An Introduction to Persistent Homology

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Descriptors of Energy Landscapes Using Topological Analysis

3N Energy Landscape (Simulation/Experiment) → Dimensionality Reduction → Topology of Reduced Energy Landscapes → Predictive Machine Learning → Accelerated Sampling

- PCA
- Non-linear Methods
- Generalized Collective Coordinates
- Morse Theory
- Persistent Homology
- Catastrophe Theory
- Singularity Theory

- Optimized Synthetic Conditions
- Phase Behavior
- Tuning Catalytic Pathways

Energy
An Introduction to Persistent Homology

1. Review of topology and homology
2. Introduction to persistent homology
3. Sublevel set persistent homology
4. Persistent homology applied to point cloud data
An Introduction to Persistent Homology

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A donut and coffee mug are “homotopy equivalent” and considered to be the same shape. You can bend and stretch (but not tear) one to get the other.
torus has a Betti sequence (1, 2, 1, 0, 1), since it has a single connected component, two different loops that cannot be deformed into a point (shown in red in the bottom panel of Figure 2c), and there is a two-dimensional surface that cannot be deformed into a point (shown in orange in Figure 2c). The Klein bottle has the same sequence as the torus (1, 2, 1, 0, 1). This shows that while two objects that are equivalent must have the same Betti sequences, two objects that are not equivalent do not necessarily have different sequences. Finally, a sphere has a sequence (1, 0, 1, 0, 1), as any one-dimensional loop on its surface can be deformed into a point. The Betti sequence therefore provides a signature (albeit not unique) of the underlying topology of the object.

These definitions work for smooth continuous objects. But suppose now that instead of a continuous rubbery object we are faced with a finite set of (noisy) points sampled from it, which may represent actual experimental data. How can one estimate the Betti numbers of the original object from these samples? The proposed method...
Topology studies shapes

Torus
Topology studies shapes

Klein bottle
Topology studies shapes

Klein bottle

Image credit: https://plus.maths.org/content/imaging-maths-inside- klein-bottle
Homology

- $i$-dimensional homology $H_i$ “counts the number of $i$-dimensional holes”
- $i$-dimensional homology $H_i$ actually has the structure of a vector space!

0-dimensional homology $H_0$: rank 6
1-dimensional homology $H_1$: rank 0


0-dimensional homology $H_0$: rank 1
1-dimensional homology $H_1$: rank 3


0-dimensional homology $H_0$: rank 1
1-dimensional homology $H_1$: rank 6
Homology

- $i$-dimensional homology $H_i$ “counts the number of $i$-dimensional holes”
- $i$-dimensional homology $H_i$ actually has the structure of a vector space!

0-dimensional homology $H_0$: rank 1
1-dimensional homology $H_1$: rank 0
2-dimensional homology $H_2$: rank 1

Be careful! (Same as torus over $\mathbb{Z}/2\mathbb{Z}$)

Image credit: https://plus.maths.org/content/imaging-maths-inside-klein-bottle
The torus has a Betti sequence (1, 2, 1, 0), since it has a single connected component, two different loops that cannot be deformed into a point (shown in red in the bottom panel of Figure 2c), and there is a two-dimensional surface that cannot be deformed into a point (shown in orange in Figure 2c). The Klein bottle has the same sequence as the torus (1, 2, 1, 0). This shows that while two objects that are equivalent must have the same Betti sequences, two objects that are not equivalent do not necessarily have different sequences. Finally, a sphere has a sequence (1, 0, 1, 0), as any one-dimensional loop on its surface can be deformed into a point. The Betti sequence therefore provides a signature (albeit not unique) of the underlying topology of the object.

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Homology equivalent shapes have the same homology!

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In the context of topological data analysis, persistent homology is a powerful tool for estimating the topology of an unknown space from a finite set of samples. This method is particularly useful in scenarios where the underlying space is complex and not easily discernible from the data alone.

The key idea behind persistent homology is to build a nested family of simplicial complexes, increasing in complexity, and then to apply persistent homology to track the birth and death of topological features as the complexes are constructed.

