Persistent homology for multivariate data visualization

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Motivation
Understanding the ‘shape’ of data

Unstructured data  Scatterplot matrix  Parallel coordinates
Agenda

1. Theory: Algebraic topology
2. Theory: Persistent homology
3. Applications
Part I

Theory: Algebraic topology
Algebraic topology is the branch of mathematics that uses tools from abstract algebra to study \textit{manifolds}. The basic goal is to find \textit{algebraic invariants} that classify topological spaces up to \textit{homeomorphism}.

Adapted from https://en.wikipedia.org/wiki/Algebraic_topology.
A d-dimensional Riemannian manifold $\mathbb{M}$ in some $\mathbb{R}^n$, with $d \ll n$, is a space where every point $p \in \mathbb{M}$ has a neighbourhood that ‘locally looks’ like $\mathbb{R}^d$. 

* 

A 2-dimensional manifold
A homeomorphism between two spaces $X$ and $Y$ is a continuous function $f: X \to Y$ whose inverse $f^{-1}: Y \to X$ exists and is continuous as well.

Intuitively, we may *stretch, bend*—but not *tear* and *glue* the two spaces.
Algebraic invariants

An invariant is a property of an object that remains unchanged upon transformations such as scaling or rotations.

Example

*Dimension* is a simple invariant: $\mathbb{R}^2 \neq \mathbb{R}^3$ because $2 \neq 3$.

In general

Let $\mathcal{M}$ be the family of manifolds. An invariant permits us to define a function $f: \mathcal{M} \times \mathcal{M} \to \{0, 1\}$ that tells us whether two manifolds are different or ‘equal’ (with respect to that invariant).

No invariant is *perfect*—there will be objects that have the same invariant even though they are different.
Betti numbers
A useful topological invariant

Informally, they count the number of holes in different dimensions that occur in a data set.

| \( \beta_0 \) | Connected components |
| \( \beta_1 \) | Tunnels |
| \( \beta_2 \) | Voids |

<table>
<thead>
<tr>
<th>Space</th>
<th>( \beta_0 )</th>
<th>( \beta_1 )</th>
<th>( \beta_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Circle</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Sphere</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Torus</td>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

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Signature property

If \( \beta^X_i \neq \beta^Y_i \), we know that \( X \not\sim Y \). The converse is not true, unfortunately:

\[
\begin{array}{c|cc}
\text{Space} & \beta_0 & \beta_1 \\
\hline
X & 1 & 1 \\
Y & 1 & 1
\end{array}
\]

We have \( \beta_0 = 1 \) and \( \beta_1 = 1 \) for \( X \) and \( Y \), but still \( X \not\sim Y \).
Simplicial complexes

0-simplex 1-simplex 2-simplex 3-simplex

Valid

Invalid
The simplicial complex representation is compact and permits the calculation of the Betti numbers using an efficient matrix reduction scheme.
Basic idea
Calculating boundaries

The boundary of the triangle is:

$$\partial_2 \{a, b, c\} = \{b, c\} + \{a, c\} + \{a, b\}$$

The set of edges does not have boundary:

$$\partial_1 (\{b, c\} + \{a, c\} + \{a, b\})$$

$$= \{c\} + \{b\} + \{c\} + \{a\} + \{b\} + \{a\}$$

$$= 0$$
Fundamental lemma

For all $p$, we have $\partial_{p-1} \circ \partial_p = 0$: **Boundaries do not have a boundary themselves.**

This permits us to calculate Betti numbers of simplicial complexes by reducing a *boundary matrix* to its *Smith Normal Form* using Gaussian elimination.
Summary

- We want to differentiate between different objects.
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Part II

Theory: Persistent homology
Real-world multivariate data

- Unstructured point clouds
- $n$ items with $D$ attributes; $n \times D$ matrix
- Non-random sample from $\mathbb{R}^D$

Manifold hypothesis

There is an unknown $d$-dimensional manifold $M \subseteq \mathbb{R}^D$, with $d \ll D$, from which our data have been sampled.

2-manifold in $\mathbb{R}^3$
Agenda

1. Convert our input data into a simplicial complex $K$.
2. Calculate the Betti numbers of $K$.
3. Use the Betti numbers to compare data sets.

(Fair warning: It won’t be so simple)
Converting unstructured data into a simplicial complex

Require: Distance measure (e.g. Euclidean distance), maximum scale threshold $\epsilon$.

Construct the Vietoris–Rips complex $\mathcal{V}_\epsilon$ by adding a $k$-simplex whenever all of its $(k - 1)$-dimensional faces are present.
Calculating Betti numbers directly from $\mathcal{V}_\varepsilon$

Unstable behaviour

$\beta_1$ 1 1 1 0
Calculating *persistent* Betti numbers

Persistent homology

\[ \varepsilon \]

\[ \beta_1 \]
How does this work in practice?

