(Largely pictorial) Intro to Topological Data Analysis

Outline

- motivation: gravitational wave detection

  → Brester & Jung (arXiv 1910.08245v1)

  → picking up signal from noise?

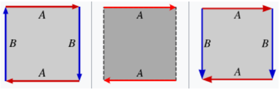
  → topological features i.e., **shape** of data
- time-series data and Takens embedding
- aspects of TDA

  → aspects of topology

  → (persistent) homology

  → topological features for machine learning pipelines
- extras if time/appetite...

Figure: Fluid flow on a Möbius strip. From Vanneste (2021), JFM.



Brester & Jung (2019)

Detection of gravitational waves using topological data analysis and convolutional neural network: An improved approach

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(Dated: October 21, 2019)

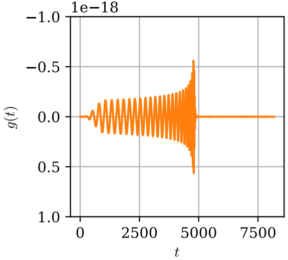
The gravitational wave detection problem is challenging because the noise is typically overwhelming. Convolutional neural networks (CNNs) have been successfully applied, but require a large training set and the accuracy suffers significantly in the case of low SNR. We propose an improved method that employs a feature extraction step using persistent homology. The resulting method is more resilient to noise, more capable of detecting signals with varied signatures and requires less training. This is a powerful improvement as the detection problem can be computationally intense and is concerned with a relatively large class of wave signatures.

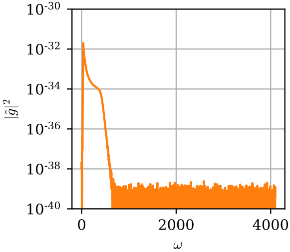
- Convolutional Neural Network (CNN) to detect GWs
- noise tends to swamp things, CNN as is generally no better than guessing...
- add **topological features**, helps it quite a bit even in low SNR regimes?

  $\rightarrow$ not terrible even when *only* topological features are included (see later)

  $\rightarrow$ only go up to H_0 and H_1 homologies here

Synthetic examples





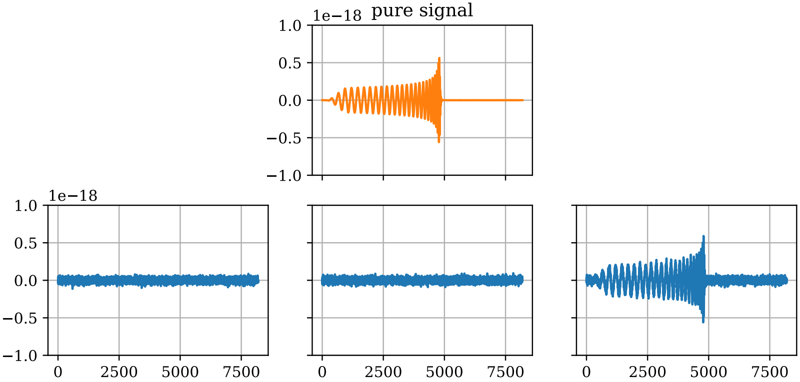
$$f = g + \frac{10^{-19}}{R}\xi, \qquad \xi \sim N(0,1)$$

- f the noisy signal
- g a synthetic gw signal

  $\rightarrow$ non-spinning binary black hole mergers here
- $R \in (0.075, 0.65)$ controls the SNR

  $\rightarrow$ SNR $\approx$ 10 or below

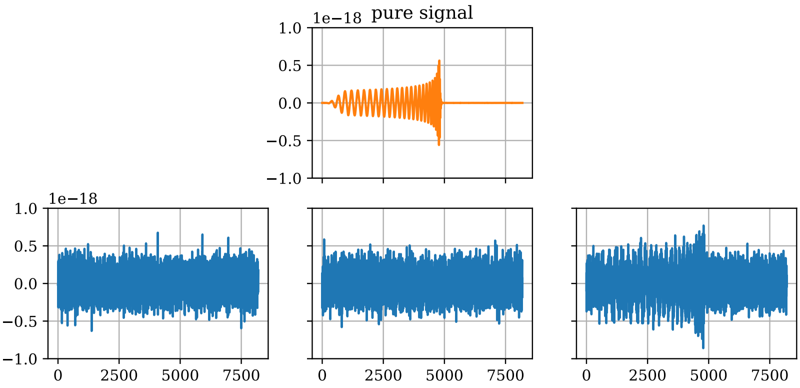
Synthetic signal



- Low noise regime ($R = 4$ because why not)

  $\rightarrow$ "obvious"

