Intrinsic persistent homology via density-based metric learning

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joint work with E. Borghini, P. Groisman and G. Mindlin

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EPSRC Centre for Topological Data Analysis

Prifysgol Abertawe
Swansea University

Image: Keenan Crane

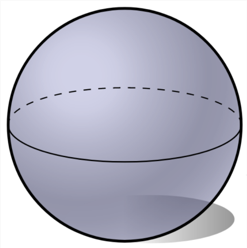
The problem

Metric learning in Riemannian manifolds

$(\mathcal{M}, g)$ a *d*-dimensional Riemannian manifold with associated Riemannian distance

$$d_{\mathcal{M}}(x, y) = \inf_{\gamma} \int_I \sqrt{g(\dot{\gamma}_t, \dot{\gamma}_t)} dt,$$

over all $\gamma : I \to \mathcal{M}$ with $\gamma(0) = x$, and $\gamma(1) = y$.



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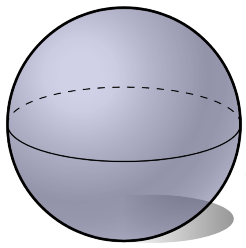
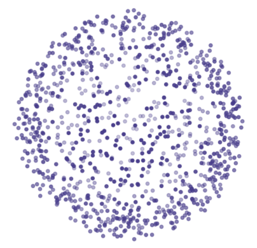


$\mathbb{X}_n = \{x_1, x_2, \dots, x_n\}$ a finite sample of $\mathcal{M}$.



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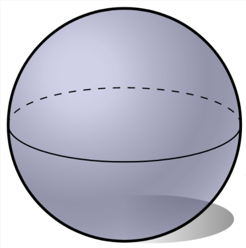
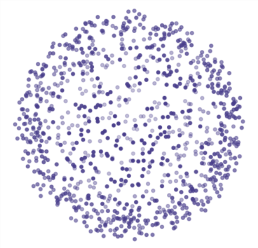


$\mathbb{X}_n = \{x_1, x_2, \ldots, x_n\}$ a finite sample of $\mathcal{M}$.

How to infer the Riemannian distance from the sample?



Inherited Riemannian metric

If $\mathcal{M}$ is embedded in $\mathbb{R}^D$ and $g(x, y) = \langle x, y \rangle$ is the **inner product in $\mathbb{R}^D$**, the associated Riemannian distance is

$$d_{\mathcal{M}}(x, y) = \inf_{\gamma} \int_I ||\dot{\gamma}_t|| dt$$

over all piecewise smooth curves $\gamma : I \to \mathcal{M}$ with $\gamma(0) = x$, and $\gamma(1) = y$.

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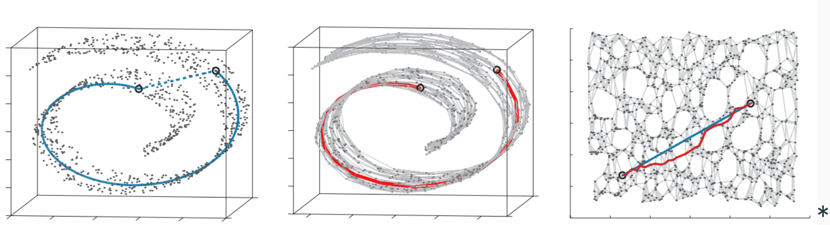
Given $\varepsilon > 0$, consider the **ε-graph** $G_\varepsilon(\mathbb{X}_n)$ and define the **estimator***

$$d_{\mathbb{X}_n,\varepsilon}(x,y) = \inf_{\gamma} \sum_{i=0}^{r} |x_{i+1} - x_i|$$

over all $\gamma = (x, x_1, \ldots, , x_r, y)$ with $(x_i, x_{i+1}) \in E(G_\varepsilon)$ for all $1 \leqslant i \leqslant r$.



* Bernstein, de Silva, Langford, Tenenbaum (2000).

Theorem (Bernstein, de Silva, Langford, Tenenbaum, 2000)

Let $\mathcal{M}$ be a closed d-dimensional Riemannian manifold embedded in $\mathbb{R}^D$ with inherited Riemannian distance $d_{\mathcal{M}}$. Let $\mathbb{X}_n$ be a finite sample of $\mathcal{M}$.

