sqrt{\frac{10}{\pi}} \frac{\| f \|_\infty}{\sigma} \right) W_1(B, B').
\]
The persistence image $I(\rho_B)$ with Gaussian distributions is stable with respect to the $1$-Wasserstein distance between diagrams. More precisely,

$$\|I(\rho_B) - I(\rho_{B'})\|_1 \leq \left( \sqrt{5} |\nabla f| + \sqrt{\frac{10}{\pi}} \frac{\|f\|_\infty}{\sigma} \right) W_1(B, B')$$

$$\|I(\rho_B) - I(\rho_{B'})\|_2 \leq \left( \sqrt{5} |\nabla f| + \sqrt{\frac{10}{\pi}} \frac{\|f\|_\infty}{\sigma} \right) W_1(B, B')$$

$$\|I(\rho_B) - I(\rho_{B'})\|_\infty \leq \left( \sqrt{5} |\nabla f| + \sqrt{\frac{10}{\pi}} \frac{\|f\|_\infty}{\sigma} \right) W_1(B, B').$$
DATA ANALYSIS
SHAPE DATA

Points sampled from six topological spaces: the solid cube, a circle, a sphere, three clusters, three clusters within three clusters, and a torus.

25 point clouds from each space, consisting of 500 points, 2 levels of noise $\eta = 0.05, 0.1$
Goal:

Compare classification accuracy and computational time of shape data for

- the PD framework equipped with the Bottleneck, 1-Wasserstein, 2-Wasserstein metrics,
- the PL framework equipped with the $L^1, L^2, L^\infty$ metrics, and
- the PI framework equipped with the $L^1, L^2, L^\infty$ metrics.

Construct $3^2 \cdot 2^2 = 36$ distance matrices of size $150 \times 150$. 

K-MEDOIDS FOR CLASSIFICATION

Depends only on distances from one point to another.

Partitions a metric space into $K$ clusters by choosing most centrally located point in a cluster, the medoid, and assigning each point to closest medoid.

Cluster score is sum of distances from each point to closest medoid.

- Ideally, want minimal clustering score.
- In practice, choose large number of random initializations (1,000 with $K/6$ for us). Return clustering with lowest score.

Compute accuracy (percentage of shape point clouds identified with a medoid of the same shape class).
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Image from QUSMA.com
**K-MEANS FOR CLASSIFICATION**

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# K-Medoids Comparison of Topological Representation

<table>
<thead>
<tr>
<th>Distance Matrix</th>
<th>Accuracy (Noise 0.05)</th>
<th>Time (Noise 0.05)</th>
<th>Accuracy (Noise 0.1)</th>
<th>Time (Noise 0.1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PD, $H_0$, $L^1$</td>
<td>96.0%</td>
<td>37346s</td>
<td>96.0%</td>
<td>42613s</td>
</tr>
<tr>
<td>PD, $H_0$, $L^2$</td>
<td>91.3%</td>
<td>24656s</td>
<td>91.3%</td>
<td>25138s</td>
</tr>
<tr>
<td>PD, $H_0$, $L^\infty$</td>
<td>60.7%</td>
<td>1133s</td>
<td>63.3%</td>
<td>1149s</td>
</tr>
<tr>
<td>PD, $H_1$, $L^1$</td>
<td>100%</td>
<td>657s</td>
<td>96.0%</td>
<td>703s</td>
</tr>
<tr>
<td>PD, $H_1$, $L^2$</td>
<td>100%</td>
<td>984s</td>
<td>97.3%</td>
<td>1042s</td>
</tr>
<tr>
<td>PD, $H_1$, $L^\infty$</td>
<td>81.3%</td>
<td>527s</td>
<td>66.7%</td>
<td>564s</td>
</tr>
<tr>
<td>PL, $H_0$, $L^1$</td>
<td>92.7%</td>
<td>29s</td>
<td>96.7%</td>
<td>33s</td>
</tr>
<tr>
<td>PL, $H_0$, $L^2$</td>
<td>77.3%</td>
<td>29s</td>
<td>82.0%</td>
<td>34s</td>
</tr>
<tr>
<td>PL, $H_0$, $L^\infty$</td>
<td>60.7%</td>
<td>2s</td>
<td>63.3%</td>
<td>2s</td>
</tr>
<tr>
<td>PL, $H_1$, $L^1$</td>
<td>83.3%</td>
<td>36s</td>
<td>80.7%</td>
<td>48s</td>
</tr>
<tr>
<td>PL, $H_1$, $L^2$</td>
<td>83.3%</td>
<td>50s</td>
<td>66.7%</td>
<td>69s</td>
</tr>
<tr>
<td>PL, $H_1$, $L^\infty$</td>
<td>74.7%</td>
<td>8s</td>
<td>66.7%</td>
<td>9s</td>
</tr>
<tr>
<td>PI, $H_0$, $L^1$</td>
<td>93.3%</td>
<td>9s</td>
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<tr>
<td>PI, $H_1$, $L^1$</td>
<td>100%</td>
<td>17s</td>
<td>95.3%</td>
<td>18s</td>
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<td>17s</td>
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1-norm regularized linear support vector machine (aka sparse SVM) classifies data by generating a separating hyperplane that depends on very few input space features.

