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How do we distinguish geometrical objects?

Figures in second row drawn by Violeta Kovacev-Nikolic
Figure: All three letters F have the same shape. The first and the second have the same shape and size. The third has a different size.
What is Topology?

One popular answer: It is the branch of mathematics which does not distinguish between a teacup and a bagel.
Classification of capital letters

- Equivalence classes by topological type
  \{D, O\}, \{E, F, T, Y\}, \{H, K\},
  \{P\}, \{Q\}, \{X\}

- Equivalence classes by homotopy type
  \{A, R, D, O, P, Q\}, \{B\},
Topology cares connectivity

Topology allows the larger group of homeomorphisms that deform an object by stretching, shrinking, bending, but neither tearing nor gluing.
Homotopy equivalent

- A circle is homeomorphic to a square.
- **Homotopy equivalent** intuitively means that one can be continuously deformed to the other.
- The figure eight and the island with two lakes are equivalent although they are not homeomorphic to each other.
- Similarly the circle, the square, and Möbius band.
Classification of capital letters

- **Equivalence classes by topological type**
  \{D, O\}, \{E, F, T, Y\}, \{H, K\},
  \{P\}, \{Q\}, \{X\}

- **Equivalence classes by homotopy type**
  \{A, R, D, O, P, Q\}, \{B\},
Algebraic topology associates to a topological space an algebraic system such as a group or a sequence of groups.

There is a natural interplay between continuous maps $f : X \to Y$ between topological spaces and algebraic homomorphisms $f_* : G(X) \to G(Y)$ on their associated groups.

There exist several ways to associate topological spaces with groups, but homology fits our interests the best.
Outline

- Simplicial Homology and Betti Numbers
- Persistent Homology and its Descriptors
- Persistence Landscape and its Applications to Maltose Binding Protein
Distinguish torus from sphere

Mission: recover topology and geometry from point cloud data.

Figures prepared by Violeta Kovacev-Nikoloc
But... set of points does not have interesting topology
How about $\epsilon$ balls? No…
Answer: Simplicial complexes
Čech Complex
Čech (Nerve) Theorem

The *Nerve lemma* states that if the ambient space is $\mathbb{R}^d(Y)$, then the Čech complex $C_\epsilon(S)$ is homotopy equivalent to the union of balls, $\bigcup_i B_\epsilon(x_i)$ (Rotman 1988).
Oriented simplex

A $p$-simplex $\sigma$ is the convex hull of $p + 1$ geometrically independent points $V = \{v_0, v_1, \ldots, v_p\}$ in $\mathbb{R}^d$. An oriented simplex $[\sigma] = [v_0, v_1, \ldots, v_p]$ is an equivalence class of particular ordering of the $p + 1$ vertices of a $p$-simplex.

Figure: 0-simplex $[v_0]$, 1-simplex $[v_0, v_1]$, 2-simplex $[v_0, v_1, v_2]$, and 3-simplex $[v_0, v_1, v_2, v_3]$. 
**Simplicial complex** \( K \)

\( p \)-simplex, \( \sigma = [v_0, \ldots, v_p] \)

Any simplex \( \tau \) spanned by a subset of \( \{v_0, \ldots, v_p\} \) is called a **face** of \( \sigma \).

A simplicial complex \( K \) in \( \mathbb{R}^d \) is a collection of simplices such that

- every face of a simplex in \( K \) also belongs to \( K \);
- the intersection of any two simplices in \( K \) is a face of each of them.
Example of simplicial complex

A simplicial complex

Non-simplicial complexes
Čech and Vietoris-Rips Complex

Figure: (Left) Čech complex, the edges are formed when two points are within $\epsilon$ and triangles are formed when three points are simultaneously within $\epsilon$ distance and so on. (Right) Vietoris-Rips complex, the two points join when they are within $\epsilon$ distance and three points join when points are pairwise within $\epsilon$ distance.

Figures prepared by Violetka Kovacev-Nikolic.
A $p$-chain is defined as $\sum_i n_i[\sigma_i], n_i \in \mathbb{Z}, \sigma_i \in K$ is a $p$-simplex.

The $p$th chain group $C_p(K)$ is the set of all $p$-chains on $K$.