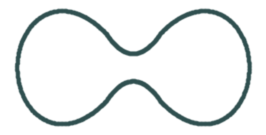
Assume $\varepsilon_n \to 0$ and $n\varepsilon_n^d \to \infty$. Then,

$$\lim_{n\to\infty} \sup_{x,y\in\mathcal{M}} |d_{\mathbb{X}_n,\varepsilon_n}(x,y) - d_{\mathcal{M}}(x,y)| = 0$$

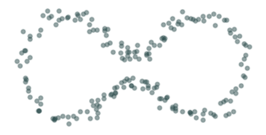
in probability, with almost sure convergence provided $n\varepsilon_n^d/\log n \to \infty$.

Dependence on ε (and density)

Manifold



Noisy sample



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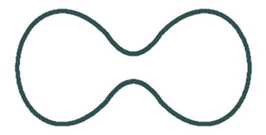

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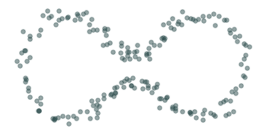
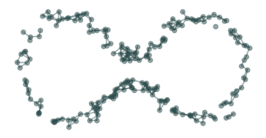
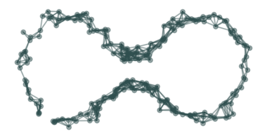


ε- graph

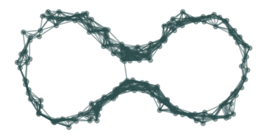
$\varepsilon = 0.2$



$\varepsilon = 0.3$



$\varepsilon = 0.4$

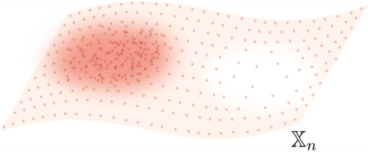


The manifold (and density) assumption

$\mathbb{X}_n = \{x_1, x_2, \ldots, x_n\}$ a finite set of points in $\mathbb{R}^D$.

We assume that:

- $\mathbb{X}_n$ lies in a d-dimensional Riemannian manifold $\mathcal{M}$,
- $\mathbb{X}_n$ is drawn according to a density f.



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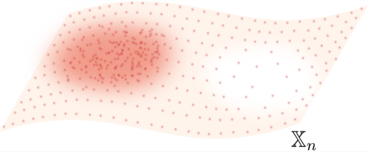
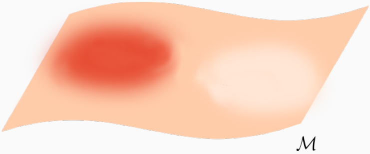


$(\mathcal{M}, g)$ a d-dimensional Riemannian manifold embedded in $\mathbb{R}^D$ with $f : \mathcal{M} \to \mathbb{R}_{>0}$ a smooth density function.



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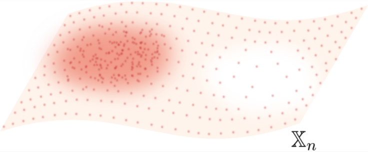

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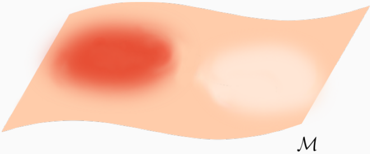

Consider a (new) Riemannian metric that depends on f.

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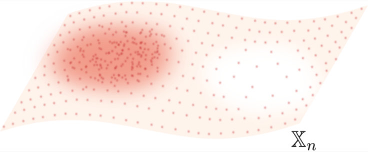
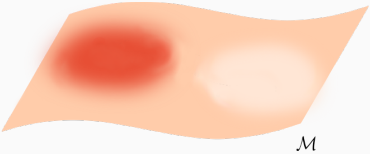


Find an estimator of the (density-based) Riemannian metric from the sample.

$(\mathcal{M}, g)$ a d-dimensional Riemannian manifold embedded in $\mathbb{R}^D$ with $f : \mathcal{M} \to \mathbb{R}_{>0}$ a smooth density function.



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Density-based metric learning

Deformed Riemannian metric

- Let $(\mathcal{M}, g)$ be a Riemannian manifold and let $f : \mathcal{M} \to \mathbb{R}_{>0}$ be a smooth density.