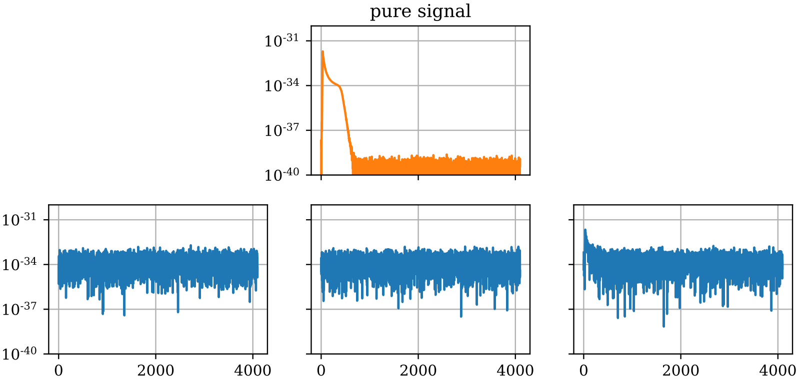
Synthetic signal



- Medium noise regime ($R = 0.65$ SNR $\approx$ 10?)

  $\rightarrow$ got lucky here, something visual

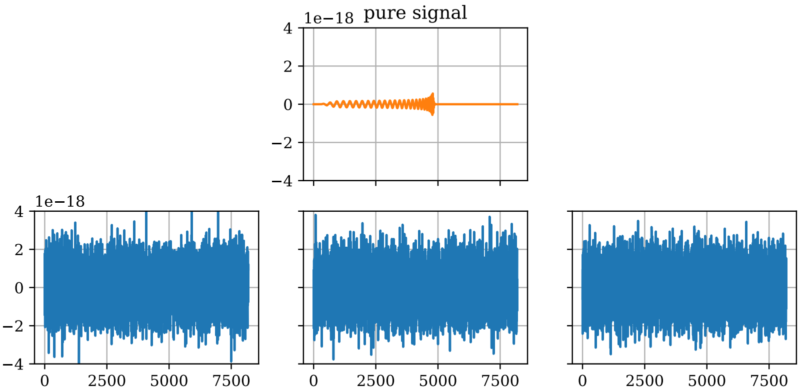
Synthetic signal



- Medium noise regime ($R = 0.65$ SNR $\approx$ 10?)

  $\rightarrow$ signal still ok in PSD

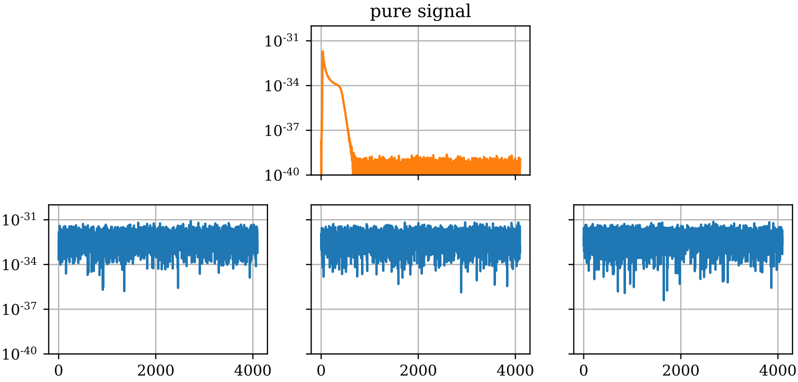
Synthetic signal



- Noisy regime ($R = 0.1$ SNR $\approx$ 3?)

  $\rightarrow$ ...nope

Synthetic signal



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  $\rightarrow$ ...still nope

Idea: shape of data

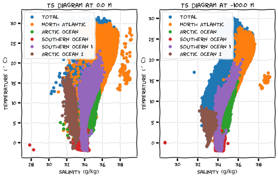

Figure: TS diagram from Argo data (with help from Fei Er Yan).

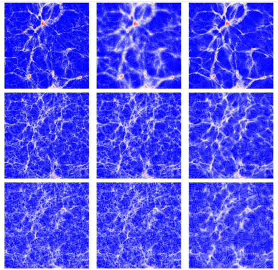

Figure: From Fig. 4 of Cheng, Chu & Tang (2015), JCAP.

- data might have a **shape**

  → noise might have one shape, structured data might have another

  → depends on embedding (a loop in 2d might be a curve in 3d)

  → topology ∼ shape information!

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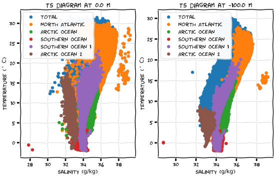

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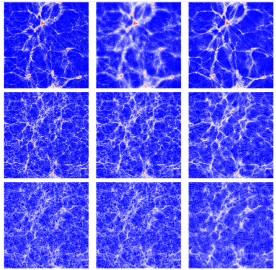

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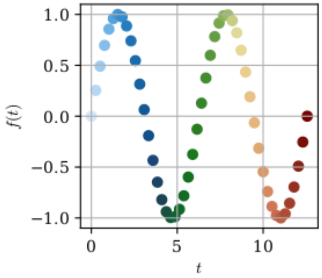
how to do this with time-series data?