The boundary homomorphism $\partial_p : C_p(K) \rightarrow C_{p-1}(K)$ is defined as, $\partial_p \sigma = \sum_i (-1)^i[v_0, v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_p]$.
Boundary operator—pictorially

\[ \partial_1[v_0, v_1] = v_1 - v_0 \]
\[ \partial_2[v_0, v_1, v_2] = [v_1, v_2] - [v_0, v_2] + [v_0, v_1] \]
\[ = [v_1, v_2] + [v_2, v_0] + [v_0, v_1] \]
The boundary operator connects the chain groups into a chain complex $C_*$:

$$\cdots \to C_{p+1} \xrightarrow{\partial_{p+1}} C_p \xrightarrow{\partial_p} C_{p-1} \cdots$$

- A $p$-chain with no boundary is a $p$-cycle; $p$th **cycle group** is the kernel of $\sigma_p$; $Z_p = \ker \partial_p = \{ c \in C_p | \partial_p c = 0 \}$.

- A $p$-chain that is the boundary of $(p + 1)$-chain is a $p$-boundary; $p$th **boundary group** $B_p = \text{im} \partial_{p+1} = \{ c \in C_p | \exists d \in C_{p+1} : c = \partial_{p+1} d \}$. 
Homology groups

- Since $\partial_p - 1 \partial_p = 0$ for all $p$, each boundary of a $p + 1$ chain is a $p$-cycle, that is, $B_p \subseteq Z_p \subseteq C_p$.

- The chains in $B_p$ are cycles that are boundaries of higher dimensional cycles.

  **We are interested in cycles that are not boundaries.**

- $p$th homology group of a simplicial complex $K$ is a quotient group $H_p(K) = Z_p(K)/B_p(K)$. 
Since $H_p$ is a finitely-generated abelian group, it decomposes uniquely into a direct sum:

$$H_p(K) \cong \bigoplus_{i=1}^{\beta_p} \mathbb{Z} \oplus \bigoplus_{j=1}^{r} \mathbb{Z}_{b_j},$$

where $\beta_p, b_j \in \mathbb{Z}$, $b_j | b_{j+1}$, $\mathbb{Z}_{b_j} = \mathbb{Z}/b_j\mathbb{Z}$.

- left sum = free subgroup and its rank is the $p$th Betti number $\beta_p$ of $H_p(K)$.
- right sum = the torsion subgroup and $b_j$ are the torsion coefficients of homology group $H_p(K)$. 
• \( \beta_0 \) counts the number of connected components of a complex \( K \).
• \( \beta_1 \) counts the number of loops/tunnels of a complex \( K \).
• \( \beta_2 \) counts the number of voids of a complex \( K \).
Our intuition and Betti numbers
Our intuition and Betti numbers

Figure: $\beta_0 = 1$, $\beta_1 = 1$, $\beta_k = 0$, $k \geq 2$
Our intuition and Betti numbers
Our intuition and Betti numbers

Figure: $\beta_0 = 1, \beta_1 = 0, \beta_2 = 1, \beta_k = 0, k \geq 3$
Our intuition and Betti numbers
Our intuition and Betti numbers

Figure: $\beta_0 = 1$, $\beta_1 = 2$, $\beta_2 = 1$, $\beta_k = 0$, $k \geq 3$
How about Möbius band and a knot?
Theorem—Munkres (1984)

For a finite simplicial complex, there are bases $e_1, \cdots, e_n$ for $C_p(K)$ and $e'_1, \cdots, e'_m$ for $C_{p-1}(K)$, relative to which the matrix of

$$
\partial_p : C_p(K) \rightarrow C_{p-1}(K)
$$

has the normal form, where $b_i \geq 1$ and $b_1 \mid b_2 \mid \cdots \mid b_r$,

\[
\begin{array}{cccccccc}
  e_1 & e_2 & \cdots & e_r & e_{r+1} & \cdots & e_n \\
  e_1' & b_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\
  e_2' & 0 & b_2 & \cdots & 0 & 0 & \cdots & 0 \\
  \vdots & 0 & 0 & \ddots & 0 & 0 & \ddots & 0 \\
  e_r' & 0 & 0 & \cdots & b_r & 0 & \cdots & 0 \\
  e_{r+1}' & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\
  \vdots & 0 & 0 & \ddots & 0 & 0 & \ddots & 0 \\
  e_m' & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\
\end{array}
\]
Facts about normal form

- \( \{e_{r+1}, \ldots, e_n\} \) is a basis for \( \mathbb{Z}_p \) and thus the rank of \( \mathbb{Z}_p \) equals the number of zero columns;
- \( \{b_1 e_1', \ldots, b_r e_r'\} \) is a basis for \( B_{p-1} \), and thus rank \( B_{p-1} \) equals the number of non-zero rows;
- the torsion coefficients of \( H_{p-1} \) are the diagonal entries \( b_i > 1 \).
- The \( p \)-th Betti number of a finite complex \( K \) is

\[
\beta_p(K) = \text{rank } C_p(K) - \text{rank } \Lambda_p - \text{rank } \Lambda_{p+1},
\]

where \( \Lambda_p \) is the matrix of \( \partial_p \) relative to bases.
Hand calculation

