Analyzing the Shape of Data

Construction of Complexes for Persistent Homology

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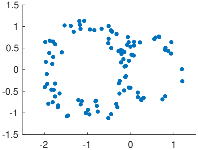
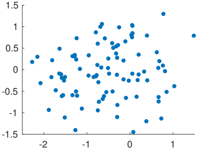
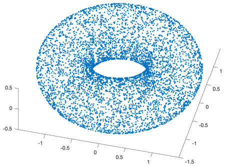
“Shape” of a data set

Here are two data sets with the same mean and covariance, but different “shapes”.

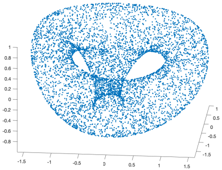




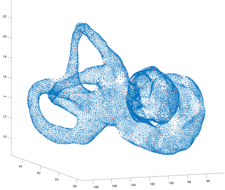
Examples of 3D data set sampled from surfaces:



torus



double torus

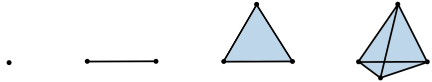


the inner ear

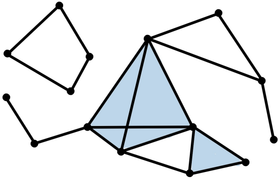
How to characterize the “shape” of a data set in terms of its **connectivity and hole structures**?

Homology of Simplicial complex

- In topology, the n-th **homology** characterizes the n-dim hole structure of a space.
- A **simplicial complex** is a collection of simplicies. A **n-simplex** is the smallest convex set containing $n+1$ points, $\sigma = [v_0, \cdots, v_n]$.



- **Simplicial homology** identifies non-trivial n-dim holes as n-cycles that are not boundary of any $n+1$ simplicies.

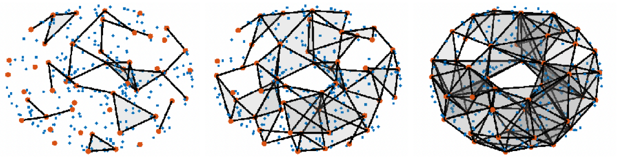


Betti number $b_n =$ # of n-dim holes

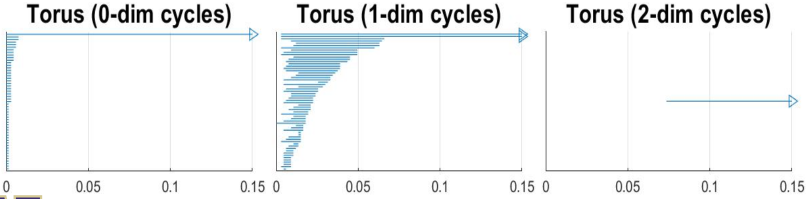
$b_0 = 2$, 2 connected components
$b_1 = 3$, 3 loop (1-dim hole)
$b_2 = 1$, 1 void (2-dim hole)

Persistent homology of filtered simplicial complex

Given a data set S, generate a sequence of simplicial complexes $\{\mathcal{K}_t\}$ that capture the topological features at different scales t. (generated by our Matlab implementation)



Then compute homology of the filtered simplicial complexes and identify the t interval in which each homology cycle persists. (computed by existing implementation JavaPlex)



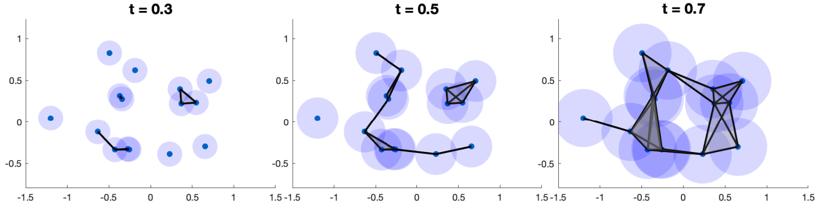
Vietoris-Rips complex

The **Vietoris-Rips complex of a set of points S at scale t** is

$$VR_t(S) = \{\sigma \subseteq S : d(v_i, v_j) \leq 2t \text{ for all } v_i, v_j \in \sigma\}.$$

- Two points are connected by a 1-simplex if their distance is $\leq 2t$.
- Three points are connected by a 2-simplex if the distance between every pair of points is $\leq 2t$.