Takens embedding: easy case

- semi-trivial example

$$f(t) = \sin(t) = [f(0), f(\Delta t), f(2\Delta t)\ldots] = [f_0, f_1, f_2, \ldots]$$



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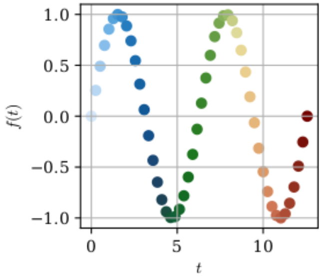
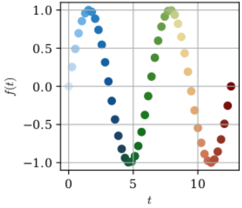
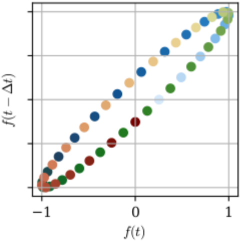


- why not

$$g(t) = \begin{pmatrix} f(t) \\ f(t-\Delta t) \end{pmatrix} = \begin{bmatrix} f_1, f_2, f_3, \ldots \\ f_0, f_1, f_2, \ldots \end{bmatrix} ?$$

Takens embedding: easy case





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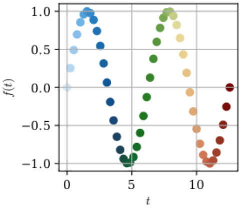

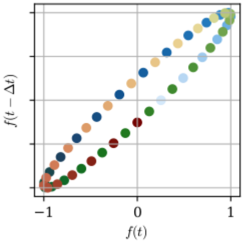

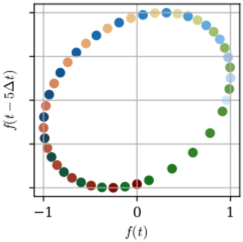

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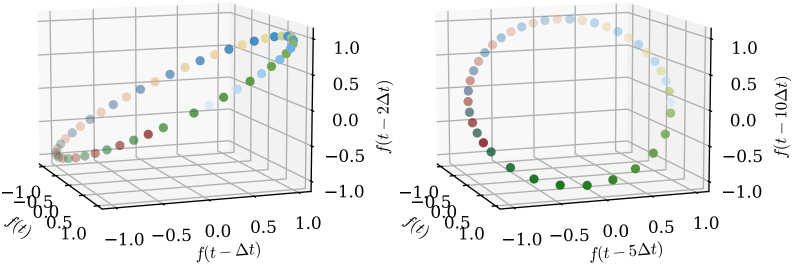
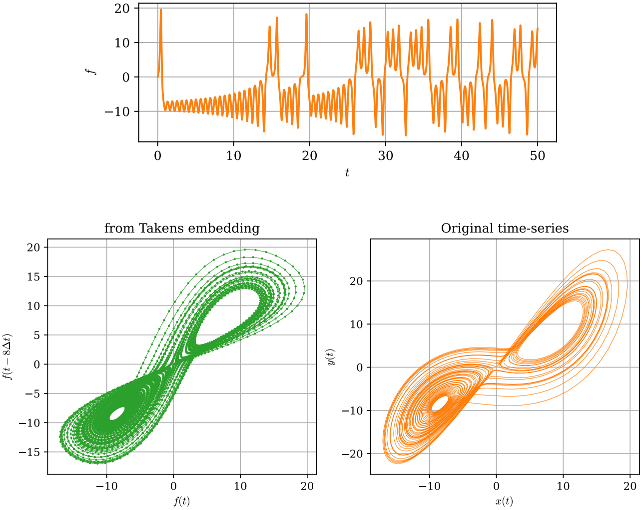


- seems to be fundamentally a 2d structure

  $\rightarrow$ embedding in 3d still 'looks' 2d (more fundamental reason for this)

  $\rightarrow$ has a 2d 'hole' (Betti number $\beta_1 = 1$, H_1 homology later)

Takens embedding: more interesting case



Takens's theorem

Takens (1981) proved that (paraphrasing a bit here):

- the delay transformation for finite dimensional manifolds is an embedding

  $\rightarrow$ think 'manifold' as that traced out by solution trajectory

  $\rightarrow$ embedding = no information loss

  $\rightarrow$ **upper bound** in dimension of delay embedding
- manifold structures are persevered up to **diffeomorphisms**

  $\rightarrow$ diffeomorphism $\Rightarrow$ topological equivalence

Figure: Floris Takens (1940-2010), Dutch mathematician + flautist.

