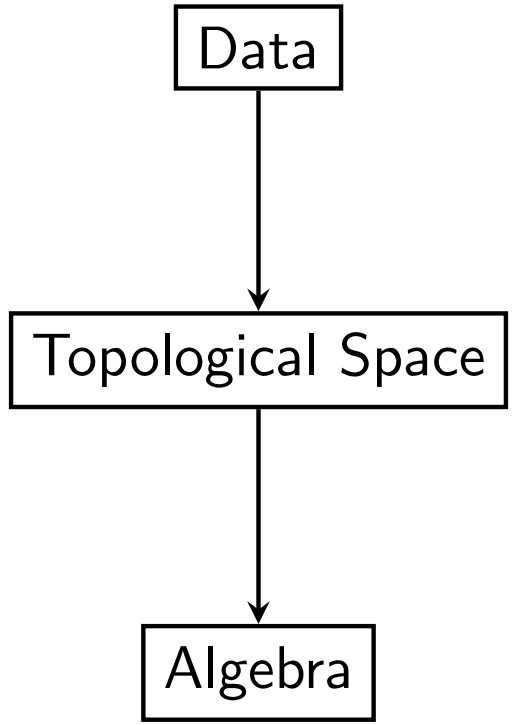
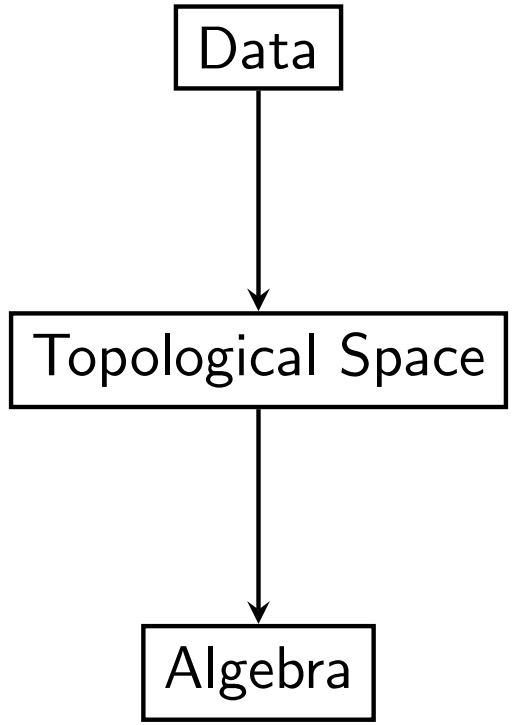
Topological Data Analysis

Graham Ellis
NUI Galway


Data
Topological Space
Algebra



General Aim: Given a finite sample S from an unknown population X we'd like to use algebra to describe/construct a topological space BS that models X.

Cluster Analysis

Consider toy data points $S = \{v_1, v_2, \ldots, v_{72}\} \subset \mathbb{R}^{262144}$

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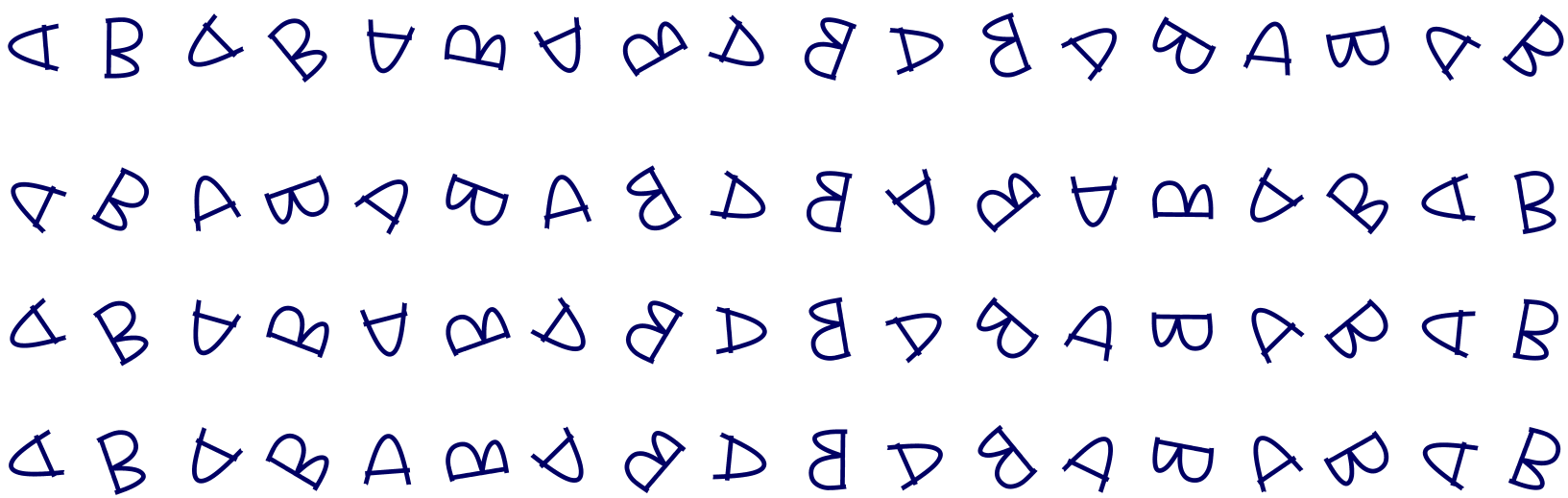
generated from