Let's consider an example. Suppose we have a dataset represented as a collection of points in a space. We can build a Vietoris–Rips simplicial complex from this dataset, where the points are the vertices of the complex, and the edges are formed between points that are within a certain distance of each other.

As we increase the threshold distance, we construct a sequence of nested complexes. Each complex in this sequence represents the topology of the underlying space at a different resolution. Persistent homology then allows us to analyze the evolution of topological features as the complexes grow.

The persistent homology barcode is a visual representation of the birth and death of these features. Each horizontal line segment in the barcode corresponds to a topological feature, and the length of the segment reflects the persistence of the feature, i.e., the range of scales over which the feature exists.

For instance, if we have a dataset that contains two loops, we would expect to see two persistent homology features in the barcode, each corresponding to one of the loops. The horizontal segments in the barcode would indicate when these loops first appear (birth) and when they disappear (death) as the distance threshold increases.

In the figure, we see four nested Vietoris–Rips complexes, each differing in the threshold distance used to define the edges of the complex. The persistent homology barcode associated with the dataset is shown below the complexes, illustrating the birth and death of topological features.

Here are the features of the barcode:
- **H_0**: Represents the number of connected components.
- **H_1**: Represents the number of 1-dimensional holes (loops).

**Input:** Increasing spaces. **Output:** Barcode. Significant features persist.

The cubic computational time is a significant consideration in practical applications of persistent homology. The complexity of the computation increases cubically with the number of simplices in the complex.
persistent homology

Significant features persist.
Cubic computation time in the number of simplices.
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Given a space $X$ and a real-valued function $f : X \rightarrow \mathbb{R}$, the sublevel set for $a \in \mathbb{R}$ consists of all the points in $X$ with $f(x) \leq a$.

Example: $f(x) = x^2 - y^2$ on $X = [-1,1] \times [-1,1]$.

Input: Real-valued function on a space. Output: barcode.
Input: Real-valued function on a space. Output: barcode.
Analysis of Kolmogorov flow and Rayleigh–Bénard convection using persistent homology by Miroslav Kramár, Rachel Levanger, Jeffrey Tithof, Balachandra Suri, Mu Xu, Mark Paul, Michael F Schatz, Konstantin Mischaikow.
Sublevel set persistent homology

Input: Real-valued function on a space. Output: barcode.
Sublevel set persistent homology

EL (PageRank) of ion-pair formation of Na\(^+\) and OH\(^-\): superlevel sets

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Nucleophilic attack EL: sublevel sets
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Question: How does sublevel set persistent homology relate to Morse-Smale complexes (and TTK)?

Answer: Sublevel set persistent homology encodes most of the topology, but little of the geometry, in the Morse-Smale complex.
Sublevel set persistent homology

• **Stability Theorem.** If \( f \) and \( g \) are real-valued functions on a space, \( X \), and \( U_f \) and \( U_g \) are the barcodes of the associated sublevel set filtrations, then

\[
d_B(U_f, U_g) \leq \|f - g\|_\infty = \max_{x \in X} |f(x) - g(x)|
\]
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Datasets have shapes

Example: Diabetes study
145 points in 5-dimensional space

An attempt to define the nature of chemical diabetes using a multidimensional analysis by G. M. Reaven and R. G. Miller, 1979
Datasets have shapes
Example: Cyclo-Octane (C₈H₁₆) data
1,000,000+ points in 24-dimensional space

*Non-Manifold Surface Reconstruction from High Dimensional Point Cloud Data*
by Shawn Martin and Jean-Paul Watson, 2010.
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What shape is this?
Definition

For metric space $X$ and scale $r \geq 0$, the Vietoris–Rips simplicial complex $\text{VR}(X; r)$ has vertex set $X$ and finite simplex when $\text{diam}(X) \leq r$. 