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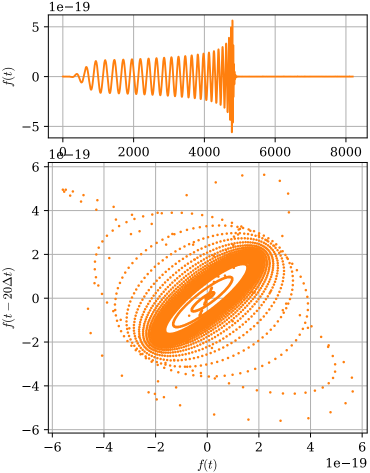
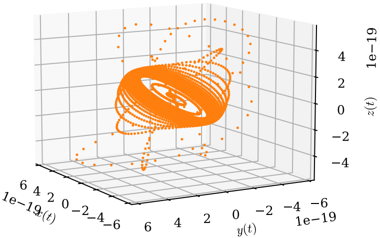
(above examples are solutions to 2d and 3d dynamical systems)

Takens embedding: gw case





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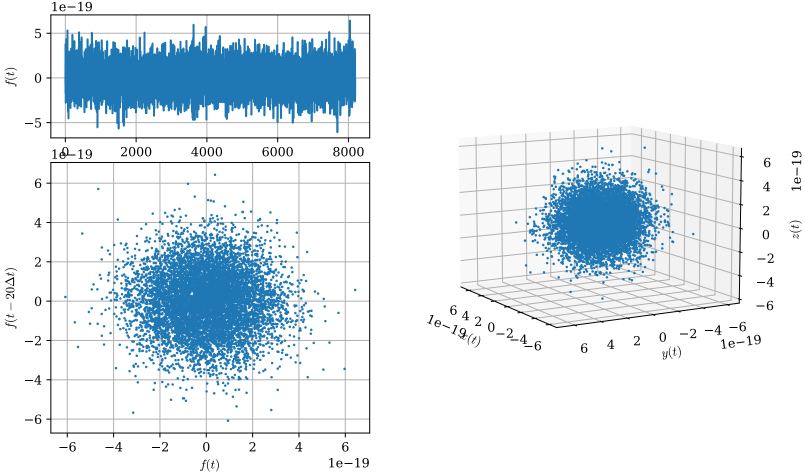

Some topology: equivalences

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Great, but how to measure the shape of data? Do something "coarser" (but more robust / global): how to measure **connectedness**?

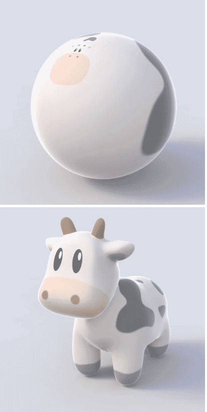

Figure: Two homotopy equivalent manifolds.

- topology, concerned with a space and **continuous** maps on it

  $\rightarrow$ two spaces are X and Y are **equivalent** if there is some map between them with appropriate properties

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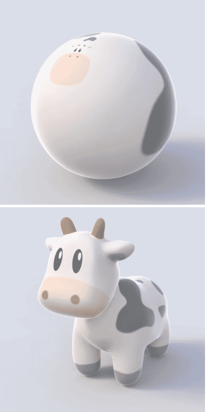

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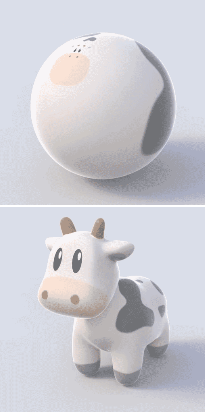

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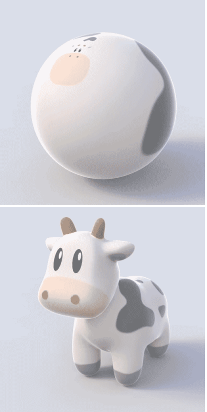

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  $\rightarrow$ cf. X and Y are homeomorphic, where $f \circ g$ and $g \circ f$ **is** the identity map

Some topology: homology and Betti numbers

- measure a topology by measuring its defects or holes

  $\rightarrow$ cf. classify a dynamical system by its singularities

  $\rightarrow$ implications if an inner product is also present (i.e., a **geometry**, e.g. **Gauss–Bonnet** linking curvature with Euler characteristic)

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- homotopic equivalence $\Rightarrow$ invariants, e.g. Betti numbers β_k:

  $\to \beta_0 =$ connected components

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(more formally, Betti numbers are the ranks of the homology group H_k with

$$H_k = \text{cycle group}/\text{boundary group} = \text{Ker } \partial_k / \text{Im } \partial_{k+1},$$

where ∂_k are boundary maps, and quotient groups are meant here)