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The clique simplicial complex $Y_t = Y(S, \epsilon_t)$ has

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- n-simplices the subsets $\sigma \subseteq S$ with $n+1$ vertices and $d(v, v') \leq \epsilon_t$ for all $v, v' \in \sigma$.

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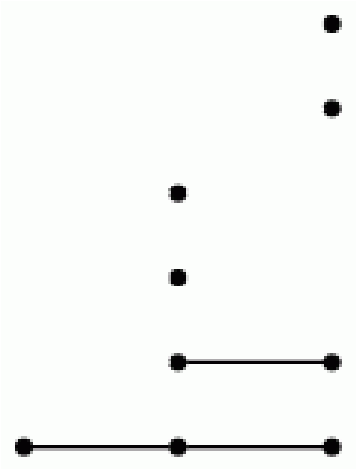
$$\beta_0^{s,t} = 0, \qquad s > t.$$

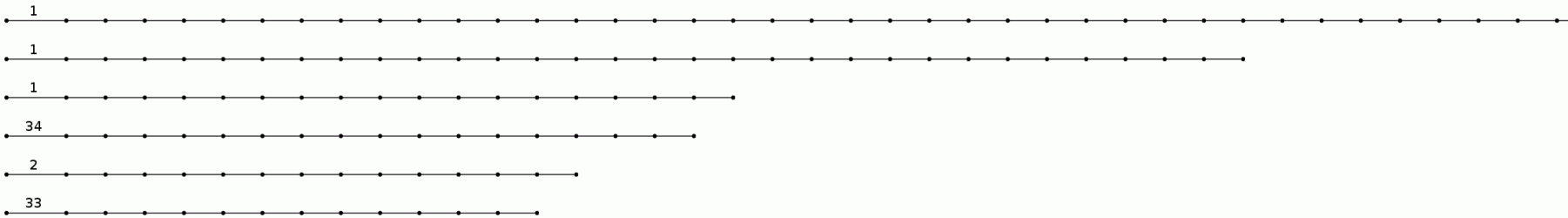
A β_n bar code has

$\beta_n^{s,t}$ *horizontal lines from column s to column t*

$$(\beta_2^{s\,t}) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 4 & 2 \\ 0 & 0 & 4 \end{pmatrix}$$



