An Introduction to Applied Topology

Henry Adams
Colorado State University
An Introduction to Applied Topology

Part I: Topology applied to data analysis
Part II: Topology applied to sensor networks
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 ($C_8H_{16}$) 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.
Datasets have shapes

Example: Cyclo-Octane \((\text{C}_8\text{H}_{16})\) data

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

\[ \begin{bmatrix}
  c_{1,1,x} & c_{2,1,x} \\
  c_{1,1,y} & c_{2,1,y} \\
  c_{1,1,z} & c_{2,1,z} \\
  \vdots & \vdots \\
  h_{1,16,x} & h_{2,16,x} \\
  h_{1,16,y} & h_{2,16,y} \\
  h_{1,16,z} & h_{2,16,z}
\end{bmatrix} \]

1,031,644

Non-Manifold Surface Reconstruction from High Dimensional Point Cloud Data
by Shawn Martin and Jean-Paul Watson, 2010.
Datasets have shapes
Topology studies shapes

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.
The 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
Topology studies shapes

Klein bottle

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

$$
\begin{align*}
\text{0-dimensional homology } H_0 & : \text{ rank } 1 \\
\text{1-dimensional homology } H_1 & : \text{ rank } 0 \\
\text{2-dimensional homology } H_2 & : \text{ rank } 1
\end{align*}
$$

$$
\begin{align*}
0\text{-dimensional homology } H_0 & : \text{ rank } 1 \\
1\text{-dimensional homology } H_1 & : \text{ rank } 2 \\
2\text{-dimensional homology } H_2 & : \text{ rank } 1
\end{align*}
$$

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

Image credit: https://plus.maths.org/content/imaging-maths-inside-klein-bottle
What shape is this?

Topology studies shapes
Definition

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

Diagram:

- A set of points arranged in a circular pattern.
- The dots represent the vertices of the simplicial complex.
- The circles around some pairs of dots indicate proximity or connectivity.

Note: The diagram visualizes the Vietoris–Rips complex with a threshold for proximity.
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 $r > 0$, the Vietoris–Rips simplicial complex $\text{VR}(X; r)$ has a vertex set $X$ if the diameter is less than or equal to $r$.
Definition

For metric space \( X \) and scale \( r > 0 \), the Vietoris–Rips simplicial complex \( VR(X; r) \) has vertex set \( X \) if the diameter of any finite simplex is less than or equal to \( r \).
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 metric space $X$ and scale $r \geq 0$, the Vietoris–Rips simplicial complex $\operatorname{VR}(X; r)$ has a finite simplex when $\operatorname{diam}(X) \leq r$. 
Definition

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

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

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- 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 $\check{\text{Cech}}(X; r)$ has

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

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- finite simplex $\{x_0, x_1, \ldots, x_k\}$ when $\cap_{i=0}^k B(x_i, r) \neq \emptyset$. 
Nerve Lemma. $\check{\text{Cech}}(X; r) \simeq \text{union of balls}$

Definition

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Persistent homology

- Significant features persist.
- Cubic computation time in the number of simplices.
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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
• Significant features persist.
• Cubic computation time in the number of simplices.
Persistent homology applied to data

Example: Cyclo-Octane ($C_8H_{16}$) data

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

Non-Manifold Surface Reconstruction from High Dimensional Point Cloud Data
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Persistent homology applied to data

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Table 2

Example run times. Here we show the run times obtained for the different examples investigated in this section. For each example we provide the number of points $n$, number of landmarks $L$, neighborhood size $k$, time in seconds for pre-processing, and time in seconds for reconstruction.

<table>
<thead>
<tr>
<th>Example</th>
<th>$n$</th>
<th>$L$</th>
<th>$k$</th>
<th>Pre-proc.</th>
<th>Recon.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>10,000</td>
<td>886</td>
<td></td>
<td>36</td>
<td>1.7</td>
</tr>
<tr>
<td>Torus</td>
<td>10,000</td>
<td>667</td>
<td>28</td>
<td>368</td>
<td>2.2</td>
</tr>
<tr>
<td>Double torus</td>
<td>20,000</td>
<td>813</td>
<td>26</td>
<td>263</td>
<td>7.1</td>
</tr>
<tr>
<td>Mobius strip</td>
<td>10,000</td>
<td>416</td>
<td>23</td>
<td>123</td>
<td>7.7</td>
</tr>
<tr>
<td>Klein figure</td>
<td>8</td>
<td>1940</td>
<td>33</td>
<td>778</td>
<td>9.0</td>
</tr>
<tr>
<td>$\mathbb{R}P^2$</td>
<td>100,000</td>
<td>753</td>
<td>35</td>
<td>11,73</td>
<td>2.0</td>
</tr>
<tr>
<td>Two spheres</td>
<td>83,646</td>
<td>1588</td>
<td>13</td>
<td>344</td>
<td>4.4</td>
</tr>
<tr>
<td>Klein immersion</td>
<td>61,440</td>
<td>4566</td>
<td>14</td>
<td>1183</td>
<td>1.7</td>
</tr>
<tr>
<td>Henneberg</td>
<td>13,637</td>
<td>1463</td>
<td>39</td>
<td>723</td>
<td>4.9</td>
</tr>
</tbody>
</table>

Fig. 7.

