Topology and data
(Gunnar Carlsson, Bulletin of the AMS, 2009)

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  - we do not trust large distances (genomic sequences differing by 100/150 entries?)
  - we trust small distances only a little bit (strength of similarity as encoded by the distance may not be significant)

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  - properties robust to changes in metrics?
  - the study of idealized versions of such properties: topology

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- connected components / clusters: zeroth order topological information

Homotopy

- connectivity: $x, y \in \mathcal{X}$, say $x \sim y$ iff $\exists$ continuous map $f : [0,1] \to \mathcal{X}$, such that $f(0) = x$, $f(1) = y$

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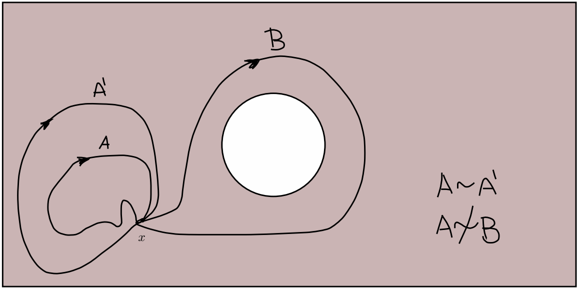
Homotopy groups

- n-th order topological information: homotopy classes of equivalence of continuous maps f from the n-dimensional sphere S^n to $\mathcal{X}$ s.t. $f(s) = x$



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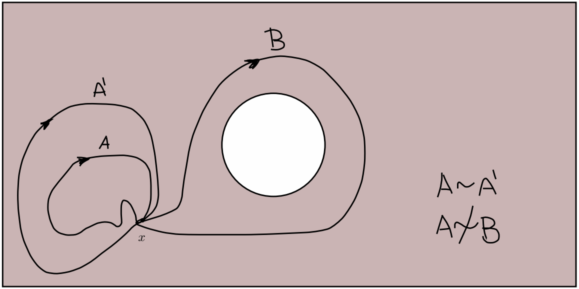
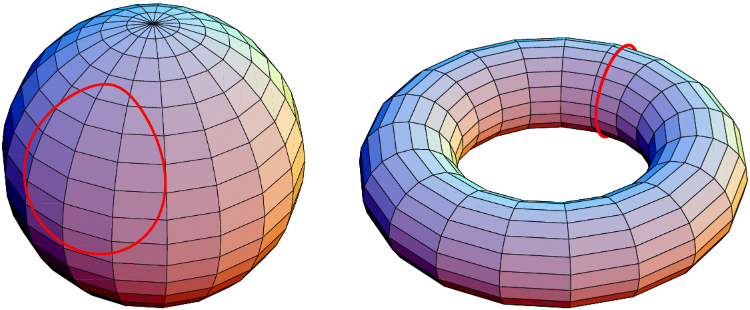


- Classes of equivalence form a group structure $\pi_n(\mathcal{X})$; for $n = 1$, **fundamental group**, e.g., $\pi_1(\mathbb{R}^n) = \{0\}$, $\pi_1(\mathbb{R}^n \backslash \{0\}) = \pi_1(S^1) = \mathbb{Z}$.

Homotopy groups



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- a friendlier alternative: **homology groups**, with an extended equivalence relation
- e.g., two loops are equivalent if there is a surface with boundary equal to the difference of two loops

Simplices and chains

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- An n-**chain** c is a formal sum of n-simplices, e.g., $[12] + [23] + [34] \in C_1$ (may occur with a multiplicity or with an opposite orientation - winding numbers):

$$c = \sum_k \alpha_k \sigma_k, \qquad \alpha_k \in A, \sigma_k \in S_n$$

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- A is an abelian group (such as $\mathbb{Z}$,$\mathbb{F}_p$); S_n is a finite set of n-simplices
- The set of all n-chains is denoted C_n; $(C_n, +)$ forms a free abelian group: $c + c' = \sum \left(\alpha_k + \alpha'_k\right) \sigma_k$ (abelian group with a "basis")

Boundary map

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- Boundary map $\partial_n : C_n \to C_{n-1}$ is a group homomorphism

Boundary map

- Example:

$$\partial_1 ([12] + [23] + [34]) = [2] - [1] + [3] - [2] + [4] - [3] = [4] - [1].$$