\[ C_{\text{VR}(X; r)} \]
Definition

For metric space $X$ and scale $r > 0$, the Vietoris–Rips simplicial complex $\text{VR}(X; r)$ has a finite simplex when $\text{diam}(X) \leq r$. 
Definition

For metric space $X$ and scale $r \geq 0$, the Vietoris–Rips simplicial complex $\text{VR}(X; r)$ has its vertex set equal to $X$ when $\text{diam}(X) \leq r$. 
Definition

For metric space \( X \) and scale \( r \geq 0 \), the Vietoris–Rips simplicial complex \( \text{VR}(X; r) \) has vertex set \( X \) finite simplex when \( \text{diam}(X) \leq r \).
Definition

For a metric space $X$ and a scale $r \geq 0$, the Vietoris–Rips simplicial complex $\mathcal{VR}(X; r)$ has the vertex set $X$ and a finite simplex when $\text{diam}(X) \leq r$. 
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For metric space $X$ and scale $r \geq 0$, the Vietoris–Rips simplicial complex $\mathcal{VR}(X; r)$ has vertex set $X$ with a finite simplex when $\text{diam}(X) \leq r$. 
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For a metric space $X$ and a scale $r \geq 0$, the Vietoris–Rips simplicial complex $VR(X; r)$ has a finite simplex when $\text{diam}(X) \leq r$. 

![Diagram of points and circles representing the Vietoris–Rips complex](image)
Definition

For a data set $X \subseteq \mathbb{R}^n$ and scale $r \geq 0$, the Čech simplicial complex $\check{\text{Čech}}(X; r)$ has

- vertex set $X$
- finite simplex $\{x_0, x_1, \ldots, x_k\}$ when $\cap_{i=0}^k B(x_i, r) \neq \emptyset$. 

Definition

For a data set $X \subseteq \mathbb{R}^n$ and scale $r \geq 0$, the Čech simplicial complex $\check{\text{C}}ech(X; r)$ has

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**Nerve Lemma.** \( \check{\text{Čech}}(X; r) \simeq \text{union of balls} \)

**Definition**

For a data set \( X \subseteq \mathbb{R}^n \) and scale \( r \geq 0 \), the \( \check{\text{Čech simplicial complex}} \) \( \check{\text{Čech}}(X; r) \) has

- vertex set \( X \)
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Persistent homology applied to data

Significant features persist.
Cubic computation time in the number of simplices.
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Example: Cyclo-Octane (C₈H₁₆) data

1,000,000+ points in 24-dimensional space

Non-Manifold Surface Reconstruction from High Dimensional Point Cloud Data
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3.5. Run times

The run times for the nine examples we have investigated are shown in Table 2. These times were obtained on a 2.26 GHz Intel Xeon dual quadcore workstation with 16 GB of RAM. The algorithm was implemented in Matlab (www.mathworks.com) using the optimization toolbox to solve the linear program in (6).

Table 2 shows that pre-processing is negligible except for the non-manifold examples. In the case of the non-manifold examples, the pre-processing is generally faster than the triangulation.

4. Application

Cyclo-octane is a saturated eight-member cyclic compound with chemical formula C_8H_16. Cyclo-octane has received attention in computational chemistry because it has multiple conformations of similar energy, a complex potential energy surface, and significant (steric) influence from the hydrogen atoms on preferred conformations [32–34]. Cyclo-octane is also interesting because there are enumerative algorithms available which can provide a dense sampling of the conformation space [35,36]. These algorithms show from first principles that the resulting conformation space has two degrees of freedom, suggesting that the space is a surface (but not necessarily a manifold).

Using dimension reduction methods, we have previously analyzed the cyclo-octane conformation space [16]. In our analysis, we used a dataset of 1,031,644 cyclo-octane conformations, enumerated using the triaxial loop closure algorithm of Coutsias et al. [35]. Each conformation is placed in Cartesian space via the 3D position coordinates of each atom in the molecule. The conformations are then aligned to a reference conformation such that the Eckart conditions are satisfied [37].