An example for $\beta_0$

- Have a function $f: \mathcal{V}_e \rightarrow \mathbb{R}$ on the vertices of the Vietoris–Rips complex.
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An example for $\beta_0$

- Have a function $f : \mathcal{V}_e \to \mathbb{R}$ on the vertices of the Vietoris–Rips complex.
- Extend it to a function on the whole simplicial complex by setting $f(\sigma) = \max\{f(\nu) \mid \nu \in \sigma\}$. 
How does this work in practice?

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- Have a function $f : V_e \rightarrow \mathbb{R}$ on the vertices of the Vietoris–Rips complex.
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- Analyse the connectivity changes in the sublevel sets of $f$, i.e. sets of the form

$$L^{-\alpha}_\alpha(f) = \{ \nu \mid f(\nu) \leq \alpha \}.$$
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- This can be done by traversing the values of $f$ in increasing order and stopping at ‘critical points’.
Persistent homology & persistence diagrams

One-dimensional example
Persistent homology & persistence diagrams

One-dimensional example
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One-dimensional example

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One-dimensional example
Uses for persistence diagrams

A persistence diagram is a multi-scale summary of topological activity in a data set. But the diagrams go well and beyond a simple comparison of Betti numbers!

*L’algèbre est généreuse, elle donne souvent plus qu’on lui demande.*

—D’Alembert
Distance calculations

\[ \text{Distance calculations} \]

\[ W(X, Y) = \sqrt{\inf_{\eta : X \rightarrow Y} \sum_{x \in X} \| x - \eta(x) \|_2} \]

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Distance calculations

\[ W^2(X, Y) = \sqrt{\sum_{x \in X} \| x - \eta(x) \|_\infty} \]
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\[ W_2(X, Y) = \sqrt{\inf_{\eta: X \to Y} \sum_{x \in X} \|x - \eta(x)\|_\infty^2} \]
Sensitivity of distances
Wasserstein versus function space distances

Only the Wasserstein distance does not distort the ‘shape’ of noise in the data.
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Part III

Applications
Published projects

Persistence rings
- Rieck, Mara, Leitte: Multivariate data analysis using persistence-based filtering and topological signatures

Simplicial chain graphs
- Rieck, Leitte: Structural analysis of multivariate point clouds using simplicial chains

Model landscapes
- Rieck, Leitte: Enhancing comparative model analysis using persistent homology

Evaluating embeddings
- Rieck, Leitte: Persistent homology for the evaluation of dimensionality reduction schemes

Agreement analysis
- Rieck, Leitte: Agreement analysis of quality measures for dimensionality reduction

Data descriptor landscapes
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Qualitative visualizations: Persistence rings
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Motivation

Analyse the connectivity of topological features for *ensembles* of data sets: Different runs of an experiment, different times at which measurements are being taken...
Central idea

Obtain geometrical descriptions of topological features (‘holes’) while calculating persistent homology.

This is known as the ‘localization problem’ in persistent homology.
Solving the localization problem

1. Define a *geodesic ball* in a simplicial complex.
2. Solve all-pairs-shortest-paths problem to find possible sites.
Advantage: The space in which we localize the features usually has a high dimension, but the graph will always be drawn in $\mathbb{R}^2$. 
Results

Data: Tropical Atmosphere Ocean Array
Lessons learned

1. We can obtain features via persistent homology that permit a comparative analysis.
2. Visualizing these features becomes abstract very quickly.
3. Need more ‘quantitative’ topological visualizations.
Quantitative visualizations: Model landscapes

Example: Solubility analysis

- 19 different mathematical models
- 1267 chemical compounds, described by 228-dimensional feature vectors
- Measured ground truth (solubility values)

Each model is a function $f: D \rightarrow \mathbb{R}$. How to evaluate similarities & differences between the models?
State-of-the-art

- Existing measures (RMSE or $R^2$) only focus on values of a model.
- The structure/shape is not being used!
- Shortcomings: Sensitivity to noise, ‘masking’ the influence of outliers…
Our approach

1 Calculate Vietoris–Rips complex $\mathcal{V}_\varepsilon$ on the molecular descriptors.
Our approach

1. Calculate Vietoris–Rips complex $\mathcal{V}_\epsilon$ on the molecular descriptors.
2. Use model values & ground truth to obtain a set of functions on $\mathcal{V}_\epsilon$.

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5. *Absolute* comparison with ground truth diagram.
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5. *Absolute* comparison with ground truth diagram.
Visualization of relative model differences

- random forest
- svm
- svm tuned
- regression trees
- m5
- cubist
- bagged trees
- rpart
- enet
- enet tuned
- pls
- pls tuned
- ridge
- ridge tuned
- rlm pca
- rlm
- rpart
- svm
- svm tuned
- cubist
- rm5
- enet
- pls
- ridge
- rlm
Why is \textit{m5} rated differently?

Comparison with \textit{cubist}
Summary

Topological methods yield quantitative and qualitative information about data sets—often, this goes well and beyond the scope of regular geometric approaches.
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Future work

1 Performance improvements: Smaller complexes, other distance measures, …
2 Ensemble data & ‘average’ topological structures
3 Connection to geometric features in data
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Future work

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2. Ensemble data & ‘average’ topological structures
3. Connection to geometric features in data

Thank you for your attention!