



INTRINSIC PERSISTENT HOMOLOGY VIA DENSITY-BASED METRIC LEARNING

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

IMSI WORKSHOP ON TOPOLOGICAL DATA ANALYSIS

28th April 2021

EPSRC Centre for Topological Data Analysis



Prifysgol
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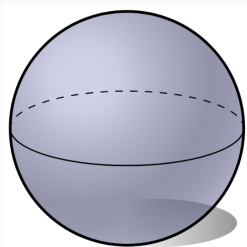
The problem

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

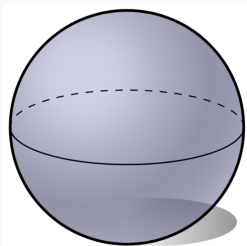


Metric learning in Riemannian manifolds

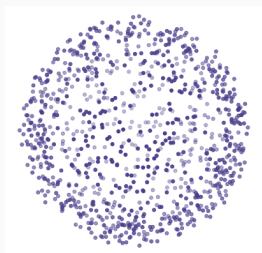
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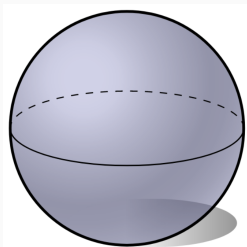


Metric learning in Riemannian manifolds

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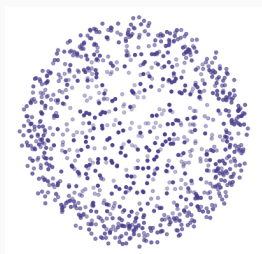
$$d_{\mathcal{M}}(x, y) = \inf_{\gamma} \int_I \sqrt{g(\dot{\gamma}_t, \dot{\gamma}_t)} dt,$$

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



$\mathbb{X}_n = \{x_1, x_2, \dots, x_n\}$ 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 $\gamma : I \rightarrow \mathcal{M}$ with $\gamma(0) = x$, and $\gamma(1) = y$.

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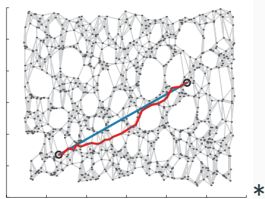
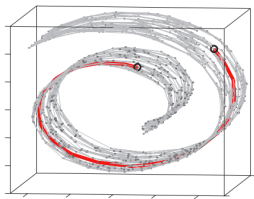
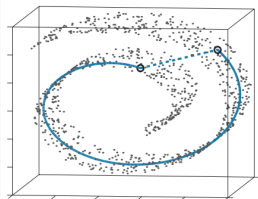
$$d_{\mathcal{M}}(x, y) = \inf_{\gamma} \int_I \|\dot{\gamma}_t\| dt$$

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

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



* 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} .

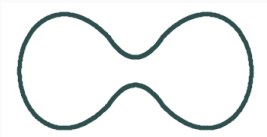
Assume $\varepsilon_n \rightarrow 0$ and $n\varepsilon_n^d \rightarrow \infty$. Then,

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

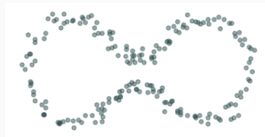
in probability, with almost sure convergence provided $n\varepsilon_n^d / \log n \rightarrow \infty$.

Dependence on ε (and density)

Manifold

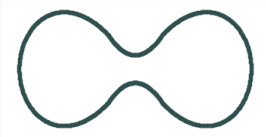


Noisy sample

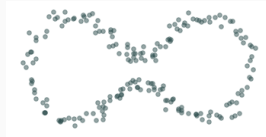


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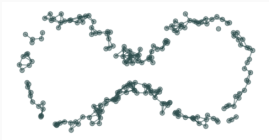


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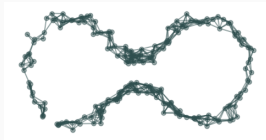


ε - graph

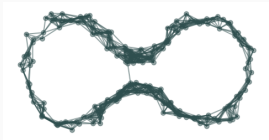
$\varepsilon = 0.2$



$\varepsilon = 0.3$



$\varepsilon = 0.4$

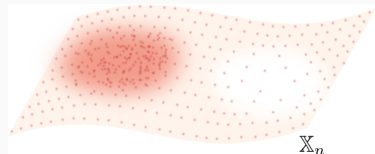


The manifold (and density) assumption

$\mathbb{X}_n = \{x_1, x_2, \dots, x_n\}$ 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 .