The final positions of a given conformation are concatenated to obtain a vector in R^{72}. The resulting collection is a dataset \{x_i\}_{i=1}^{1,031,644} \subset R^{72} which is presumed to describe a surface. In Brown et al. [16] we applied a variety of dimension reduction methods to the cyclo-octane dataset, one of which was Isomap [38]. A summary of our analysis using the Isomap reduction is shown in Fig. 7.

Beyond dimension reduction, the next step in our analysis is surface reconstruction. Unfortunately, the Isomap representation of the cyclo-octane conformation space is only a visualization, and is not accurate enough for use with a 3D surface reconstruction method. Therefore we applied Freedman's algorithm for surface reconstruction in the original high-dimensional conformation space. Freedman's method failed because the surface had self-intersections of the type discussed in this paper. Thus we developed our method for non-manifold surface reconstruction and applied it to the cyclo-octane dataset.

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• Stability Theorem.
  If $X$ and $Y$ are metric spaces, then

$$d_b \left( \text{PH}(\check{\text{Cech}}(X)), \text{PH}(\check{\text{Cech}}(Y)) \right) \leq 2d_{GH}(X, Y)$$
Why is applied topology popular when few datasets have Klein bottles?

- Many datasets have clusters & flares (as in the diabetes example)
- Motivates interesting questions in many pure disciplines: mathematics, computer science (computational geometry), statistics
- Interest from domain experts in biology, neuroscience, computer vision, dynamical systems, sensor networks, ...
- Materials science, pattern formation
- Machine learning: small features matter
- Agent-based modeling (swarming)

Possible answer: Persistent homology measures both the local geometry and the global topology of a dataset.

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Conclusions

- Persistent homology can be applied to any increasing sequence of spaces, measuring some of the local and global topology.
- The two most common versions of persistent homology are sublevel set persistence and persistence applied to point cloud data.

“Topology! The stratosphere of human thought! In the twenty-fourth century it might possibly be of use to someone …”

- Aleksandr Solzhenitsyn, *The First Circle*
Topology applied to image data
The receptive fields of cells in our primary visual cortex (V1) are related to the statistics of natural images.

*Independent component filters of natural images compared with simple cells in primary visual cortex* by JH van Hateren and A van der Schaaf, 1997
Persistent homology applied to data

3x3 high-contrast patches from images
Points in 9-dimensional space, normalized to have average color gray and contrast norm one (on 7-sphere).

Persistent homology applied to data

1. Densest patches according to a global estimate
Persistent homology applied to data

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Interpretation: nature prefers linearity
Persistent homology applied to data

2. Densest patches according to an intermediate estimate
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2. Densest patches according to an intermediate estimate

Interpretation: nature prefers horizontal and vertical directions
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3. Densest patches according to a local estimate
Persistent homology applied to data

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3. Densest patches according to a local estimate
3. Densest patches according to a local estimate

Interpretation: nature prefers linear and quadratic patches at all angles

Image credit: https://plus.maths.org/content/imaging-maths-inside-klein-bottle
Zigzag persistent homology

Form zigzag module for $X \to I$ with $(d - 1)$–dimensional homology.
Zigzag persistent homology

Form zigzag module for $X \to I$ with $(d - 1)$-dimensional homology.
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Form zigzag module for $X \to I$ with $(d - 1)$–dimensional homology.
**Zigzag persistent homology**

Form zigzag module for $X \to I$ with $(d-1)$-dimensional homology.

- **Theorem.**
  If there is an evasion path then there is a full-length bar.
Where can I find resources if I am interested in applied topology?

- You may be interested in the Applied Algebraic Topology Research Network. Become a member to receive email invites to the online research seminars. Recorded talks are available at the YouTube Channel. There is also a forum.
- Another source of applied topology news is appliedtopology.org.
- A second online research seminar is GEOTOP-A: Applications of Geometry and Topology.
- Mailing lists with announcements in applied topology include WinCompTop and ALGTOP-L.

https://www.math.colostate.edu/~adams/advising
Thank you!