Fundamental Lemma of Homology

- The boundary of the boundary of a simplex is empty:

$$
\begin{aligned}
\partial_n \partial_{n+1} [i_0 \dots i_{n+1}] &= \partial_n \left(\sum_{j=0}^{n+1} (-1)^j \left[i_{\setminus j} \right] \right) \\
&= \sum_{j<l} \left[(-1)^{j+l-1} - (-1)^{l+j} \right] \left[i_{\setminus l,j} \right] \\
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- Therefore, the boundary of the boundary of a chain is also empty, i.e., $\partial_n \partial_{n+1} C_{n+1} \equiv 0 \Rightarrow \mathrm{im} \partial_{n+1} \subset \ker \partial_n$

Cycles and boundaries

- An **n-cycle** is a chain with no boundary, e.g., $[12] + [23] + [34] + [41]$. The set of cycles: $Z_n = \ker \partial_n$ is a subgroup of C_n

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- Some cycles (not all) are **boundaries** of higher order chains, e.g., $[23] + [31] + [12] = \partial_2 [123]$. The set of **n-boundaries**: $B_n = \mathrm{im}\partial_{n+1}$ is a subgroup of Z_n

Cycles and boundaries

- n-th Homology group: $H_n = Z_n/B_n = \ker \partial_n / \mathrm{im}\partial_{n+1}$, i.e., it is a factor group of equivalence classes, given by:

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- two cycles are equivalent (**homologous**) if they differ by a boundary, say $z_1 = [12] + [23] + [34] + [41]$, $z_2 = [12] + [23] + [34] + [45] + [51]$, then:

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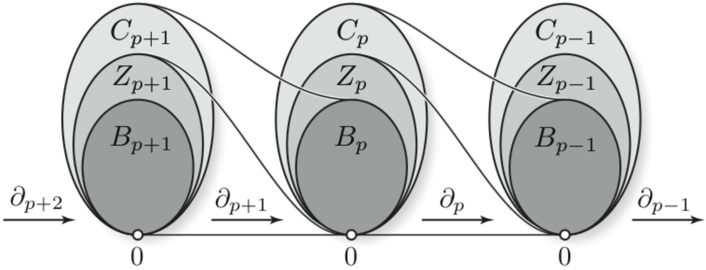
- rank of H_n (roughly) counts the number of n-dimensional holes in the space

Chains, cycles and boundaries



Homology groups

- In general $H_n = H_n(\mathcal{X}, A)$ is a **free abelian group** which depends on the underlying topological space **and** the choice of the underlying abelian group A of winding numbers in the definition of the chain

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- In general $H_n = H_n(\mathcal{X}, A)$ is a **free abelian group** which depends on the underlying topological space **and** the choice of the underlying abelian group A of winding numbers in the definition of the chain
- **Functoriality**: tranforming topological problems into algebraic problems. If $f : \mathcal{X} \to \mathcal{Y}$ is continuous then there is an induced homomorphism $H_n(f, A) : H_n(\mathcal{X}, A) \to H_n(\mathcal{Y}, A)$, with
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- If f and g are homotopic then $H_n(f, A) = H_n(g, A)$, i.e., **if topological spaces** $\mathcal{X}$ and $\mathcal{Y}$ **are homotopy equivalent then** $H_n(g, A) \circ H_n(f, A) = H_n(g \circ f, A) = H_n(id_{\mathcal{X}}, A) = id_{H_n(\mathcal{X},A)}$, i.e., **their homology groups** $H_n(\mathcal{X}, A)$ and $H_n(\mathcal{Y}, A)$ **are isomorphic**

Homology vector spaces

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- If two spaces are homotopy equivalent, then all their Betti numbers are equal

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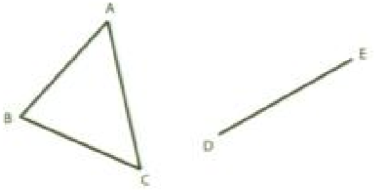
- Given the sets of n-simplices S_n, we form
  - the chain finite-dimensional vector spaces C_n
  - boundary homomorphisms (linear maps) $\partial_n : C_n \to C_{n-1}$, which can be expressed as a sequence of matrices D_n, with

$$(D_n)_{\tau\sigma} = \begin{cases} (-1)^j & \tau \text{ is a face of } \sigma \\ 0 & \text{otherwise} \end{cases}$$