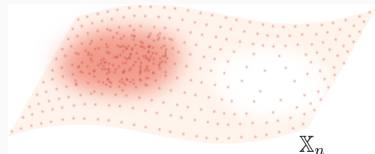


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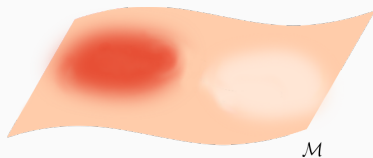
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(\mathcal{M}, g) a d -dimensional Riemannian manifold embedded in \mathbb{R}^D with $f : \mathcal{M} \rightarrow \mathbb{R}_{>0}$ a smooth density function.

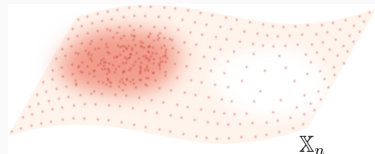


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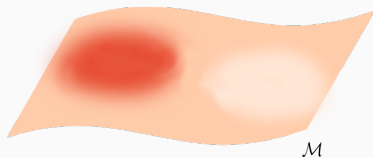
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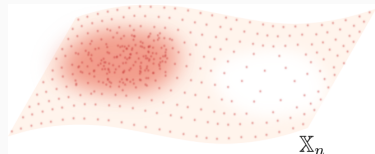
Consider a (new) Riemannian metric that depends on f .

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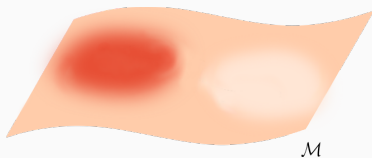
We assume that:

- \mathbb{X}_n lies in a d -dimensional Riemannian manifold \mathcal{M} ,
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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 $f : \mathcal{M} \rightarrow \mathbb{R}_{>0}$ a smooth density function.



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

Density-based metric learning

Deformed Riemannian metric

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

Deformed Riemannian metric

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

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

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

Deformed Riemannian metric

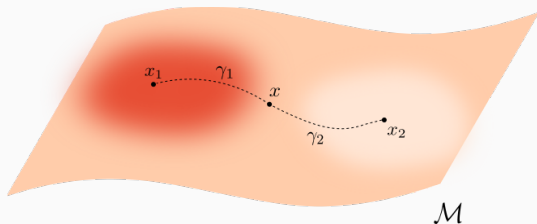
- Let (\mathcal{M}, g) be a **Riemannian manifold** and let $f : \mathcal{M} \rightarrow \mathbb{R}_{>0}$ be a smooth **density**.
- For $q > 0$, and consider the **deformed metric tensor**

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

- 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 $\gamma : I \rightarrow \mathcal{M}$ with $\gamma(0) = x$ and $\gamma(1) = y$.



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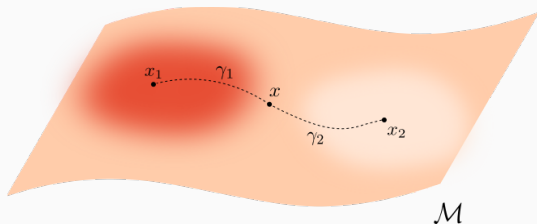
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Fermat distance

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

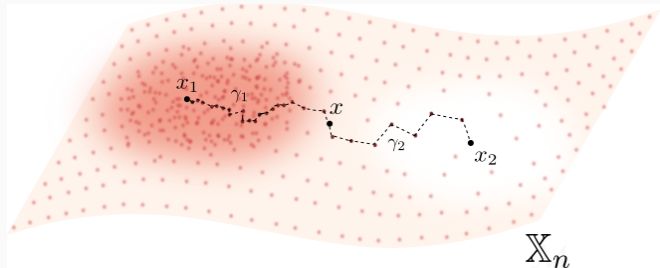
[†]Groisman, Jonckheere, Sapienza (2018), McKenzie and Damelin (2019).