Example. VR complexes of 15 points drawn from a 2D Gaussian distribution (plot generated by our Matlab implementation)



Cons of VR cx: computationally expensive, it generates large number of simplices.

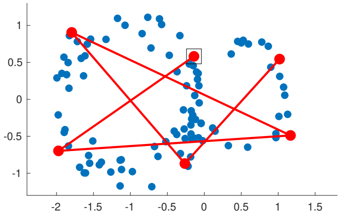
Witness Complex - landmark points

Motivation: Generate smaller number of simplices to speed up the construction of filtered simplicial complexes.

Idea: Choose a subset of data points, called **landmarks**, that can still capture the shape of the original data set.

Algorithm: Sequential MaxMin Method (Farthest-first traversal).

Example. 100 points synthesized from a figure 8 curve, generate 6 landmark points.



$\ell_1 =$ RANDOMIZED-SELECTED-POINT

for $i = 2, \cdots, k$ **do**

$$\ell_i = \operatorname*{argmax}_{v \in S} \left(\operatorname*{argmin}_{j \in \{1, \cdots, i-1\}} d(v, \ell_j) \right)$$

Witness complex - construction

At each filtration value t, two landmarks ℓ_i and ℓ_j are connected by a 1-simplex if there exists a **witness** point w such that:

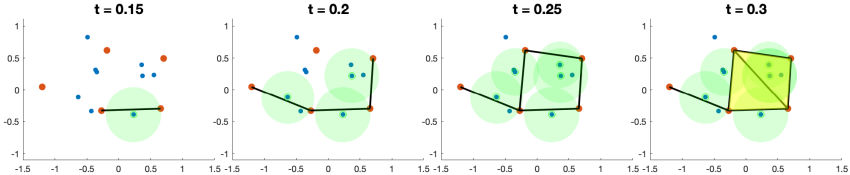
$$\max\{d(\ell_i, w), d(\ell_j, w)\} \leq t + \nu(w)$$

where $\nu(w)$ is the distance between w and its nearest landmark point.

Three landmarks are connected by a 2-simplex if every pair has been connected.

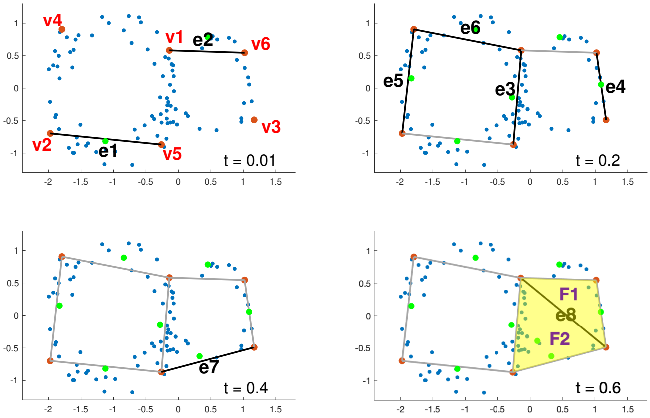
- When $t = 0$, two landmarks ℓ_i and ℓ_j are connected by a 1-simplex if there exists a witness point w such that $d(\ell_i, w) = d(\ell_j, w) = \nu(w)$.

Example. Witness complexes of 15 points and 5 landmarks, $t = 0.15, 0.2, 0.25, 0.3$.