Homology vector spaces

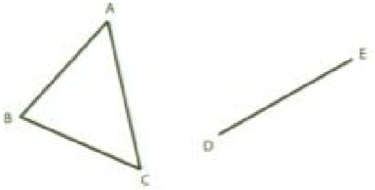
$$\begin{aligned}
\beta_n(\mathcal{X}, F) &= \dim H_n(\mathcal{X}, F) \\
&= \dim \ker \partial_n - \dim \mathrm{im}\partial_{n+1} \\
&= \dim C_n(\mathcal{X}, F) - \dim \mathrm{im}\partial_n - \dim \mathrm{im}\partial_{n+1} \\
&= \dim C_n(\mathcal{X}, F) - \mathrm{rank} D_n - \mathrm{rank} D_{n+1}
\end{aligned}$$



	AB	AC	BC	DE
A	1	1	0	0
B	1	0	1	0
C	0	1	1	0
D	0	0	0	1
E	0	0	0	1

- D_1 = incidence matrix, S_0-vertices, S_1-edges

rank-nullity in graph theory



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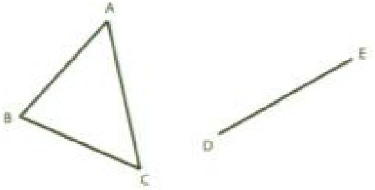

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- #connected components=#nodes-rank(D_1)
- #loops=#edges-rank(D_1)

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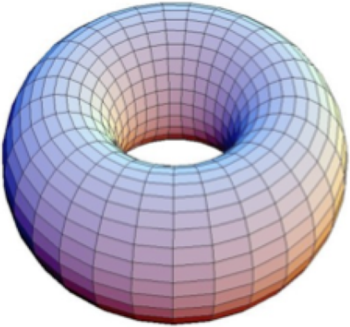
$$\beta_0 = 1,\ \beta_1 = 1,\ \beta_k = 0, \text{ for } k \geq 2$$

Betti numbers



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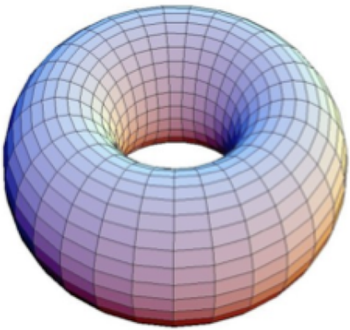

$$\beta_0 = 1,\ \beta_1 = 2,\ \beta_2 = 1,\ \beta_k = 0 \text{ for } k \geq 3$$

The story so far

- If someone gave us the topological space $\mathcal{X}$ which consists of sets of points, edges, triangles, ..., n-simplices, we can compute its Betti numbers over, say, $\mathbb{F}_2$ using linear algebra (simplicial homology)

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- Only got 0-simplices - we have to build the higher order structure into data, i.e. form the **simplicial complex**

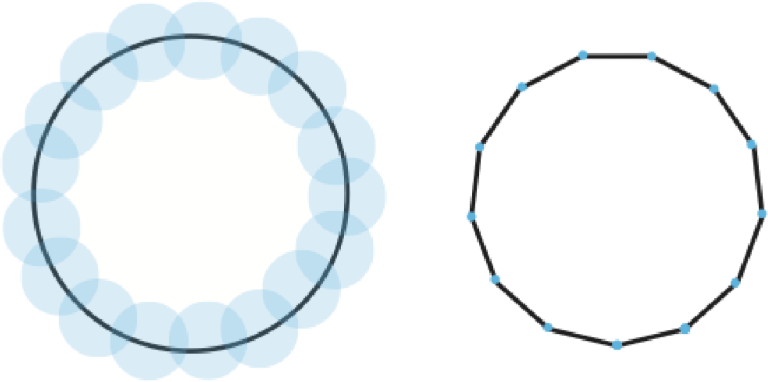
Čech complex

- Čech complex (**nerve**) $\check{\mathfrak{C}}(\epsilon)$ of data $\{Y_i\}_{i=1}^N$ contains:
  - 0-simplices $[i]$
  - 1-simplices $[ij]$ whenever $\|Y_i - Y_j\| \leq \epsilon$
  - n-simplices $[i_0 \ldots i_n]$ whenever $\bigcap_{j=0}^n U_{i_j} \neq \emptyset$,
    $U_{i_j} = \{y \in \mathcal{Y} \ : \ \|y - Y_{i_j}\| \leq \epsilon\}$