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



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

Example

Manifold

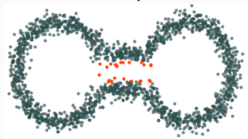


Example

Manifold



Sample

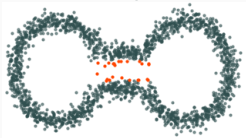


Example

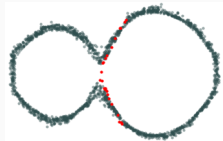
Manifold



Sample



Isomap

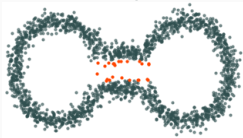


Example

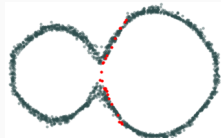
Manifold



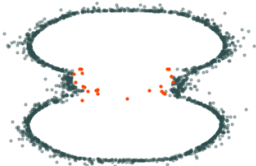
Sample



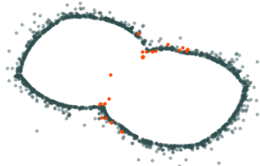
Isomap



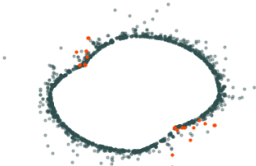
Fermat $p = 1.5$



Fermat $p = 2.0$



Fermat $p = 2.5$



Fermat $p = 3.0$



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 $f : \mathcal{M} \rightarrow \mathbb{R}_{>0}$.

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

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

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 $\varphi : \bar{S} \rightarrow \mathbb{R}^D$ such that $\varphi(\bar{S}) = \mathcal{M}$ and $\varphi : \bar{S} \rightarrow \mathcal{M}$ is a Riemannian isometry.

Previous work

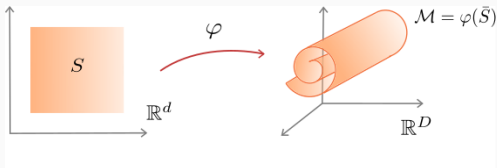
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Theorem (Hwang, Damelin, Hero (2016))

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 $f : \mathcal{M} \rightarrow \mathbb{R}_{>0}$.

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

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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 $b > 0$

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

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 $\gamma = (x_0, \dots, x_{r+1})$ with $x_0 = x$, $x_{r+1} = y$ and $\{x_1, \dots, x_r\} \subseteq \mathbb{X}_n$.

Density-based metric learning

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 $f : \mathcal{M} \rightarrow \mathbb{R}_{>0}$.

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

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

for n large enough.

'Metric space' learning

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

'Metric space' learning

- Population metric space: $(\mathcal{M}, d_{f,q})$.
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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 $\lambda \in ((p - 1)/pd, 1/d)$ and $\varepsilon > 0$ there exist $\theta > 0$ satisfying

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

for n large enough.

Proof. Thm 1 + some additional work.

Intrinsic persistent homology

Convergence of persistence diagrams

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

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Theorem 3 (Borghini, F., Groisman, Mindlin, 2020)

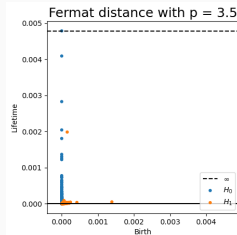
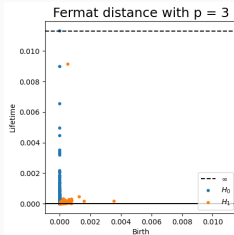
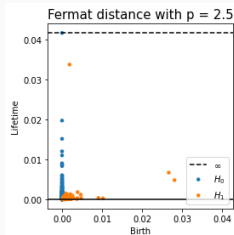
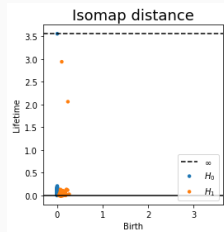
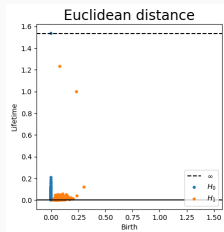
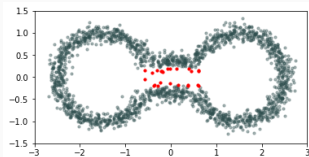
Given $p > 1$ and $q = (p - 1)/d$, there exists a constant $\mu = \mu(p, d)$ such that for every $\lambda \in ((p - 1)/pd, 1/d)$ and $\varepsilon > 0$ there exist $\theta > 0$ satisfying

$$\begin{aligned} \mathbb{P}\left(d_b(\text{dgm}(\text{Filt}(\mathcal{M}, d_{f,q})), \text{dgm}(\text{Filt}(\mathbb{X}_n, \frac{n^q}{\mu} d_{\mathbb{X}_n,p}))) > \varepsilon\right) \\ \leq \exp\left(-\theta n^{(1-\lambda d)/(d+2p)}\right) \end{aligned}$$

for n large enough.