Can reduce data dimension and/or select discriminatory features.

Linear SSVM feature selection implemented on vectors (such as PIs to select discriminatory pixels during classification).
EXTRACTING FEATURES WITH SPARSE SVM

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- Can reduce data dimension and/or select discriminatory features.

- Linear SSVM feature selection implemented on vectors (such as PIs to select discriminatory pixels during classification).

**Goal:**

Use Sparse SVM to simultaneously classify data and select input space features that contribute to the classification process.

- Adopt the one-against-all SSVM to separate one class from members of all other classes of PIs of the shape classes using resolution $20 \times 20$, variance $0.0001$, and noise level $0.05$. 
Figure: $H_1$ PIs of shape data with selected pixels marked by blue crosses. (a) Solid cube (b) Torus (c) Sphere (d) Three clusters (e) Three clusters within three clusters (f) Circle
ANISOTROPIC KURAMOTO-SIVASHINSKY (AKS) EQUATION
ANISOTROPIC KURAMOTO-SIVASHINSKY (AKS) EQUATION

- Partial differential equation for a function $u(x, y, t)$ of spatial variables $x, y,$ and time $t$.
- Kuramoto-Sivashinsky equation derived in problems involving pattern formation such as surface nanopatterning by ion-beam erosion, epitaxial growth, and solidification from a melt.
- Anisotropic Kuramoto-Sivashinsky (aKS) Equation is given by
  \[
  \frac{\partial}{\partial t} u = -\nabla^2 u - \nabla^2 \nabla^2 u + r \left( \frac{\partial}{\partial x} u \right)^2 + \left( \frac{\partial}{\partial y} u \right)^2,
  \]
  where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$, and the real parameter $r$ controls the degree of anisotropy.
- For a fixed time $t^*$, $u(x, y, t^*)$ is a patterned surface (periodic in both $x$ and $y$) defined over the $(x, y)$-plane.
Figure: Plots of $u(x, y, \cdot)$ from simulations of the aKS equation. Columns represent parameters $r = 1, 1.25, 1.5, 1.75$ and $2$. Rows represent time: $t = 3$ (top) and $t = 5$ (bottom).
PARAMETER OF THE AKS EQUATION

Figure: Plots of $u(x, y, \cdot)$ from simulations of the aKS equation. Columns represent parameters $r = 1, 1.25, 1.5, 1.75$ and $2$. Rows represent time: $t = 3$ (top) and $t = 5$ (bottom).

Figure: Surfaces $u(x, y, 3)$ for $r = 1.75$ or $r = 2$. Can you group the images by eye?
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Figure: Surfaces $u(x, y, 3)$ for $r = 1.75$ or $r = 2$. Can you group the images by eye?

Answer: (from left) $r = 1.75, 2, 1.75, 2$. 
AKS CLASSIFICATION METHODS

Goal:

Classify (150, 30 for each parameter) trials of the aKS Equation by parameter (5 values) using snapshots of the surfaces $u(x, y, \cdot)$ as they evolve in time (5 values).