β_0 barcode for the toy data S



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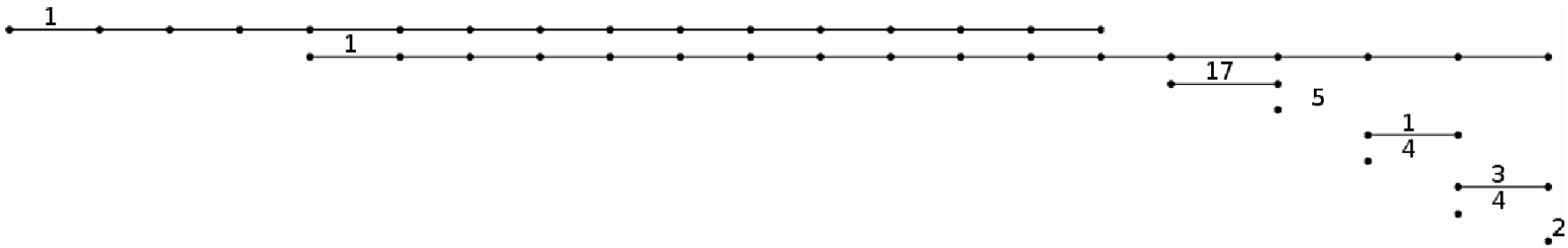
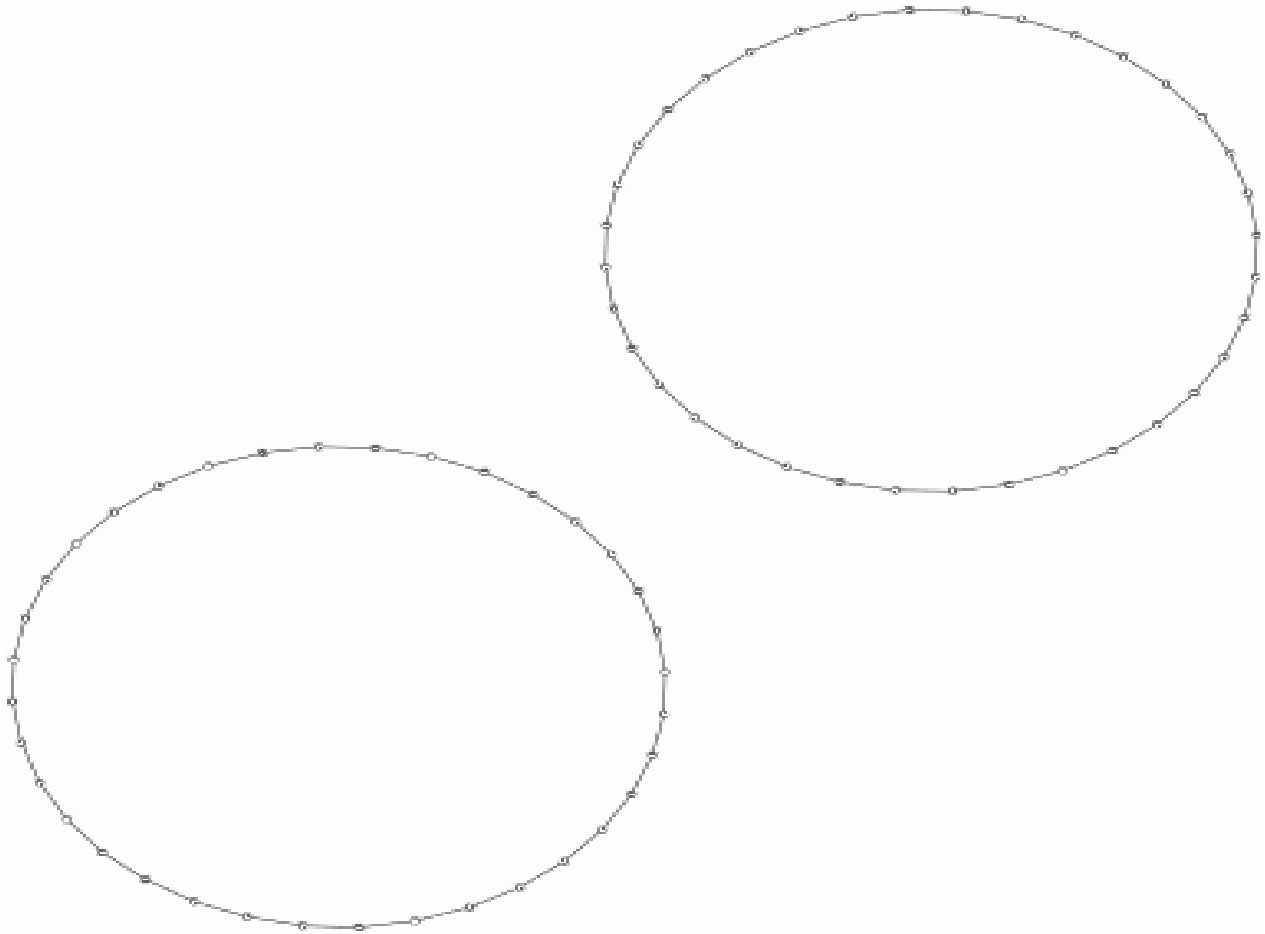
$$H_n(Y, \mathbb{F}) = \ker(\mathbb{F}^{s_n} \xrightarrow{\partial_n} \mathbb{F}^{s_{n-1}}) / \mathrm{im}(\mathbb{F}^{s_{n+1}} \xrightarrow{\partial_{n+1}} \mathbb{F}^{s_n})$$