Čech complex

- Čech complex (**nerve**) $\check{\mathfrak{C}}(\epsilon)$ of data $\{Y_i\}_{i=1}^N$ contains:
  - 0-simplices $[i]$
  - 1-simplices $[ij]$ whenever $\|Y_i - Y_j\| \leq \epsilon$
  - n-simplices $[i_0 \ldots i_n]$ whenever $\bigcap_{j=0}^n U_{i_j} \neq \emptyset$,
    $U_{i_j} = \{y \in \mathcal{Y} \,:\, \|y - Y_{i_j}\| \leq \epsilon\}$
- **The nerve theorem**: In a general topological space $\mathcal{X}$, the nerve $N(\mathcal{U})$ is associated to an open covering $\mathcal{U} = \{U_i\}_{i \in I}$. $N(\mathcal{U})$ is homotopy equivalent to $\mathcal{X}$ whenever every U_i is contractible (homotopy equivalent to a point).

Čech complex



Vietoris-Rips complex

- VR complex $VR(\epsilon)$ contains:
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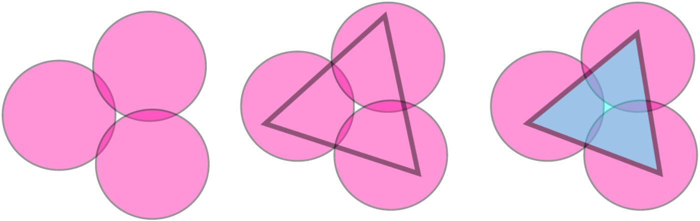
- $\check{\mathfrak{C}}(\epsilon) \subseteq VR(2\epsilon) \subseteq \check{\mathfrak{C}}(2\epsilon)$

$\check{\mathfrak{C}}(\epsilon)$ vs $VR(\epsilon)$



- Vietoris-Rips is the maximal simplicial complex that can be built on top of the 1-simplicial skeleton (*flag complex*)

Witness complexes

- Choose a set of **landmark points** $\mathcal{L} \subset \{Y_i\}_{i=1}^N$ - this is the set of 0-simplices
- Strong witness complex:
  - $[l_0 \dots l_n] \in W^s(\epsilon)$ iff $\exists Y$ (a strong witness): $d(Y, l_j) \leq d(Y, \mathcal{L}) + \epsilon$, $\forall j = 0, \dots, n$
- Weak witness complex:
  - $[l_0 \dots l_n] \in W^w(\epsilon)$ iff $\exists Y$ (a weak witness): $d(Y, l_j) \leq d(Y, \mathcal{L} \backslash \{l_0 \dots l_n\}) + \epsilon$, $\forall j = 0, \dots, n$

How to choose ϵ?

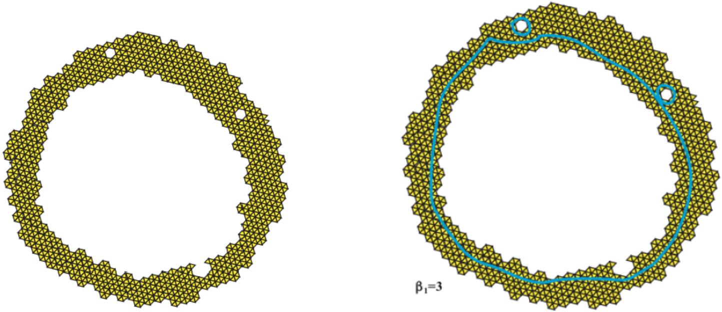


Figure: Scale ϵ_1: $\beta_0 = 1$, $\beta_1 = 3$

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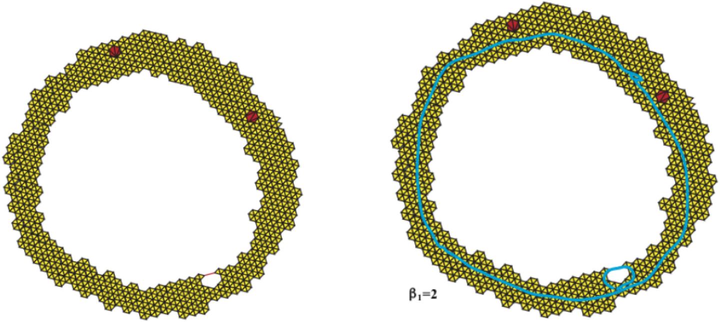