Methods of classification:
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Methods of classification:

1. Surfaces viewed as points in $\mathbb{R}^{266144}$. Reduce resolution to $10 \times 10$ by coarsening the discretization of the spatial domain. Classify with Subspace Discriminant Ensemble.
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(a)  

(b)
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2. Parameter $r$ influences mean and amplitude of pattern. Use a normal distribution-based classifier built on the variances of the surface heights.
3. Sublevel set filtration PD. Generate PIs with resolution $10 \times 10$ and variance 0.01. Classify $H_0, H_1$ and concatenated PIs using Subspace Discriminant Ensemble.
<table>
<thead>
<tr>
<th>Classification Approach</th>
<th>Time t=3</th>
<th>Time t=5</th>
<th>Time t=10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subspace Discriminant Ensemble, Resized Surfaces</td>
<td>26.0 %</td>
<td>19.3%</td>
<td>19.3 %</td>
</tr>
<tr>
<td>Variance Normal Distribution Classifier</td>
<td>20.74%</td>
<td>75.2%</td>
<td>77.62 %</td>
</tr>
<tr>
<td>Subspace Discriminant Ensemble, ( H_0 ) PIs</td>
<td>58.3 %</td>
<td>96.0 %</td>
<td>94.7 %</td>
</tr>
<tr>
<td>Subspace Discriminant Ensemble, ( H_1 ) PIs</td>
<td>67.7 %</td>
<td>87.3 %</td>
<td>93.3 %</td>
</tr>
<tr>
<td>Subspace Discriminant Ensemble, ( H_0 ) and ( H_1 ) PIs</td>
<td>72.7 %</td>
<td>95.3 %</td>
<td>97.3 %</td>
</tr>
</tbody>
</table>
TOPOLOGY EVOLVING IN TIME
In many natural systems, particles, organisms, or agents interact locally according to rules that produce aggregate behavior.
Alignment Order Parameter: \( \varphi(t) = \frac{1}{Nv_0} \left| \sum_{i=1}^{N} \vec{v}_i(t) \right| \)
CLASSIC WAY TO ANALYZE BIOLOGICAL AGGREGATIONS

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Goal: Use topology to analyze the collective behavior of interacting agents' positions and velocities as time evolves.
CLASSIC WAY TO ANALYZE BIOLOGICAL AGGREGATIONS

Alignment Order Parameter: \( \varphi(t) = \frac{1}{N_{v_0}} \left| \sum_{i=1}^{N} \vec{v}_i(t) \right| \)
Goal:

Use topology to analyze the collective behavior of interacting agents’ positions and velocities as time evolves.
1. Envision data as a point cloud
   - e.g. position-velocity for on snapshot in time

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   - build simplicial complex

3. Determine topological structure of complex
   - compute homology (measure # holes)

4. Vary proximity parameter to assess different scales
   - calculate persistent homology

5. Evolve in time
   - CROCKER plots
COMPUTE PERSISTENT HOMOLOGY
COMPUTE PERSISTENT HOMOLOGY

Proximity Parameter $\varepsilon$
COMPUTE PERSISTENT HOMOLOGY
Compute the $k$th Betti number $b_k(\varepsilon, t)$,
Compute the $k$th Betti number $b_k(\varepsilon, t)$,

CROCKER plot

VICSEK MODEL

- Highly cited dynamical system in discrete time and continuous space.
- Describes motion of interacting point particles in a square with periodic boundary conditions.
- Model written as:

\[
\begin{align*}
\theta_i(t + \Delta t) &= \frac{1}{N} \left( \sum_{|\vec{x}_i - \vec{x}_j| \leq R} \theta_j(t) \right) + U(-\eta/2, \eta/2) \\
\vec{v}_i(t + \Delta t) &= v_0 \left( \cos \theta_i(t + \Delta t), \sin \theta_i(t + \Delta t) \right) \\
\vec{x}_i(t + \Delta t) &= \vec{x}_i(t) + \vec{v}_i(t + \Delta t) \Delta t
\end{align*}
\]
VICSEK MODEL

- Highly cited dynamical system in discrete time and continuous space.
- Describes motion of interacting point particles in a square with periodic boundary conditions.
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TOPOLOGY OF INITIAL CONDITION

Three-torus $T^3$: $b/\text{equalx}(1,3,3,1,0,...)$
Three-torus $T^3$: $b = (1, 3, 3, 1, 0, \ldots)$
DIFFERENT LONG-TERM BEHAVIORS OF VICSEK MODEL

(A) Clusters?