The standard bases for the chain groups of the bow-tie (お話) are

\[ C_0(お話) = \{a, b, c, d, e\}, \quad C_1(お話) = \{ba, ac, cb, dc, ce, ed\}, \quad C_2(お話) = \{0\}. \]

The matrix \( \Lambda_1 \) of the boundary homomorphism \( \partial_1 \) is then

\[
\Lambda_1 = \begin{pmatrix}
1 & -1 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -1 & 1 & -1 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & -1 & 0
\end{pmatrix}.
\]
The matrix $\Lambda_1$ is reduced to $\tilde{\Lambda}_1$ with new bases;

\[
\tilde{\Lambda}_1 = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix},
\]

where $z_1 = ba + ac + cb$ and $z_2 = dc + ce + ed$ form a basis for $Z_1$ and \{a \, \text{--} \, b, \, c \, \text{--} \, a, \, c \, \text{--} \, d, \, e \, \text{--} \, c\}$ form a basis for $B_0$. 

(TDA workshop)
Example

- $C_0(\blacktriangleleft) = \{a, b, c, d, e\}$, $C_1(\blacktriangleleft) = \{ba, ac, cb, dc, ce, ed\}$, $C_2(\blacktriangleleft) = \{0\}$. The ranks of $C_0$, $C_1$, and $C_2$ are 5, 6 and 0, respectively.
- The rank $\hat{\Lambda}_1 = 4$.
- Since $\Lambda_0 : C_0 \rightarrow \{0\}$ and $\Lambda_2 : \{0\} \rightarrow C_1$, rank $\Lambda_0 = \text{rank } \Lambda_2 = 0$.
- Therefore $\beta_0 = 5 - 0 - 4 = 1$ and $\beta_1 = 6 - 4 - 0 = 2$. 
Which $\varepsilon$?

Figure: Converting point cloud data set into a global complex (e.g. Rips or Čech) requires a choice of parameter $\varepsilon$. For $\varepsilon$ sufficiently small, the complex is a discrete set; for $\varepsilon$ sufficiently large, the complex is a single high dimensional simplex. Is there an optimal choice for $\varepsilon$ which best captures the topology of the data set? Answer: a particular $\varepsilon$ is insufficient; Betti numbers are not enough.
Let $X_1, X_2, \ldots, X_n$ be $n$ independent points randomly sampled from $X \subseteq \mathbb{R}^d$.

- Replace each point of discrete data set in $\mathbb{R}^d$ by a ball of a fixed radius $\varepsilon$;
- Obtain simplicial complexes from the balls;
- Construct filtered simplicial complexes as $\varepsilon$ increases;
- **Compute persistent homology (topological feature vs noise).**
Filtered Rips Complex with 25 Points-PLEX
Filtered Rips Complex with 25 Points (PLEX)
Rips Complex: $\varepsilon = 0.5$
Rips Complex: $\varepsilon = 0.7$
Rips Complex: $\varepsilon = 1.0$
Rips Complex: $\varepsilon = 1.4$
Persistent homology–schematic

\[ \beta_0 \text{-barcode is } \{(0, \infty), [0, 1), [0, 3), [0, 2)\}; \beta_1 \text{-barcode is } \{(2, 4), [4, 5)\}; \text{ and } \beta_2 \text{-barcode is } [6, 7). \]
Persistent complex (Edelsbrunner et al. (2002), Zomorodian and Carlsson (2005))

- Model the homological history of a space as a sequence of nested spaces (filtration)

\[ \emptyset = K^0 \subseteq K^1 \subseteq \cdots K^{\ell-1} \subseteq X^\ell = K \]

- A filtration produces a natural inclusion map

\[ \emptyset = K^0 \hookrightarrow K^1 \rightarrow K^{\ell-1} \rightarrow K^\ell \]

- **Persistent complex** $C = \{C_*, f^i\}$ is a family of chain complexes $\{C^i_*\}$ with chain maps $f^i : C_*^i \rightarrow C_*^{i+1}$.

