Topological data analysis and the construction of intrinsic circle-valued coordinates.

Mikael Vejdemo-Johansson

11-1-11
Data has shape

What is data?

Data comes as numerical values: for instance physiological measurements from patients in a study.

Captured as point clouds in $\mathbb{R}^d$.

What is shape?
Shape matters

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Homology

One major tool for describing these shapes comes from topology:

The \textit{i}th homology with coefficients in a field \( k \) assigns to a topological space \( X \) a vector space \( H_i(X; k) \).

Easiest description is through Betti numbers \( \beta_i = \dim_k H_i(X; k) \). Counts the number of \( i \)-dimensional voids. (almost)

Pleasant to use because computable with matrix arithmetic.
Homology – intuitively

\[
\begin{align*}
\beta_0 &= 1 \\
\beta_1 &= 1 \\
\beta_0 &= 1 \\
\beta_1 &= 2 \\
\beta_0 &= 1 \\
\beta_1 &= 0 \\
\beta_2 &= 1 \\
\beta_0 &= 1 \\
\beta_1 &= 2 \\
\beta_2 &= 1
\end{align*}
\]
Homology — why algebra?

Even if we only work with $\beta_i$, the algebra provided by using vector spaces remains important.

At the core: Noether’s principle. Along topological maps, the homology groups change with linear maps.

$$ X \xrightarrow{f} Y $$

$$ H_i(X; k) \xrightarrow{H_i(f; k)} H_i(Y; k) $$

Vector space structures carry additional information that can be leveraged for computation or analysis. This functoriality property will reappear later.
Simplicial topology: continuous made discrete

Definition
A simplicial complex is a family of simplices: vertices, edges, triangles, tetrahedra, ... such that any two simplices intersect in a subsimplex.

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An abstract simplicial complex is a family of subsets of a given set $V$, such that all subsets of a member are members.
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Simplicial complexes: discrete made continuous

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The Vietoris-Rips complex is an abstract simplicial complex \( VR_\epsilon(X) \) for \( \epsilon \in \mathbb{R}_+ \) and \( X \) a finite metric space:

- Contains one vertex for each element in \( X \).
- Contains a simplex \((x_0, \ldots, x_k)\) exactly when \( d(x_i, d_j) < \epsilon \) for all \( i, j \in [k] \).
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Computing homology

Given a simplicial complex $S$ we can compute its homology using matrix operations.

- To $S$ we assign a vector space $CS = \bigoplus_{\sigma \in S} \sigma \cdot k$.
- On $CS$ we define a linear boundary map $\partial : CS \to CS$. Each simplex is mapped to a (signed) sum of the maximal simplices on its boundary.
- From the algebra (and geometry) at hand follows $\partial(\partial\sigma) = 0$ for all simplices $\sigma$. So $\partial(S) \subseteq \ker \partial$.
- We define the homology $H(S; k) = \ker \partial / \partial(S)$.
- Restricting to $i$-dimensional simplices yields $H_i(S; k)$; the $i$-dimensional homology group.
Example: pointcloud of a circle

First idea: pick some nice $\epsilon$ to work with $VR_\epsilon(X)$. 
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$\beta_1 = 3$
Example: pointcloud of a circle

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$\beta_1=2$
Example: pointcloud of a circle

Better approach: study changes in $H_i(VR_\epsilon(X); k)$ for different values of $\epsilon$.

If $\epsilon < \epsilon'$, then $VR_\epsilon(X) \subset VR_{\epsilon'}(X)$. By functoriality of $H_i$, the inclusion map of simplicial complexes induces a map $H_i(VR_\epsilon(X); k) \to H_i(VR_{\epsilon'}(X); k)$.

We can summarize with a diagram of vector spaces and linear maps

$$
H_i(VR_{\epsilon_0}(X)) \to H_i(VR_{\epsilon_1}(X)) \to \cdots \to H_i(VR_{\epsilon_k}(X))
$$

A diagram like this we’ll call a persistent vector space.
Some algebra

There is an equivalence between persistent vector spaces and graded $k[t]$-modules.

$$V_0 \xrightarrow{t} V_1 \xrightarrow{t} \ldots \xrightarrow{t} V_k \quad \Rightarrow \quad \bigoplus_{i} V_i =: V_*$$

The module structure is given by determining the action of $t$.