Some topology: homology and Betti numbers

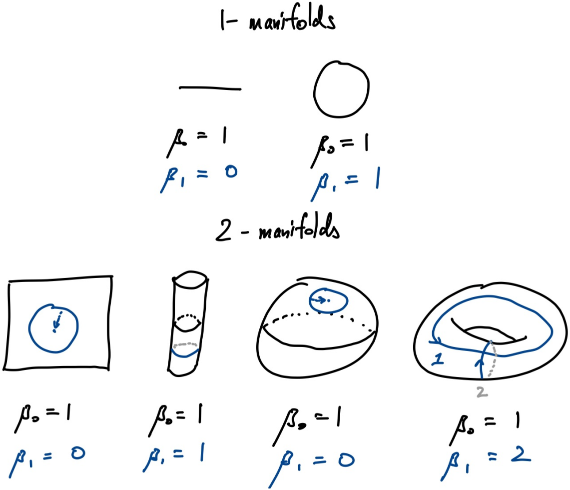
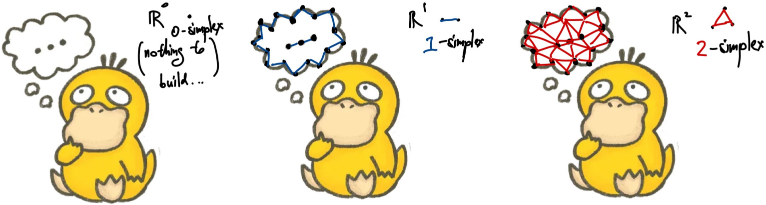


Figure: Some example manifolds and corresponding β_0 and β_1 values.

Some topology: simplicial complexes

- above is still by inspection, more algorithmically?
  → build up a manifold with simplicies (cf. a basis of sorts)



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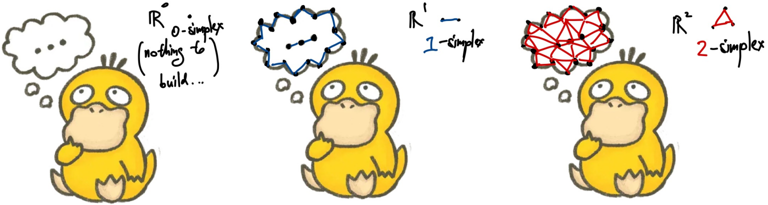

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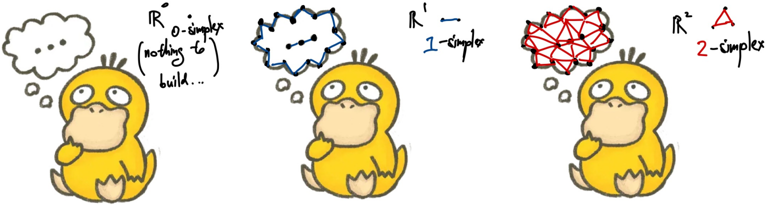

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  → β_0 number of connected components (disjoint chains)
  → β_1 the number of **closed** 1-chains (i.e. 1-cycles) that are NOT part of 2-simplicies
  → β_2 the number of 2-cycles that are NOT part of 3-simplicies etc.

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- so far we have a manifold split into simplicies, so how to use this for data that are point clouds to probe the underlying manifold?

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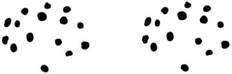

$\beta_0 = 15$
$\beta_1 = 0$

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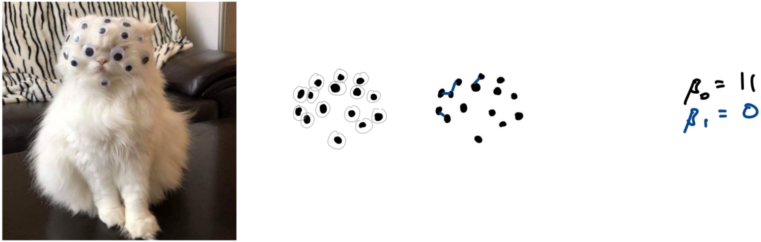

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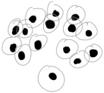

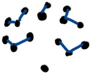

$\beta_0 = 6$
$\beta_1 = 0$

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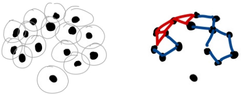

$\beta_0 = 2$
$\beta_1 = 3$

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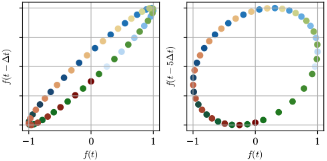
Some topology: persistent homology