*Hwang, Damelin, Hero (2016), Groisman, Jonckheere, Sapienza (2018)

Deformed Riemannian metric

- Let $(\mathcal{M}, g)$ be a Riemannian manifold and let $f : \mathcal{M} \to \mathbb{R}_{>0}$ be a smooth density.
- For $q > 0$, and consider the deformed metric tensor

$$g_q = f^{-2q} g.^*$$

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Deformed Riemannian metric

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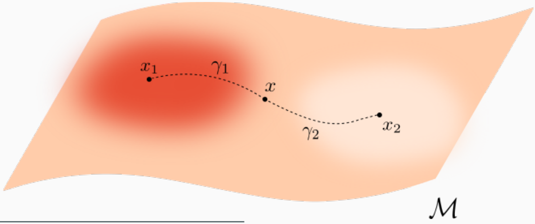
- For $q > 0$, and consider the deformed metric tensor

$$g_q = f^{-2q} g.^*$$

- The induced **deformed Riemannian distance** in $\mathcal{M}$ is

$$d_{f,q}(x, y) = \inf_{\gamma} \int_I \frac{1}{f(\gamma_t)^q} \sqrt{g(\dot{\gamma}_t, \dot{\gamma}_t)} dt$$

over all $\gamma : I \to \mathcal{M}$ with $\gamma(0) = x$ and $\gamma(1) = y$.



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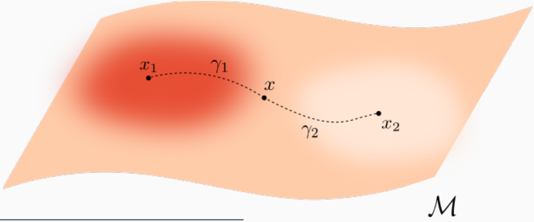

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Fermat distance

- Let $\mathbb{X}_n \subseteq \mathbb{R}^D$ a sample of points.

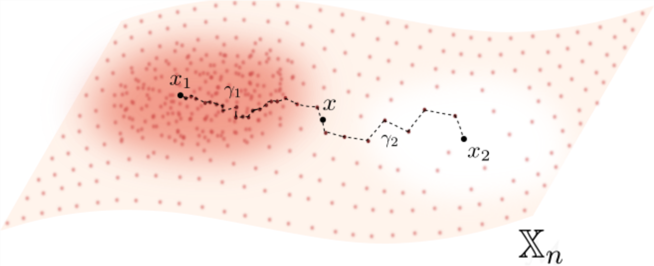
† Groisman, Jonckheere, Sapienza (2018), Mckenzie and Damelin (2019).

Fermat distance

- Let $\mathbb{X}_n \subseteq \mathbb{R}^D$ a sample of points.
- For $p > 1$, the (sample) **Fermat distance**[†] between $x, y \in \mathbb{R}^D$ is defined by

$$d_{\mathbb{X}_n,p}(x,y) = \inf_{\gamma} \sum_{i=0}^{r} |x_{i+1} - x_i|^p$$

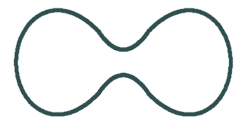
over all paths $\gamma = (x_0, \ldots, x_{r+1})$ of finite length with $x_0 = x$, $x_{r+1} = y$ and $\{x_1, x_2, \ldots, x_r\} \subseteq \mathbb{X}_n$.



[†] Groisman, Jonckheere, Sapienza (2018), Mckenzie and Damelin (2019).

Example

Manifold



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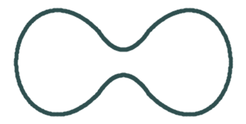
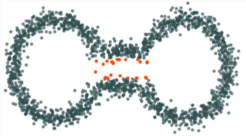


Sample



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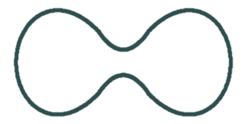

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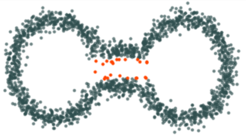
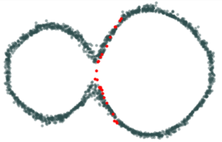


Isomap



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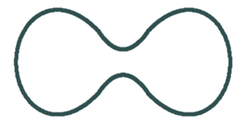
Manifold



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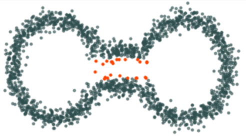