Proof. Thm 2 + Stability Thm.

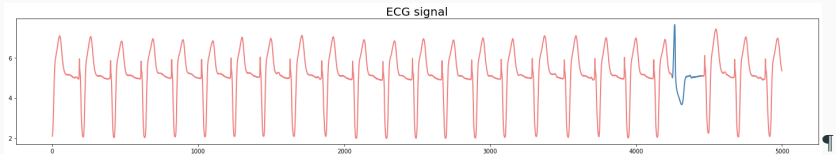
Example



Applications

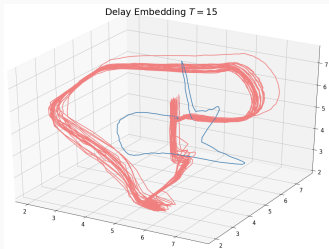
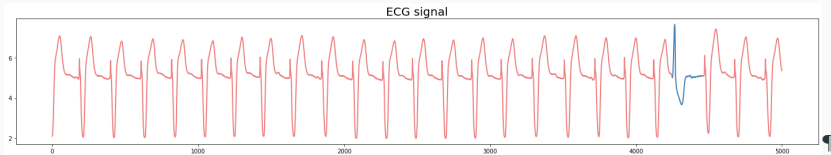
Time series: Anomaly detection

Electrocardiogram signal with abnormal heartbeat (arrhythmia).



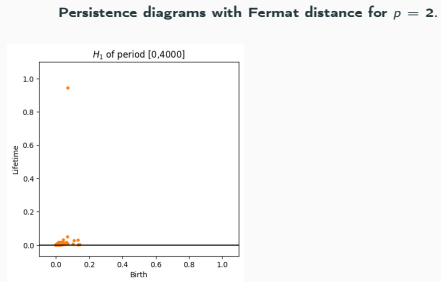
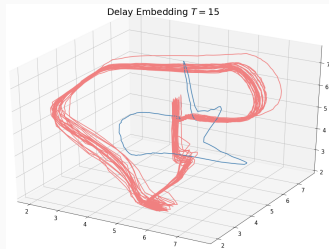
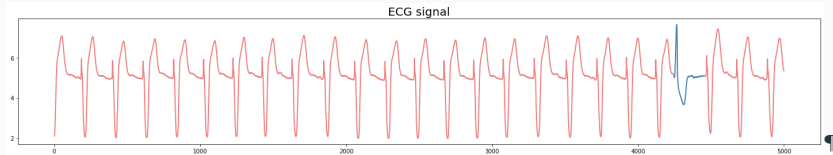
Time series: Anomaly detection

Electrocardiogram signal with abnormal heartbeat (arrhythmia).



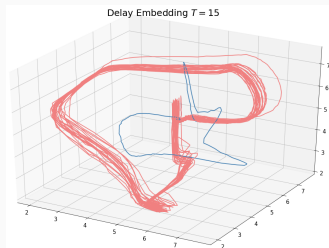
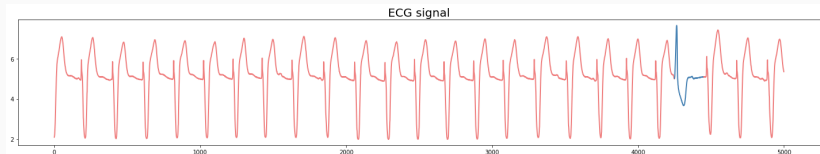
Time series: Anomaly detection

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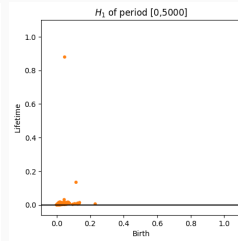
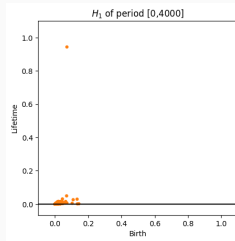


Time series: Anomaly detection

Electrocardiogram signal with abnormal heartbeat (arrhythmia).

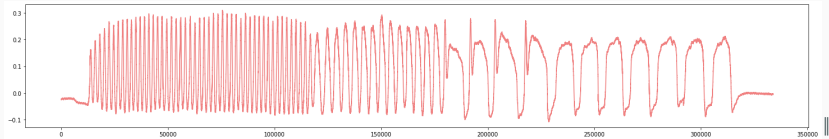


Persistence diagrams with Fermat distance for $p = 2$.