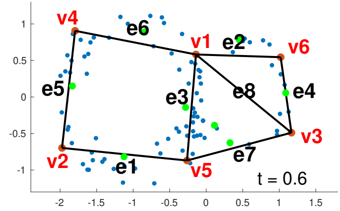


From witness complex to persistent homology

Example. 100 data points synthesized from a figure 8 curve,
6 landmarks points, $t = 0.01, 0.2, 0.4, 0.6.$



Boundary Matrix - 1-simplices



$$B(k,j) = 1 \text{ if } [v_k] \in \partial[e_j]$$

$$\begin{array}{c|cccccccc}
 & e1 & e2 & e3 & e4 & e5 & e6 & e7 & e8 \\
\hline
v1 & & 1 & 1 & & & 1 & & 1 \\
v2 & 1 & & & & 1 & & & \\
v3 & & & & 1 & & & 1 & 1 \\
v4 & & & & & 1 & 1 & & \\
v5 & 1 & & 1 & & & & 1 & \\
v6 & & 1 & & 1 & & & &
\end{array}$$

For each column e_j, $L(e_j) =$ largest row index of nonzero entry in column e_j

for column $j = 1$ to n **do**

    while $i < j$ with $L(i) = L(j)$ **do**

        add column i to column j

    end while

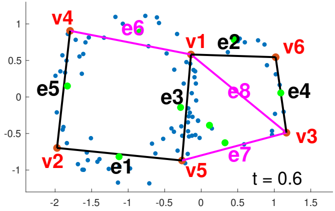
end for

$$\partial[e_3] \xrightarrow{+\partial[e_1]} [v_1] + \cancel{[v_5]} + [v_2] + \cancel{[v_5]}$$

$$\partial[e_6] \xrightarrow{+\partial[e_5]} [v_1] + \cancel{[v_4]} + [v_2] + \cancel{[v_4]}$$

$$\partial[e_6] \xrightarrow{+\partial[e_5]} \cancel{[v_1]} + \cancel{[v_2]} + \cancel{[v_1]} + \cancel{[v_2]}$$

Boundary matrix - reduction and interpretation



Reduced boundary matrix:

	$e1$	$e2$	$e3$	$e4$	$e5$	$e6$	$e7$	$e8$
$v1$		1	1	1		0	0	0
$v2$	1		1		1	0	0	0
$v3$				1		0	0	0
$v4$					1	0	0	0
$v5$	1					0	0	0
$v6$		1				0	0	0

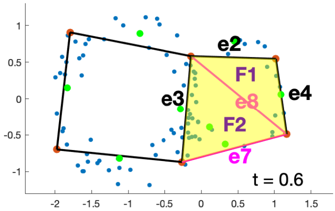
$L(e_j) = v_i \Leftrightarrow$ The occurrence of 1-simplex $[e_j]$ at time t kills the 0-dim cycle (connected component) of v_i by connecting it with an earlier point.

At $t = 0.01$, $[e_2]$ kills the component of $[v_6]$ by connecting $[v_6]$ with $[v_1]$.

$L(e_j) = \emptyset \Leftrightarrow$ The occurrence of 1-simplex $[e_j]$ at time t creates a 1-dim cycle.

At $t = 0.2$, $[e_6]$ creates the 1-dim cycle $[e_1] + [e_3] + [e_5] + [e_6]$ by closing up the loop.

Boundary matrix - 2-simplices



$$
\begin{array}{c} \\ e2 \\ e3 \\ e4 \\ e7 \\ e8 \end{array}
\begin{array}{c} \begin{array}{cc} F1 & F2 \end{array} \\ \begin{pmatrix} 1 & \\ & 1 \\ 1 & \\ & 1 \\ 1 & 1 \end{pmatrix} \end{array}
\rightarrow
\begin{array}{c} \\ e2 \\ e3 \\ e4 \\ e7 \\ e8 \end{array}
\begin{array}{c} \begin{array}{cc} F1 & F2 \end{array} \\ \begin{pmatrix} 1 & 1 \\ & 1 \\ 1 & 1 \\ & 1 \\ 1 & \end{pmatrix} \end{array}
$$

$L(F_j) = e_i$ and $L(e_i) = \emptyset$ $\Leftrightarrow$ The occurrence of 2-simplex $[F_j]$ at time t kills the 1-dim cycle created by $[e_i]$ by covering the loop.