Conformation space of cyclo-octane. Here we show how the set of conformations of cyclo-octane can be represented as a surface in a high-dimensional space. On the left, we show various conformations of cyclo-octane as drawn by PyMol (www.pymol.org). In the center, these conformations are represented by the 3D coordinates of their atoms. The coordinates are concatenated into vectors and shown as columns of a data matrix. As an example, the entry $c_{1,1,x}$ of the matrix denotes the $x$-coordinate of the first carbon atom in the first molecule. On the right, the Isomap method is used to obtain a lower-dimensional visualization of the data.

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 $\text{C}_8\text{H}_{16}$. 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 $\mathbb{R}^{72}$. The resulting collection is a dataset $\{x_i\}_{i=1}^{1,031,644} \subset \mathbb{R}^{72}$ 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 methods. 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.

Persistent homology applied to data

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Example: Equilateral pentagons in the plane

Image credit: Clayton Shonkwiler
Persistent homology applied to data

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Persistent homology applied to data

- **Stability Theorem.**
  - If $X$ and $Y$ are metric spaces, then
  
  $$d_b(\text{PH}(\check{\text{Cech}}(X)), \text{PH}(\check{\text{Cech}}(Y))) \leq 2d_{\text{GH}}(X, Y)$$
Topology applied to image data
The receptive fields of cells in our primary visual cortex (V1) are related to the statistics natural images.

*Independent component filters of natural images compared with simple cells in primary visual cortex* by JH van Hateren and A van der Schaar, 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

![Graphs showing persistent homology](image-url)
Persistent homology applied to data

1. Densest patches according to a global estimate

Interpretation: nature prefers linearity
Persistent homology applied to data

2. Densest patches according to an intermediate estimate
Persistent homology applied to data

2. Densest patches according to an intermediate estimate

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

Persistence homology applied to data
Persistent homology applied to data

3. Densest patches according to a local estimate
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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
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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Agent-Based Modeling

Collective phenomenon, self-organization
Dutch Starling murmuration
filmed by Roald van Stijn

https://www.youtube.com/watch?v=YjDYE5CUb7Q
Takens’ Theorem

Roughly speaking: Let $M$ be a $d$-dimensional compact manifold, let $\phi: M \rightarrow M$ be a flow, and let $f: M \rightarrow \mathbb{R}$ be a measurement. Then generically,

$$m \mapsto (f(m), f(\phi(m), f(\phi^2(m), \ldots, f(\phi^{2d}(m)))$$

is an embedding $M \hookrightarrow \mathbb{R}^{2d+1}$.

Detecting strange attractors in turbulence by Floris Takens, 1982
Conley index theory
Conclusions for Part I

- Datasets have shape, which are reflective of patterns within.
- Persistent homology is a way to measure some of the local geometry and global topology of a dataset.
Evasion Paths in Mobile Sensor Networks
Topology applied to sensor networks

- Sensors move in a ball-shaped domain $B \subset \mathbb{R}^d$ over time interval $I = [0, 1]$. Fixed sensors cover the boundary.
- Measure only the Čech complex.
- Is there an evasion path?

Coordinate-free Coverage in Sensor Networks with Controlled Boundaries via Homology by V. de Silva and R. Ghrist
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Topology applied to sensor networks

- Let $X \subset B \times I$ be the covered region.
- An *evasion path* is a time-preserving map from $I$ to the uncovered region.

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Coordinate-free Coverage in Sensor Networks with Controlled Boundaries via Homology

• Let $X \subset B \times I$ be the covered region.

• An *evasion path* is a time-preserving map from $I$ to the uncovered region.

• **Evasion Problem.** Using the time-varying Čech complex, can we determine if an evasion path exists?
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- **Theorem (de Silva, Ghrist).** If there is an \( \alpha \in H_d(SC, \partial B \times I) \) with \( 0 \neq \partial \alpha \in H_{d-1}(\partial B \times I) \), then no evasion path exists.
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- Not sharp. Can it be sharpened?

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Coordinate-free Coverage in Sensor Networks with Controlled Boundaries via Homology by V. de Silva and R. Ghrist
Zigzag persistent homology

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

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

• Theorem.
  
  If there is an evasion path then there is a full-length bar.
Zigzag persistent homology

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Zigzag persistent homology

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

- **Theorem.**
  If there is an evasion path then there is a full-length bar.
- **Streaming computation.**
Dependence on embedding $X \hookrightarrow B \times I$

- The time-varying Čech complex of $X$ does not determine if an evasion path exists!
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Dependence on embedding \( X \hookrightarrow B \times I \)
Dependence on embedding $X \leftrightarrow B \times I$

- The two covered regions are “topologically indistinguishable in a time-preserving way”, but the uncovered regions are not!
Zigzag persistence

- Caution 2.9 of *Zigzag Persistence*. Not every submodule isomorphic to an interval corresponds to a summand.
Zigzag persistence

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Dependence on embedding $X \hookrightarrow B \times I$

- The two covered regions are “topologically indistinguishable in a time-preserving way”, but the uncovered regions are not!
Conclusions for Part II

- There is a streaming one-sided criterion for the evasion problem using zigzag persistence.
- Čech complex insufficient. Alpha complex with rotation information suffices. What about the Čech complex with rotation information?
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!