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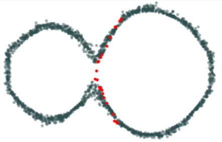
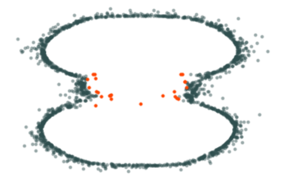
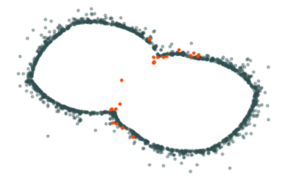


Fermat p = 1.5



Fermat p = 2.0



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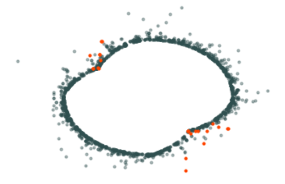
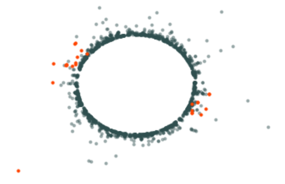


Fermat p = 3.0



Previous work

Theorem (Groisman, Jonckheere, Sapienza (2018))

Let $(\mathcal{M}, g)$ be an **isometric**[‡] C^1 d-dimensional Riemannian manifold embedded in $\mathbb{R}^D$ with inherited metric tensor. Let $\mathbb{X}_n \subseteq \mathcal{M}$ be a set of n independent sample points with common smooth density $f : \mathcal{M} \to \mathbb{R}_{>0}$.

Given $p > 1$, there exists $\mu = \mu(p, d) > 0$ such that for any $x, y \in \mathcal{M}$,

$$\lim_{n \to +\infty} \frac{n^q}{\mu} d_{\mathbb{X}_n, p}(x, y) = d_{f,q}(x, y) \text{ almost surely}$$

with $q = (p-1)/d$.

[‡] $\mathcal{M}$ is an **isometric** d-dimensional C^1 manifold embedded in $\mathbb{R}^D$ if there exists $S \subseteq \mathbb{R}^d$ an open connected set and $\varphi : \bar{S} \to \mathbb{R}^D$ such that $\varphi(\bar{S}) = \mathcal{M}$ and $\varphi : \bar{S} \to \mathcal{M}$ is a Riemannian isometry.

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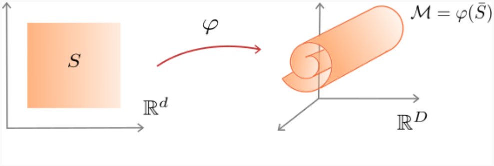

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Theorem (Hwang, Damelin, Hero (2016))

Let $(\mathcal{M}, g)$ be a closed smooth d-dimensional manifold with associated Riemannian distance $d_{\mathcal{M}}$. Let $\mathbb{X}_n \subseteq \mathcal{M}$ be a set of n independent sample points with common smooth density $f : \mathcal{M} \to \mathbb{R}_{>0}$.

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§ $L_{\mathbb{X}_n,p}(x,y) = \inf_{\gamma} \sum_{i=0}^{r} d_{\mathcal{M}}(x_{i+1}, x_i)^p$ over all paths $\gamma = (x_0, \ldots, x_{r+1})$ with $x_0 = x$, $x_{r+1} = y$ and $\{x_1, \ldots, x_r\} \subseteq \mathbb{X}_n$.

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Given $p > 1$ (and $q = (p-1)/d$), there exists $\mu = \mu(p, d) > 0$ such that for all $\varepsilon > 0$ and $b > 0$

$$\mathbb{P}\left(\sup_{x,y : d_{\mathcal{M}}(x,y) \geqslant b} \left| \frac{\frac{n^q}{\mu} L_{\mathbb{X}_n,p}(x,y)^{\S}}{d_{f,q}(x,y)} - 1 \right| > \varepsilon \right) \leqslant \exp(-\theta n^{1/(d+2p)})$$

for some $\theta = \theta(\varepsilon) > 0$ and sufficiently large n.

$^{\S} L_{\mathbb{X}_n,p}(x,y) = \inf_{\gamma} \sum_{i=0}^{r} d_{\mathcal{M}}(x_{i+1}, x_i)^p$ over all paths $\gamma = (x_0, \ldots, x_{r+1})$ with $x_0 = x$, $x_{r+1} = y$ and $\{x_1, \ldots, x_r\} \subseteq \mathbb{X}_n$.