- for the periodic signal example, expect H_1 hole to be persistent

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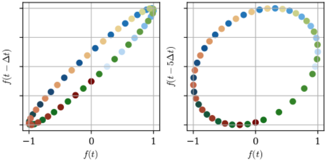
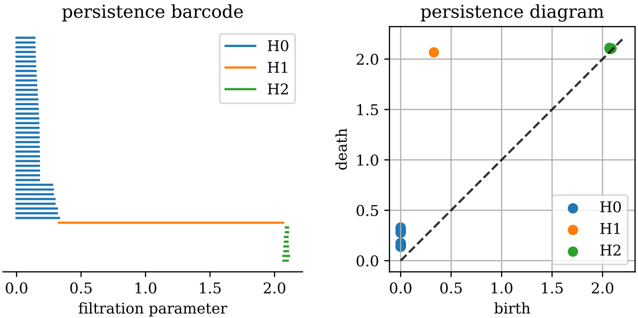
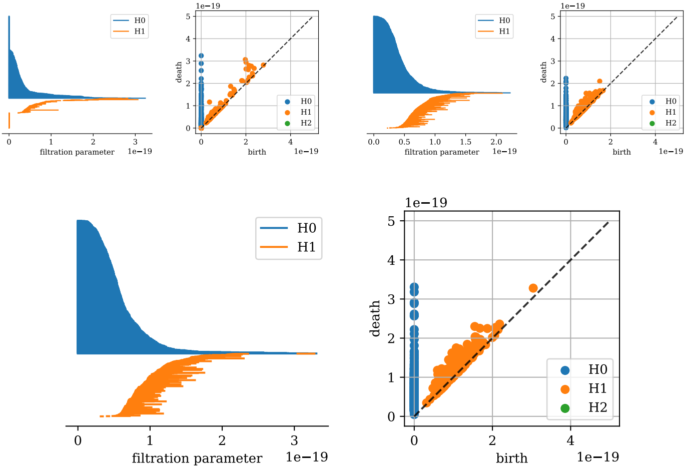


- for the periodic signal example, expect H_1 hole to be persistent
  $\rightarrow$ codify in a persistence barcode and diagram



Back to the GW case ($R = 0.65$)



Machine Learning pipeline

- lower R (high noise) case feature less obvious visually...

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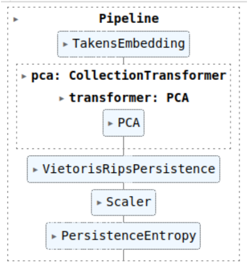
- ...but maybe who cares? Could throw that in a Machine Learning algorithm to train a classifier, e.g.,



Machine Learning pipeline

- simple demonstration with **logistic regression**

  $\rightarrow$ 1000 randomly generated samples, just topological features here

- ROC = Receiver operating characteristic, true positive rate against the false positive rate at each threshold setting
- AUC = Area under the ROC Curve, score for calculating, measure of skill for binary classifier (0.5 is crap, 0.9 onwards is pretty good, 1 is perfect)

In [49]:
```
print_scores(model)
```

```
Accuracy on train: 0.719
ROC AUC on train: 0.776
Accuracy on valid: 0.69
ROC AUC on valid: 0.769
```

In [50]:
```
#  1 = 1 - 0, so if model predicts signal when there isn't one (false positive)
#  0 = 1 - 1 or 0 - 0, when it did it right
# -1 = 0 -1, so if model fails to predict a signal when it is there (false negative)

dummy = model.predict(features) - labels
print(f" correct predictions {np.sum(dummy ==  0)} / {len(dummy)}")
print(f"   false positives   {np.sum(dummy ==  1)} / {len(dummy)}")
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```

```
 correct predictions 716 / 1000
   false positives   84 / 1000
   false negatives   200 / 1000
```

Machine Learning pipeline

- simple demonstration with **logistic regression**

  → 1000 randomly generated samples, just topological features here

  - ROC = Receiver operating characteristic, true positive rate against the false positive rate at each threshold setting
  - AUC = Area under the ROC Curve, score for calculating, measure of skill for binary classifier (0.5 is crap, 0.9 onwards is pretty good, 1 is perfect)

In [49]:
```
print_scores(model)
```