Time series: Periodicity

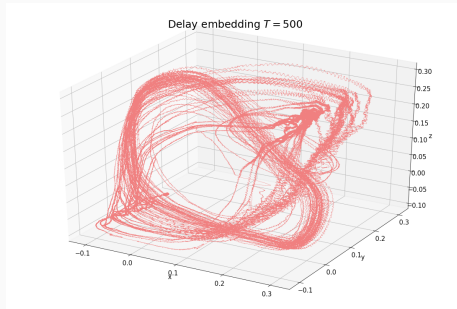
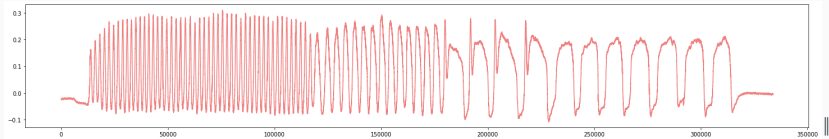
Observation of the pressure in the air sacs of a canary during singing.



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

Time series: Periodicity

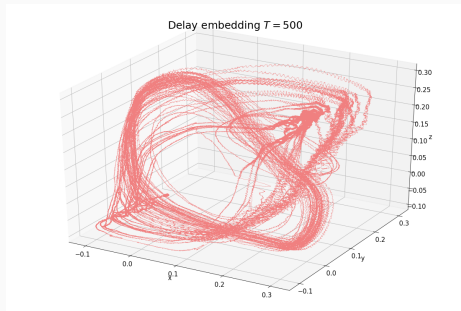
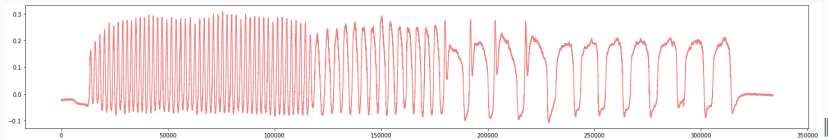
Observation of the pressure in the air sacs of a canary during singing.



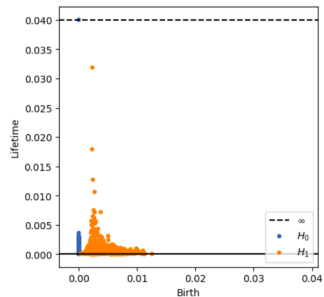
|| Data from experimental records, Laboratory of Dynamical Systems, Physics Department, University of Buenos Aires.

Time series: Periodicity

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



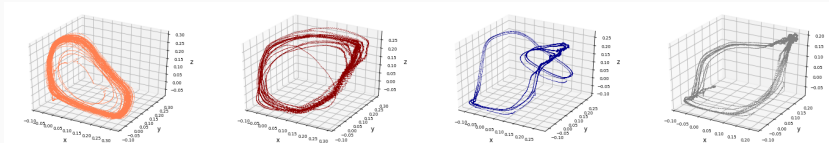
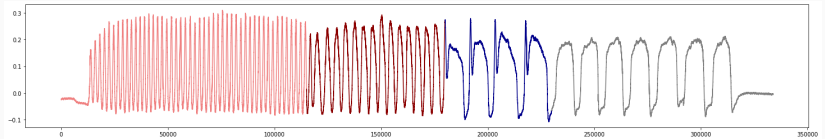
Persistence diagram Fernet distance $\rho = 1.5$.



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

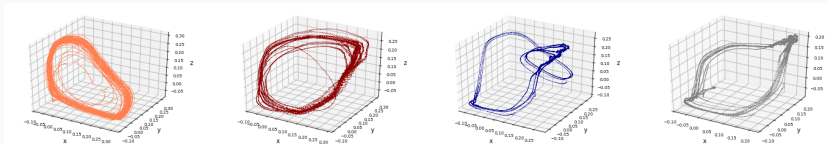
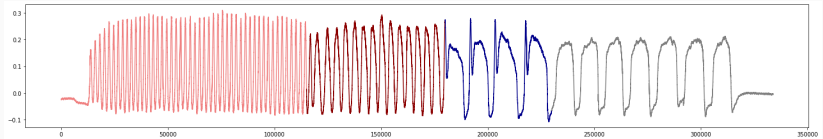
Time series: Periodicity

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



Time series: Periodicity

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



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

- *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!