Theorem 1 (Borghini, F., Groisman, Mindlin, 2020)

Let $(\mathcal{M}, g)$ be a closed smooth d-dimensional Riemannian manifold embedded in $\mathbb{R}^D$ with inherited metric tensor. Let $\mathbb{X}_n \subseteq \mathcal{M}$ be a set of n independent sample points with common smooth density $f : \mathcal{M} \to \mathbb{R}_{>0}$.

Given $p > 1$ and $q = (p-1)/d$, there exists a constant $\mu = \mu(p, d)$ such that for every $\lambda \in \big((p-1)/pd, 1/d\big)$ and $\varepsilon > 0$ there exist $\theta > 0$ satisfying

$$\mathbb{P}\left(\sup_{x,y\in\mathcal{M}} \left|\tfrac{n^q}{\mu} d_{\mathbb{X}_n,p}(x,y) - d_{f,q}(x,y)\right| > \varepsilon\right) \leqslant \exp\left(-\theta n^{\frac{1-\lambda d}{d+2p}}\right)$$

for n large enough.

‘Metric space’ learning

- **Population metric space**: $(\mathcal{M}, d_{f,q})$.
- **Sample metric space:** $\left(\mathbb{X}_n, \frac{n^q}{\mu} d_{\mathbb{X}_n,p}\right)$.

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- **Sample metric space:** $\left(\mathbb{X}_n, \frac{n^q}{\mu} d_{\mathbb{X}_n,p}\right)$.

Theorem 2 (Borghini, F., Groisman, Mindlin, 2020)

Given $p > 1$ and $q = (p-1)/d$, there exists a constant $\mu = \mu(p, d)$ such that for every $\lambda \in \big((p-1)/pd, 1/d\big)$ and $\varepsilon > 0$ there exist $\theta > 0$ satisfying

$$\mathbb{P}\left(d_{GH}\left(\left(\mathcal{M}, d_{f,q}\right), \left(\mathbb{X}_n, \tfrac{n^q}{\mu} d_{\mathbb{X}_n,p}\right)\right) > \varepsilon\right) \leqslant \exp\left(-\theta n^{(1-\lambda d)/(d+2p)}\right)$$

for n large enough.

Proof. Thm 1 + some additional work.

Intrinsic persistent homology

Convergence of persistence diagrams

- **Population persistence diagram**: $\mathrm{dgm}(\mathrm{Filt}(\mathcal{M}, d_{f,q}))$.
- **Sample persistence diagram**: $\mathrm{dgm}(\mathrm{Filt}(\mathbb{X}_n, \frac{n^q}{\mu} d_{\mathbb{X}_n,p}))$.

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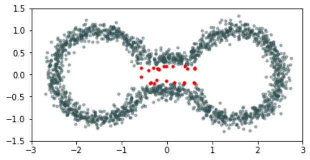
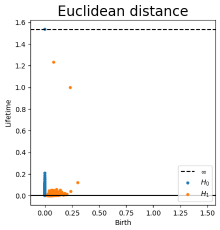
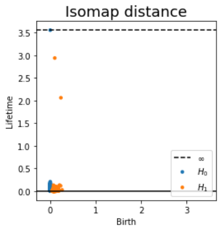
for n large enough.

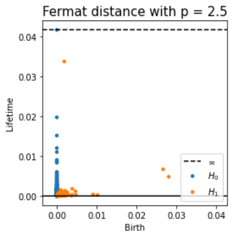
Proof. Thm 2 + Stability Thm.

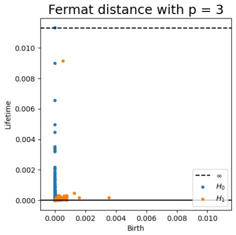
Example

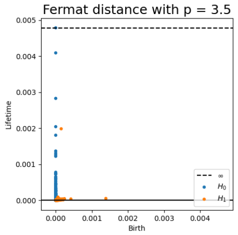



Euclidean distance
Lifetime
Birth
∞
H_0
H_1


Isomap distance
Lifetime
Birth
∞
H_0
H_1


Fermat distance with p = 2.5
Lifetime
Birth
∞
H_0
H_1

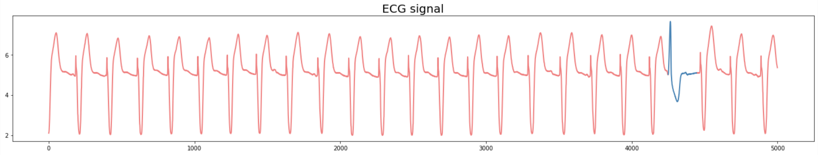

Fermat distance with p = 3
Lifetime
Birth
∞
H_0
H_1


Fermat distance with p = 3.5
Lifetime
Birth
∞
H_0
H_1

Applications

Time series: Anomaly detection

Electrocardiogram signal with abnormal heartbeat (arrhythmia).