```
Accuracy on train: 0.719
ROC AUC on train: 0.776
Accuracy on valid: 0.69
ROC AUC on valid: 0.769
```

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- not complete garbage...? (certainly better than just doing it raw with the signal)

  → Brester & Jung do it with a CNN, larger ensemble of samples, include signal <u>and</u> topological features; works fairly well

Summary

- some concepts in TDA

  → convert signal to point cloud via Takens embedding

  → filtrations to generate a hierarchy of nested simplicial complexs

  → compute persistent homology, compute their ranks, and track their birth/death as a function of filtration

  → encode in persistence barcodes/diagrams

- topology fairly robust with noise

  → stability theorems of persistent features (not covered here)

  → add topological features into ML pipeline

Things not talked about + other ideas

- choice of complexes and/or persistence?

  $\rightarrow$ showed Čech, but Vietoris–Rips actually computed

  $\rightarrow$ other choices possible, depends on problem and nature of data

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  $\to$ barcodes (lines) and diagrams (dots) here

  $\to$ landscapes, Betti curves, images...(even better for ML features?)

  $\to$ talk about distances, statistics, (dis)similarities between features?

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  $\rightarrow$ essentially matrix reduction (extra slides if wanted)

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- links with category theory?

  $\rightarrow$ persistent homology as a functor

Credit + questions

Description here to aid in developing intuition, likely have holes in rigour. See following for more + extensions:

- online lectures/tutorials by Henry Adams, Bastian Grossenbacher Rieck, Robert Ghrist + Vidit Nanda
- "A user's guide to Topological Data Analysis" by Elizabeth Munch (short article)
- "Algebraic Topology for Data Scientists" by Michael Polstol (on arXiv)
- `giotto-tda` software package (`giotto-ai.github.io`)

Figure: Questions and/or headaches?

Extras: definitions

(Assuming some background in algebra)

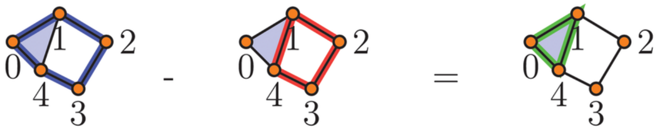

Figure: Example of homologous cycles. From Topaz, Ziegelmeier & Halverson (2014).

- σ a k-simplex with vertices $\{v_i\}_{i=0}^{k}$ with an ordering

  $\rightarrow$ assuming equivalence if ordering differ by an even permutation (i.e. element of S_k)

  $\rightarrow$ denote it $[v_0, v_1, \ldots v_k]$ (e.g., $[0, 1, 4]$ above is a 2-simplex)

  $\rightarrow$ a collection of these simplicies would be a simplicial complex K

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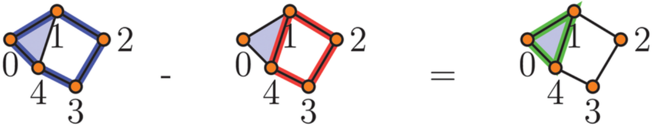

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  $\rightarrow$ a collection of these simplicies would be a simplicial complex K
- a k-chain is some formal sum

$$\sum_i n_i \sigma_i, \qquad n_i \in \mathbb{Z}, \quad \sigma_i \in K$$

(e.g. $2[0, 1] - 3[1, 2]$ above is a possible 1-chain)

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- can add chains together and still get a chain, i.e. **closure** under a **binary operation**

  $\rightarrow$ can show associativity, existence of inverse and identity element, so forms the chain group $C_k(K)$

  $\rightarrow$ if dim K is the highest dimension of a simplex in K, then $C_k(K) = 0$ for $k > \dim K$ or $k < 0$

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  $\rightarrow$ cycles form a subgroup of the chain group

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- a homomorphism known as the boundary operator ∂_k is such that

$$\partial_k : C_k(K) \rightarrow C_{k-1}(K), \quad [v_0, \dots v_k] \mapsto \sum_{i=0}^{k} (-1)^i [v_0, \dots \hat{v}_i, \dots v_k],$$

  i.e. an alternating sum ignoring each vertex $\hat{v}_i$

  (e.g. for a 2-simplex $[1, 2, 3]$, $\partial_2 [1, 2, 3] = [2, 3] - [1, 3] + [1, 2]$, which is a 1-cycle and boundary of the original 2-simplex, i.e. ∂_k guts the innards)

  $\rightarrow$ boundary cycles also form a subgroup of the chain group

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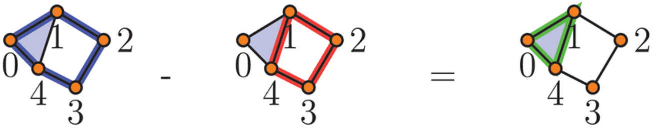

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- want to count "holes"

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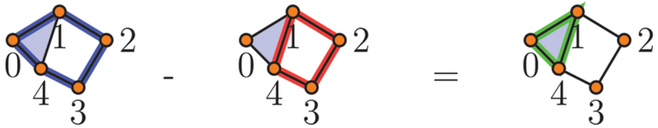

Figure: Example of homologous cycles. From Topaz, Ziegelmeier & Halverson (2014).

- want to count "holes"

  $\rightarrow$ "holes" being things that are not filled in
- argue here that the two cycles here encompass the same "hole"

  $\rightarrow$ cycles can be deformed into another via crossing the filled in 2-simplex (cf. homotopy)

  $\rightarrow$ two cycles here are homologous, count them as one under an equivalence relation

Extras: definitions

- want to count "holes"

  $\rightarrow$ want the number of k-cycles that are <u>NOT</u> boundaries of $(k+1)$-simplicies, i.e. throw away homologous cycles, i.e.,