Figure: Scale ϵ_1: $\beta_0 = 1$, $\beta_1 = 2$

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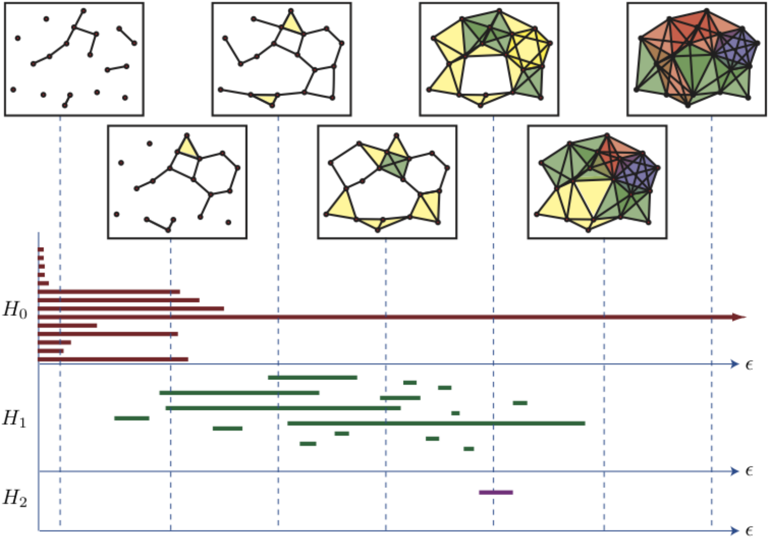
- incremental computation of Betti numbers

Persistent homology barcode



Natural image statistics

- 3x3 patches from a database of black and white images - each datapoint is a vector in $\mathbb{R}^9$

Carlsson et al, *On the local behaviour of spaces of natural images*, International Journal of Computer Vision 2008

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- exploring the high-density regions, using the k-codensity proxy $\delta_k(x) = \|x - \nu_k(x)\|$

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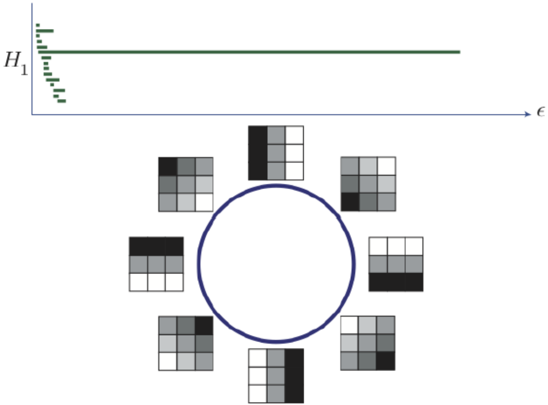
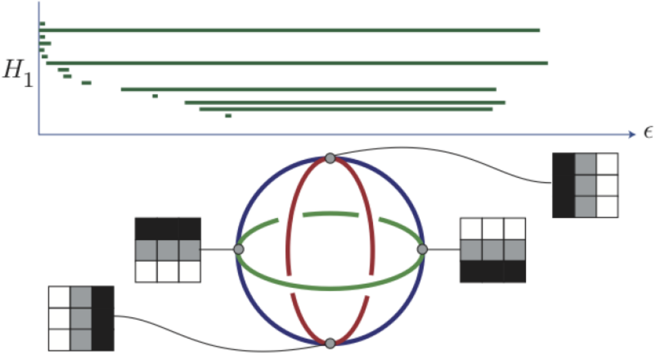


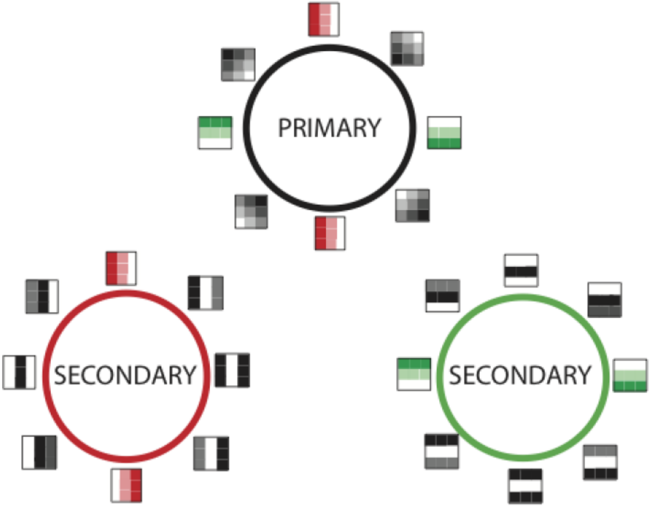
- $k = 300$, top 25% “densest points” - the underlying space appears to form a circle