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¶ Data from Physionet database, MIT Laboratory for Computational Physiology.

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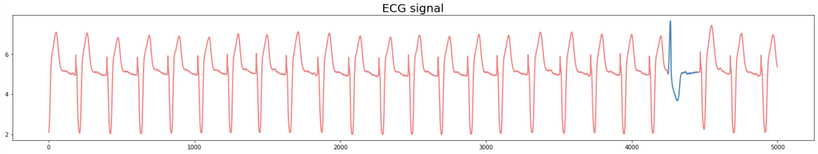

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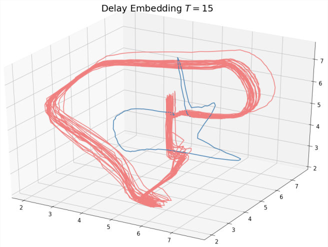

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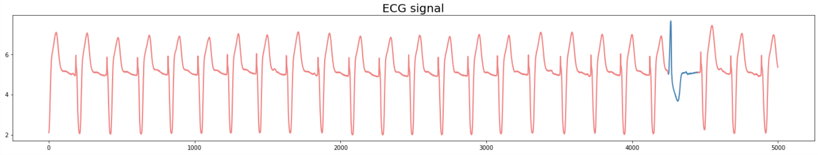

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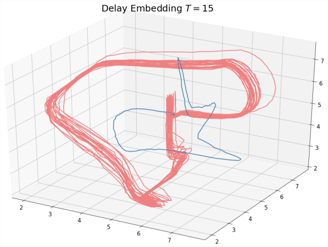
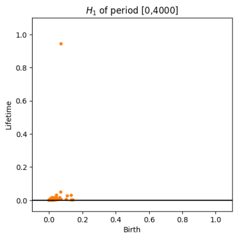
Persistence diagrams with Fermat distance for $p = 2$.





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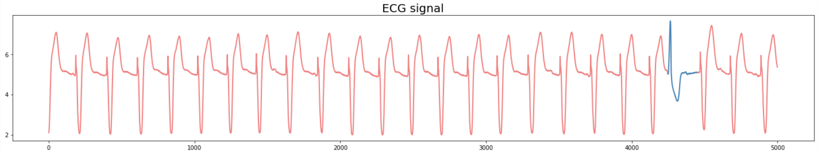

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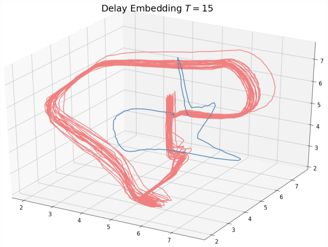

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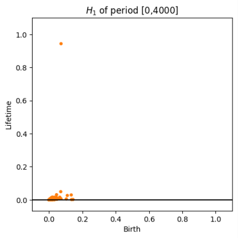
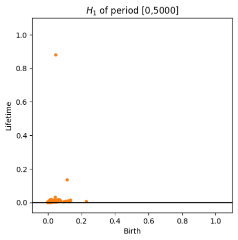
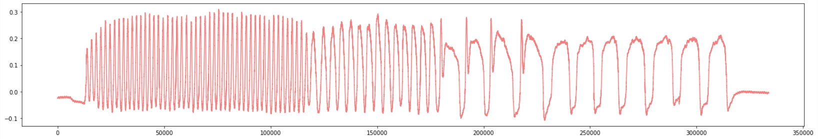




¶Data from Physionet database, MIT Laboratory for Computational Physiology.

Time series: Periodicity

Observation of the pressure in the air sacs of a canary during singing.



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‖ Data from experimental records, Laboratory of Dynamical Systems, Physics Department, University of Buenos Aires.