  $$H_k = \frac{k\text{-cycles}}{k\text{-cycles that are boundaries of } (k+1)\text{-simplices}}$$

  under the homology equivalence relation
- with the boundary map ∂_k:

  $\rightarrow$ k-cycles if no boundaries, i.e. Ker ∂_k

  $\rightarrow$ boundaries of $(k+1)$-simplices are all the results of ∂_{k+1}, i.e., Im ∂_{k+1}

  $$\Rightarrow \boxed{H_k = \text{Ker } \partial_k / \text{Im } \partial_{k+1}},$$

  and $\beta_k = \text{rank}(H_k)$

Extras: computation

- suppose we have a triangle with $K = \{[1], [2], [3], [1, 2], [1, 3], [2, 3]\}$

  $\rightarrow$ note this triangle is not filled in, since we don't have $[1, 2, 3]$

1) For H_0,

- since $\partial_0 : C_0(K) \rightarrow C_{-1}(K) = \{0\}$, Ker ∂_0 is full rank and spanned by $\{[1], [2], [3]\}$
- Im ∂_1 is spanned by $\{[2] - [1], [3] - [1], [3] - [2]\}$, but $[3] - [2] = ([2] - [1]) + ([3] - [1])$, so rank of Im $\partial_1 = 2$
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2) For H_1,

- note that for Ker ∂_1 we want

$$
\begin{aligned}
0 &= n_1([2] - [1]) + n_2([3] - [1]) + n_3([3] - [2]) \\
&= -(n_1 + n_2)[1] + (n_1 - n_3)[2] + (n_2 + n_3)[3],
\end{aligned}
$$

  so if $n_3 = n_1$, we have $n_2 = -n_1$, so one degree of freedom, thus rank 1
- $C_2(K) = 0$ so Im ∂_2 is trivial
- so $\beta_1 = 1 - 0 = 1$, as expected

Extras: computation

- suppose triangle is filled in so $K = K + \{[1,2,3]\}$, then

1) For H_0,

- as before, $\beta_0 = 1$, as expected

2) For H_1,

- Ker ∂_1 is the same, but Im ∂_2 is now spanned by $\{[2,3] - [1,3] + [1,2]\}$, so has rank 1 (we have a 1-cycle)
- $\beta_1 = 1 - 1 = 0$, as expected, since there is no hole

3) For H_2,

- kernel is trivial and rank 0 since only a zero coefficient will make above span to be zero (or because there are no 2-cycles)
- image is trivial because there are no 3-simplicies
- $\beta_2 = 0 - 0 = 0$, also expected

Extras: computation

Not entirely elegant, but since we are talking about span, maybe we can leverage linear algebra to do some stuff

- there is a vector space structure, so the following is in fact justified
- for K the non-filled triangle, note that we have the boundary matrices

$$\partial_0(K) = \begin{array}{c} \begin{array}{ccc} [1] & [2] & [3] \end{array} \\ \begin{pmatrix} 0 & 0 & 0 \end{pmatrix} \end{array}, \qquad \partial_1(K) = \begin{array}{cc} \begin{array}{ccc} [1,2] & [1,3] & [2,3] \end{array} & \\ \begin{pmatrix} -1 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 1 \end{pmatrix} & \begin{array}{c} [1] \\ [2] \\ [3] \end{array} \end{array}$$

$$\partial_2(K) = \begin{array}{cc} [1,2,3] & \\ \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} & \begin{array}{c} [1,2] \\ [1,3] \\ [2,3] \end{array} \end{array}$$

(e.g., $\partial_1([1,2]+[2,3]-[1,3]) = \partial_1(1,-1,1)^T = 0$, as it should be since it is a 1-cycle)

Extras: computation

- reduce down to a Smith normal form (cf. Gaussian elimination), e.g. for ∂_1 above,

$$\begin{pmatrix} -1 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 1 \end{pmatrix} \to \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 1 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & -1 \\ 0 & 1 & 1 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

- can then just read stuff off

  $\to$ rank Ker ∂_k = number of zero columns of ∂_k

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- if K has filled in triangle, then $\partial_2 = (1, 0, 0)^T$ in the Smith normal form, so $\beta_1 = 1 - 1 = 0$, and $\beta_2 = 0 - 0 = 0$ as before

Extras: persistent homology

For a filtration of a complex K^i (indexed by i),

- p-persistent k^{th}- homology group is

$$H_k^{i,p} = \frac{k\text{-cycles}}{k\text{-boundaries} \cap k\text{-cycles}} = \frac{Z_k^i}{B_k^{i+p} \cap Z_k^i}$$

- the persistent Betti numbers $\beta_k^{i,p}$ associated with $H_k^{i,p}$ can be defined accordingly

  $\rightarrow$ the rank of the free part of $H_k^{i,p}$

- persistent homology is stable in a precise sense

  $\rightarrow$ persistence diagrams have bounded difference in the bottleneck distance to perturbations in input filtration (Cohen-Steiner, Edelsbrunner & Harer, 2006)

Extras: categories and functors

- a category $C = (\text{object}, \text{morphism})$

  $\rightarrow$ morphisms are maps between the objects in a category, e.g.

  $\rightarrow$ groups and homomorphisms

  $\rightarrow$ topological spaces and continuous maps

  $\rightarrow$ sets and functions

  $\rightarrow$ vector spaces and linear transformations

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- functors map categories to each other

  $\rightarrow$ homology mapping category of topological spaces to category of graded groups

- idea (?)

  $\rightarrow$ results from category-theoretic studies apply generally

  $\rightarrow$ results in other fields can have analogs in other fields

  (e.g. used a lot in computer science, applications in categorical quantum mechanics and quantum information)