\[ \emptyset = C_p(K^0) \xrightarrow{f^0} C_p(K^1) \xrightarrow{f^1} \cdots \rightarrow C_p(K^{\ell-1}) \xrightarrow{f^{\ell-1}} C_p(K^\ell) \]
Persistent complex

\[ \partial_3 \downarrow \quad \partial_3 \downarrow \quad \partial_3 \downarrow \]
\[ C_2^0 \quad \overset{f^0}{\longrightarrow} \quad C_2^1 \quad \overset{f^1}{\longrightarrow} \quad C_2^2 \quad \overset{f^2}{\longrightarrow} \quad \cdots \]
\[ \partial_2 \downarrow \quad \partial_2 \downarrow \quad \partial_2 \downarrow \]
\[ C_1^0 \quad \overset{f^0}{\longrightarrow} \quad C_1^1 \quad \overset{f^1}{\longrightarrow} \quad C_1^2 \quad \overset{f^2}{\longrightarrow} \quad \cdots \]
\[ \partial_1 \downarrow \quad \partial_1 \downarrow \quad \partial_1 \downarrow \]
\[ C_0^0 \quad \overset{f^0}{\longrightarrow} \quad C_0^1 \quad \overset{f^1}{\longrightarrow} \quad C_0^2 \quad \overset{f^2}{\longrightarrow} \quad \cdots \]

**Figure:** By expanding the chain complex \( C_*^i \), we see the part of the persistence complex \( C \), where the chain maps \( f^i \) are associated with filtration horizontally and the boundary operators indicated vertically.
Persistent homology (Zomorodian and Carlsson (2005))

Definition

The $q$-th persistent homology of $\mathcal{C}$ is defined to be the image of the induced homomorphism $f_{i,*}^{i,q} : H_*(C_i) \rightarrow H_*(C_{i+q})$. That is, the $q$-th homology group of $K^i$ is $H_*^{i,q} = Z_*/(B_{i+q} \cap Z_*)$. 
Taking a particular chain maps \( t : C_*^i \rightarrow C_*^{i+1} \), for a finite persistence module \( C = \{ C_*, t \} \) with field \( F \) coefficients,

\[
H_*(C, F) \cong \bigoplus_i t^{r_i} F[t] \oplus \left( \bigoplus_j t^{s_j} F[t]/(t^{n_j} F[t]) \right).
\]

Multiplying simplices by \( t^m \) records the filtration ordering. For example, vertex \( c \) enters the filtration at time 0. To shift this simplex along the grading, we multiply the simplex by \( t \), so \( t^1 c \) exists at time 1, and \( t^2 c \) at time 2.
Barcode

free : $t^{r_i} \cdot F[t]$

torsion : $t^{s_j} \cdot (F[t]/(t^{n_j} \cdot F[t]))$

- The left sum provides $[r_i, \infty)$ corresponding to a topological feature that is created at time $r_i$ and remains until the end of filtration.
- The right sum $[s_j, s_j + n_j)$ corresponding to a feature that is created at time $s_j$ and dies after time $n_j$.
- The multiset of intervals is called a barcode.
- The longer the interval, the more significant the feature.
Example

\[ \Lambda_1 = \begin{pmatrix} a & b & d & a & c & c \\ d & 0 & t^2 & t^2 & 0 & t^4 \\ c & 0 & 0 & 0 & t^3 & -t^4 \\ b & t & -t^2 & 0 & 0 & 0 \\ a & -t & 0 & -t^2 & -t^3 & 0 \end{pmatrix} \]

\[ \hat{\Lambda}_1 = \begin{pmatrix} b & d & a & c & a & b & z_1 & z_2 \\ d & t^2 & 0 & 0 & 0 & 0 \\ c & 0 & t^3 & 0 & 0 & 0 \\ b & t^2 & 0 & t & 0 & 0 \\ a & 0 & -t^3 & -t & 0 & 0 \end{pmatrix} \]
How do we calculate the mean and variance?
Can we apply it to hypothesis testing?
New descriptor (Bubenik (2012))
Statistical topology using persistence landscapes

Figure: For \((a, b)\), define \(f_{(a,b)}: \mathbb{R} \to \mathbb{R}\) by 
\[ f_{(a,b)}(t) = \min(t - a, b - t)_+ \]
Persistence Landscape

Figure: For \( \{(a_i, b_i)\}_{i=1}^m \), \( \{\lambda(k, t) = k^{th} \text{ largest value of } \{f(a_i, b_i)(t)\}_{i=1}^m \} \)

Figure: For \( \{(a_i, b_i)\}_{i=1}^m \), \( \{\lambda(k, t) = k^{th} \text{ largest value of } \{f(a_i, b_i)(t)\}_{i=1}^m \} \)
New Development: Bubenik (2012)

The persistence landscapes are functions from $\mathbb{N} \times \mathbb{R} \to \mathbb{R}$, and are bounded and nonzero on a bounded domain. Hence, persistence landscapes belong to $L^p(\mathbb{N} \times \mathbb{R})$ with the metric induced by $p$-integrable functions, which is a separable Banach space.