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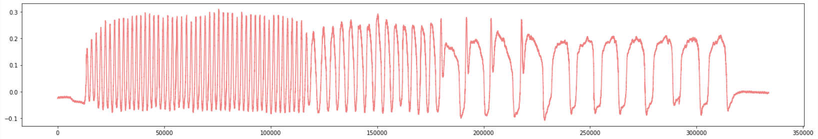

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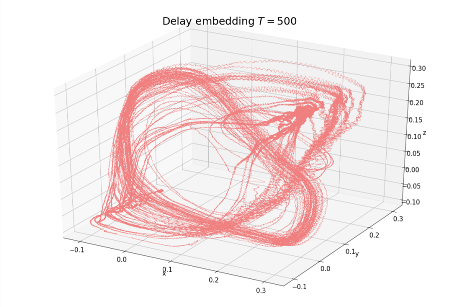

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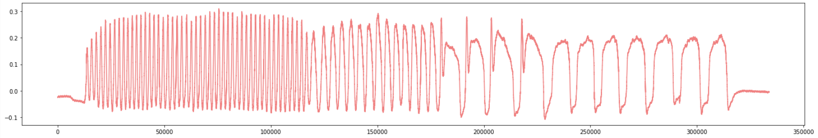

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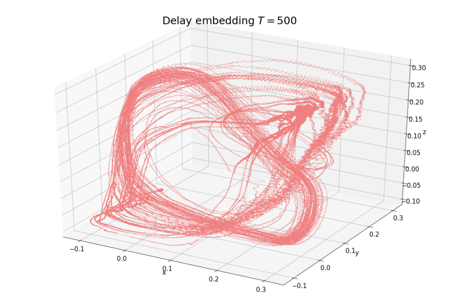
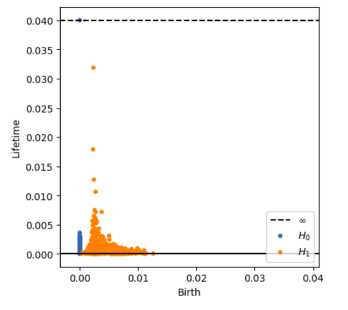


Persistence diagram Fermat distance $p = 1.5$.



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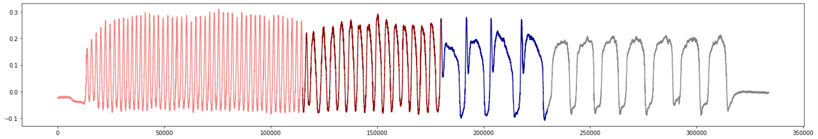
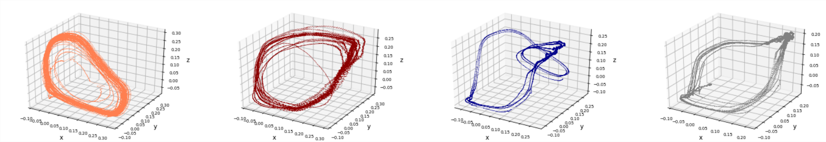
A canary song is composed by a concatenation of different syllabus patterns in the pressure in their air sacs.





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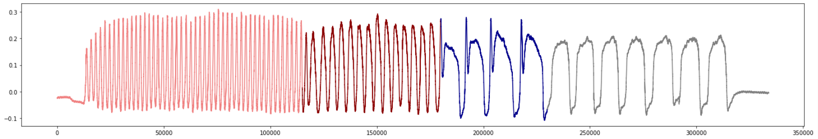

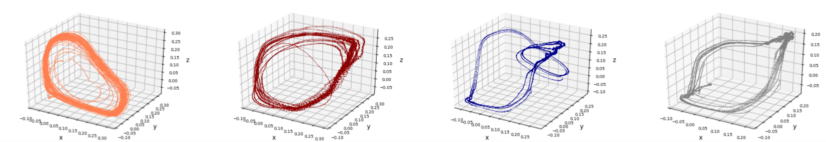

Work in progress: Fit parameters of physical models of the underlying dynamical system using this correspondence between pressure patterns and 1-dimensional cycles.

References

- *Preprint:* E. Borghini, X. F., P. Groisman, G. Mindlin. *Intrinsic persistent homology via density-based distance learning.* arXiv:2012.07621 (2020)
- *Code: https://github.com/ximenafernandez/intrinsicPH*
- *Python library:* `fermat`.

email: `x.l.fernandez@swansea.ac.uk`

Thanks for your attention!