Three-circle model



- $k = 15$, top 25% "densest points" leads to $\beta_1 = 5$
- green and red circles do not touch, each touches the blue circle

Three-circle model



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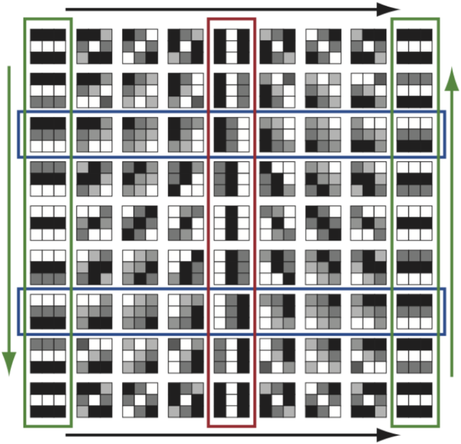
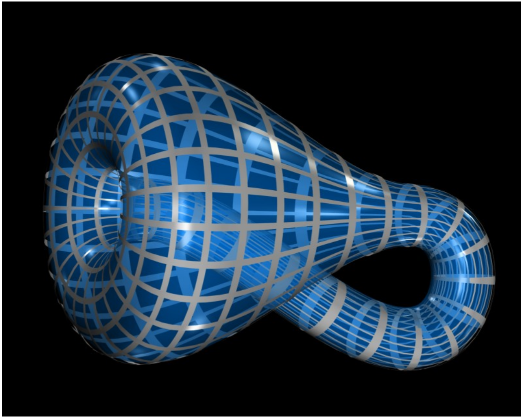


Klein bottle!



A mathematician named Klein

Thought the Möbius band was divine.

Said he: "If you glue

The edges of two,

You'll get a weird bottle like mine."

V1 data

- recordings from 10x10 electrode arrays from the V1 in Macaque monkeys (20-30 minutes):
  - **spontaneuous** / no stimulus presented
  - **evoked** / video sequences presented

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- five neurons with highest firing rate: data point cloud $\mathcal{X}$ is 200 points in $\mathbb{R}^5$
- For each data segment, construct a *witness complex*, and obtain its Betti signature $(\beta_0, \beta_1, \beta_2)$

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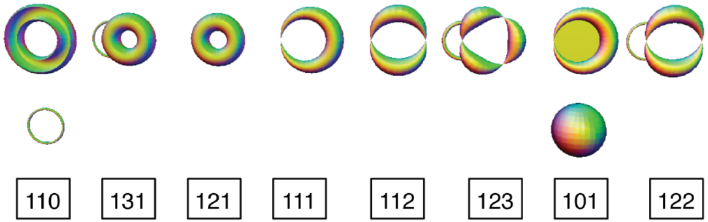
V1 data - the observed signatures



- the most frequently occurring signatures are 110 (circle) and 101 (sphere)

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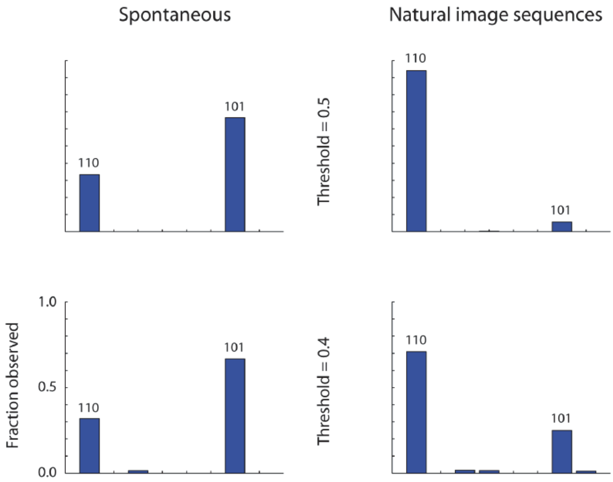

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- topology distinguishes both data sets from the Poisson model and from each other; the nature of the "circular" topological phenomenon?
- not likely due to periodicity of body's natural rhytms - no peaks in the amplitude spectrum observed

Code

- Toolbox: JPlex (http://comptop.stanford.edu/)
    - Java version of Plex, work with Matlab
    - Rips, Witness complex, Persistence Homology, barcodes
- Other Choices: Plex 2.5/Matlab (not maintained any more), Dionysus (Dimitry Morozov)