Theorem

Let $X$ be a mean zero random variable such that $\mathbb{E}(\|X\|^2) < \infty$ with values in a separable Banach space of ‘type 2’. Then $X$ satisfies the CLT. (Ledoux and Talagrand (1991))
Examples of Banach Space

$p, q \in \mathbb{R}, 1 \leq p, q, \leq \infty, 1/p + 1/q = 1.$

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Table: $c_0$ is a subspace of $\ell^\infty$ consisting of those elements $x$ for which $\lim_{i\to\infty} x_i = 0$. $C(X)$ is the space of all continuous functions on a compact metric space $X$. 
Tests

- t-test: \( \sum_{k=1}^{K} \int (\lambda_k^A(t) - \lambda_k^B(t)) \, dt \).
- Multivariate test (Hotellings \( T^2 \) test):
  Consider a vector, \( (\int (\lambda_1^A - \lambda_1^B), \int (\lambda_2^A - \lambda_2^B), \ldots, \int (\lambda_k^A - \lambda_k^B)) \),
  where \( k \) is chosen so that, \( k << n_1 + n_2 - 2 \).
Figure: Open structure (PDB 2FWO) and closed structure (PDB 2FVY) with TMR probes (red) attached via Cys residues to the upper and lower domains. Figures from Der and Dattelbaum 2008
MBP: 1OMP (open-apo) vs 1MPD (closed-holo)

**Figure:** Maltose binding proteins: (left) 1OMP open and ligand-free; (right) 1MPD closed and ligand-bound. Figures from PDB.
MBP structures with corresponding ligands

| No. | code   | ligand       | structure   | ref. | | No. | code   | ligand       | structure   | ref. |
|-----|--------|--------------|-------------|------| |-----|--------|--------------|-------------|------|
| 1   | 1ANF   | maltose      | closed-holo | r₃   | | 8   | 1EZ9  | maltotetraitol | open-holo   | r₅   |
| 2   | 1FQC   | maltotriitol | closed-holo | r₄   | | 9   | 1FQA  | maltotetraitol | open-holo   | r₄   |
| 3   | 1FQD   | maltotetraitol | closed-holo | r₄   | | 10  | 1FQB  | maltotetraitol | open-holo   | r₄   |
| 4   | 1MPD   | maltose      | closed-holo | r₂   | | 11  | 1JW4  | -            | open- apo   | r₅   |
| 5   | 3HPI   | sucrose      | closed-holo | r₇   | | 12  | 1JW5  | maltose      | open- holo  | r₅   |
| 6   | 3MBP   | maltotriose  | closed-holo | r₃   | | 13  | 1LLS  | -            | open- apo   | r₆   |
| 7   | 4MBP   | maltotetraose | closed-holo | r₃   | | 14  | 1OMP  | -            | open- apo   | r₁   |

Ligand triggers the binding site of the biomolecule to switch to a different, energetically more suitable conformation.
Is there significant difference between open and closed maltose binding proteins?

- Seven open and seven closed maltose binding proteins
- Each protein consists of 370 amino acid residues
- DATA: Correlations between 370 amino acid residues
Active sites and flexibility (1MPD)

Figure: Obtained using the ANM web server
Barcode

1MPD (closed-\textit{holo} conformation)  
\begin{align*}
\beta_0 & \quad \beta_0 \\
\beta_1 & \quad \beta_1 \\
\beta_2 & \quad \beta_2 \\
\end{align*}

1OMP (open-\textit{apo} conformation)  
\begin{align*}
\beta_0 & \quad \beta_0 \\
\beta_1 & \quad \beta_1 \\
\beta_2 & \quad \beta_2 \\
\end{align*}
The **allosteric path** is the set of highly correlated and mutually interacting amino acid residues that do not lie close to each other in the space.

**Figure:** Two shortest allosteric paths, 66-64-330-328-327/66-64-329-328-327. **AlloPathFinder** software (Tang *et al* 2007)
Binding sites and allosteric path ($\beta_1$)

Figure: 1MPD: Majority of active sites (red) and allosteric path residues (purple) stretch along the rim of the most prominent loop.
We analyzed the maltose binding proteins of open and closed structures using a conventional elastic network model along with persistent homology.

Both traditional and new methods are able to distinguish open from closed structure.

Persistent homology reveals patterns in the amino acid residues of the binding sites and the allosteric path: they are located along the rim of the most persistent loop (1 dimensional topological feature).

This result provides a preliminary screening method for identifying the residues that are susceptible to ligand binding.
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References