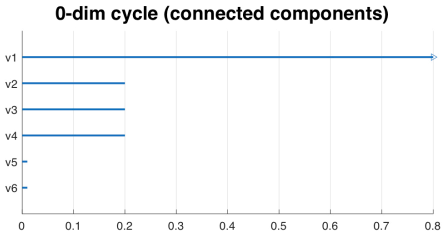
At $t = 0.6$, $[F1]$ kills the 1-dim cycle $[e_2] + [e_4] + [e_8]$ created by $[e_8]$.

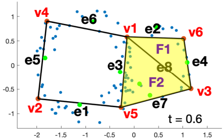
At $t = 0.6$, $[F2]$ kills the 1-dim cycle $[e_2] + [e_3] + [e_4] + [e_7]$ created by $[e_7]$.

Persistent homology

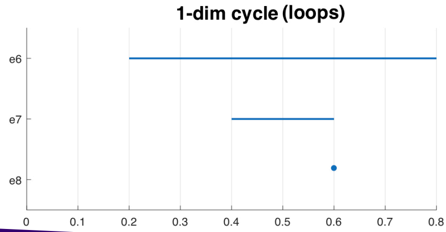
The **"barcode"** of each cycle illustrates the time interval $[t_b, t_d]$ from its birth to death. The longer it persists, the more significant the feature is.

	$e1$	$e2$	$e3$	$e4$	$e5$	$e6$	$e7$	$e8$
$v1$		1	1	1		0	0	0
$v2$	1		1		1	0	0	0
$v3$				1		0	0	0
$v4$					1	0	0	0
$v5$	1					0	0	0
$v6$		1				0	0	0





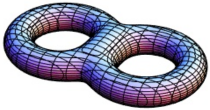
	$F1$	$F2$
$e2$	1	1
$e3$		1
$e4$	1	1
$e6$		
$e7$		1
$e8$	1	



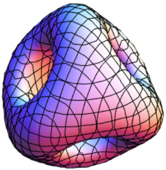
Experiment with 3D data synthesized from genus g surfaces

A compact orientable surface of genus g is a connected sum of g copies of tori.

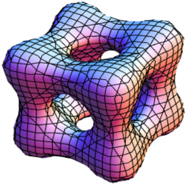
Betti numbers of genus g surface: $b_0 = 1,\ b_1 = 2g,\ b_2 = 1$



$g = 2$



$g = ?$



$g = ?$

- sample synthesized data points from implicit surface equations.
- generate and plot Witness complexes of the data points using our Matlab/Python implementation.
- used JavaPlex to compute persistent homology within ”appropriate” maximum filtration value t.

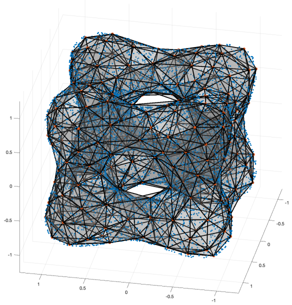
Witness complexes and persistent homology of 3D data points

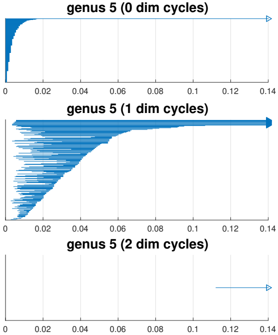
Example. Witness complexes generated by 10000 data points sampled from

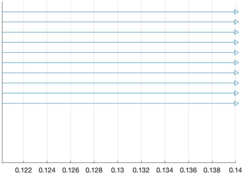
$$\textbf{genus 5 surface:}\ \ 3 + 8(x^4 + y^4 + z^4) = 8(x^2 + y^2 + z^2)$$

with 300 landmark points generated by Sequential Max-Min.

We choose maximum filtration value around $t = 0.14$, observing that additional 2-cycles starts to form after $t = 0.15$.







References

[1] N. Otter, M. Porter, U. Tillmann, P. Grindrod, H. Harrington, A Roadmap for the Computation of Persistent Homology, *EPJ Data Science*, (2017) 6:17.

[2] H. Adams, A. Tausz, JavaPlex tutorial, https://www.math.colostate.edu/ adams/research/javaplex tutorial.pdf