$$t \cdot (v_0, v_1, \ldots, v_k) = (0, tv_0, tv_1, \ldots, tv_{k-1})$$
Some algebra

The ring $k[t]$ is a graded PID, and thus graded modules over $k[t]$ have unique decompositions:

$$V_* = \bigoplus_i t^{a_i} k[t] \oplus \bigoplus_j t^{b_j} k[t]/t^{c_j}$$
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$[a_i, \infty)$

$[b_j, b_j + c_j)$
Some algebra

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where

- $[a_i, \infty)$
- $[b_j, b_j + c_j)$
Interpreting the barcode

Barcodes of betti numbers of Vietoris-Rips complexes of point clouds tell us which homological properties are significant, and which result from noise.

The length of an interval corresponds to the size of the corresponding feature.
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Example: natural images

Lee-Mumford-Pedersen investigated whether a statistically significant difference exists between natural and random images.

Natural images form a “subspace” of all images. Dimension of ambient space e.g. \(640 \times 480 = 307200\).

This space of natural images should have:

- high dimension: there are many different images.
- high codimension: random images look nothing like natural ones.
Natural 3x3 patches

Instead of studying entire images, we consider the distribution of 3 × 3 pixel patches.

Most of these will be approximately constant in natural images. Allowing these drowns out structure.

Lee-Mumford-Pedersen chose 8,500,000 patches with high contrast from a collection of black-and-white images used in cognition research. Each 3 × 3-patch is considered a vector in $\mathbb{R}^9$.

Normalised brightness: $\mathbb{R}^9 \to \mathbb{R}^8$. Normalised contrast: $\mathbb{R}^8 \to S^7$.

Subsequent topological analysis by Carlsson–de Silva–Ishkanov–Zomorodian.
Pixel patches in $S^7$

The resulting patches are dense in $S^7$ – so we consider high-density regions.

Pick out 25% densest points. We can pick a parametrised method to measure density:

**Definition**

$k$-codensity $\delta_k(x)$ of a point $x$ is the distance to its $k$th nearest neighbour.

$k$-density $d_k(x)$ is $1/\delta_k(x)$.

High $k$ yields a smoothly changing density measure capturing global properties. Low $k$ yields a wilder density measure capturing local properties. $k$ acts as a kind of focus control.
300-density
300-density
15-density
15-density
Three circles
Identifying the subspace of natural pixel patches

Raising the cut-off bar yields, with coefficients in $\mathbb{F}_2$

$$\beta_0 = 1 \quad \beta_1 = 2 \quad \beta_2 = 1$$

Assuming the shape is a surface, this corresponds to one of
Identifying the subspace of natural pixel patches

Raising the cut-off bar yields, with coefficients in $\mathbb{F}_3$

$$\beta_0 = 1 \quad \beta_1 = 1$$

Thus, the relevant shape is:
Klein bottle of pixel patches
Applications of this analysis

Image compression

A $3 \times 3$-cluster may be described using 4 values:

- Position of its projection onto the Klein bottle
- Original brightness
- Original contrast

Texture analysis

Textures yield distributions of occurring patches on the Klein bottle. Rotating the texture corresponds to translating the distribution. [J Perea]
Coordinatization methods

My own work is on automating the above process by finding topological methods to recover intrinsic coordinate maps.

Idea

- Starting from a dataset $X$: compute its persistent homology $H(VR_*(X); k)$
- Guess a simplicial complex $Y$ with corresponding homology
- Find maps $X \to Y$ or $VR_*(X) \to Y$ that lift to the expected correspondance.
First results

Joint with Vin de Silva and Dmitriy Morozov.

We can use that the circle is an Eilenberg-Mac Lane space, and thus

$$H^1(X; \mathbb{Z}) = [X, S^1]$$

We have established a definition of persistent cohomology, and produced techniques, algorithms and software for computing circle-valued coordinate functions using cohomology and a smoothing step.
Future directions

- Approach more generic coordinatizations by studying optimal chains in $H_0(\text{hom}(CX, CY)) = \bigoplus_p \text{hom}(H_pX, H_pY)$.
- Apply the circular coordinates work to periodic and recurrent systems and signals. Currently looking at data sets from: meteorology, climate research, gait research, music.
- Use circular coordinates for quality control on existing analysis methods for periodic signals.
Delay embedding of a window from a clarinet tone, using circular coordinates and a persistence diagram to quality control the delay embedding.