(B) Loose alignment?

(C) Strong alignment?
VICSEK SIMULATION A ANALYSIS

(A) Order Parameter $\phi$

(B) Proximity Parameter $\epsilon$

(C) Proximity Parameter $\epsilon$
VICSEK SIMULATION B ANALYSIS

- **Order Parameter $\phi$**
  - $b_0 \geq 5$
  - $b_0 = 1$

- **Proximity Parameter $\varepsilon$**
  - $b_1 \geq 5$
  - $b_1 = 0$
  - $b_1 = 2$
  - $b_1 = 3$

- Simulation Time $t$

---

(A) Graph showing the order parameter $\phi$ over simulation time $t$.

(B) Graph showing the proximity parameter $\varepsilon$ over simulation time $t$ for different levels.

(C) Graph showing the proximity parameter $\varepsilon$ over simulation time $t$ for different levels.
VICSEK SIMULATION C ANALYSIS

(A) Order Parameter $\phi$

(B) Proximity Parameter $\epsilon$

(C) Proximity Parameter $\epsilon$

- $b_0 \geq 5$
- $b_0 = 1$
- $b_0 = 2$
- $b_1 \geq 5$
- $b_1 = 2$
Goal:

Given simulated data from the Vicsek model, can we use machine learning algorithms to recover the unknown underlying noise parameter?
Goal:
Given simulated data from the Vicsek model, can we use machine learning algorithms to recover the unknown underlying noise parameter?

- Generate 100 simulations of different parameter choices
- Compute alignment order parameter and $H_0$ and $H_1$
- CROCKER plots
- Compare pairwise (Euclidean) distances between simulations
- Cluster with $K$-medoids
EXPERIMENT 1

Noise parameters:

$$\eta = 0.01, 0.1, 1$$

Pairwise Distance Matrices:

Alignment Order Parameter

H0 CROCKER  H1 CROCKER  H0&1 CROCKER
EXPERIMENT 2

Noise parameters:

\[ \eta = 0.01, 0.02, 0.03, 0.05, 0.1, 0.19, 0.2, 0.21, 0.3, 0.5, 1, 1.5, 1.9, 1.99, 2 \]

Pairwise Distance Matrices:
EXPERIMENT 3

Noise parameters:

\[ \eta = 0.01, 0.5, 1, 1.5, 2 \]

Pairwise Distance Matrices:

Alignment Order Parameter
### K-Medoids Clustering Results

<table>
<thead>
<tr>
<th></th>
<th>Exp 1</th>
<th></th>
<th>Exp 2</th>
<th></th>
<th>Exp 3</th>
<th></th>
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<tbody>
<tr>
<td></td>
<td>$H_{0&amp;1}$</td>
<td>Align</td>
<td>$H_{0&amp;1}$</td>
<td>Align</td>
<td>$H_{0&amp;1}$</td>
<td>Align</td>
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<td>Accuracy</td>
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<td>23.3%</td>
<td>14.3%</td>
<td>99.6%</td>
<td>63.0%</td>
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<td>0.43</td>
<td>0.3</td>
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</tbody>
</table>
CONCLUSION
Persistence Images

PIs present a method for vectorization of topological characteristics of data that:

- have an interpretable connection to PDs
- are stable
- can be incorporated with a variety of metrics and machine learning tools

CROCKER Plots

CROCKER plots present a method for vectorization of topological characteristics of time-varying (or two parameter) data that:

- are simple
- can provide higher classification accuracy than classic order parameters
- can be incorporated with a variety of metrics and machine learning tools
Thank you!

Persistence Images
Henry Adams, Sofya Chepushtan nova, Tegan Emerson, Eric Hanson, Michael Kirby, Francis Motta, Rachel Neville, Chris Peterson, and Patrick Shipman

CROCKER Plots and Viscek Model
Henry Adams, Tom Halverson, Chad Topaz, and Lu Xian

Lori Ziegelmeier
lziegel1@macalester.edu
Department of Mathematics, Statistics, and Computer Science