$s_n =$ number of n-simplices in Y

β_1 barcode for the toy data S



Data Model: A homotopy retract $Y \subset Y_{20}$



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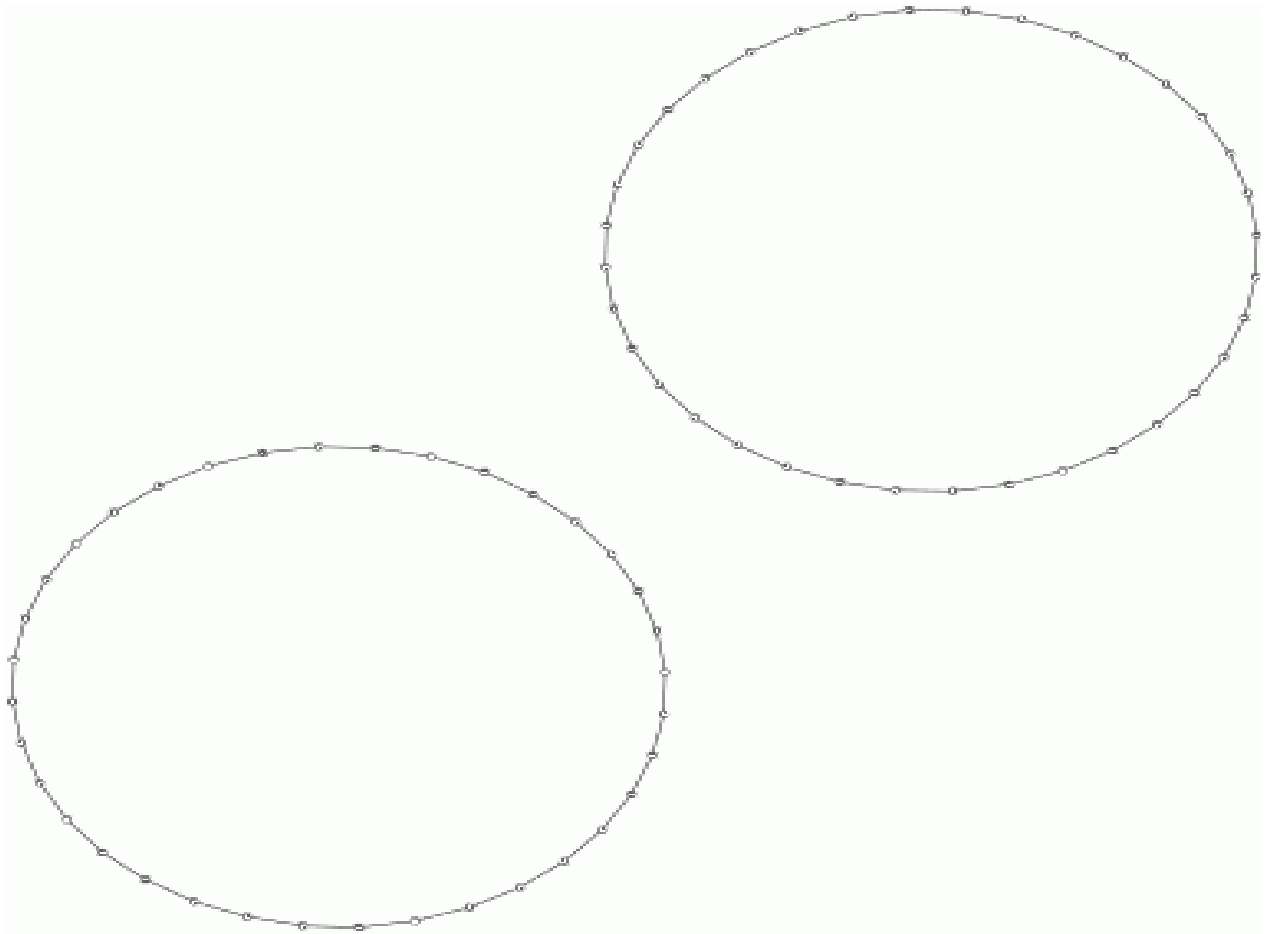

$$Y \simeq S^1 \sqcup S^1$$

Caveat

Kan-Thurston: For any space X there is a map

$$K(G,1) \to X$$

inducing

$$H_*(K(G,1),\mathbb{Z}) \cong H_*(X,\mathbb{Z}).$$

Basic Mapper Cluster Analysis

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Input:

Distances $d_X(v, v')$ for $v, v' \in S \subset X$, X an unknown metric space.

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Simplicial nerve of $\mathcal{V}$.

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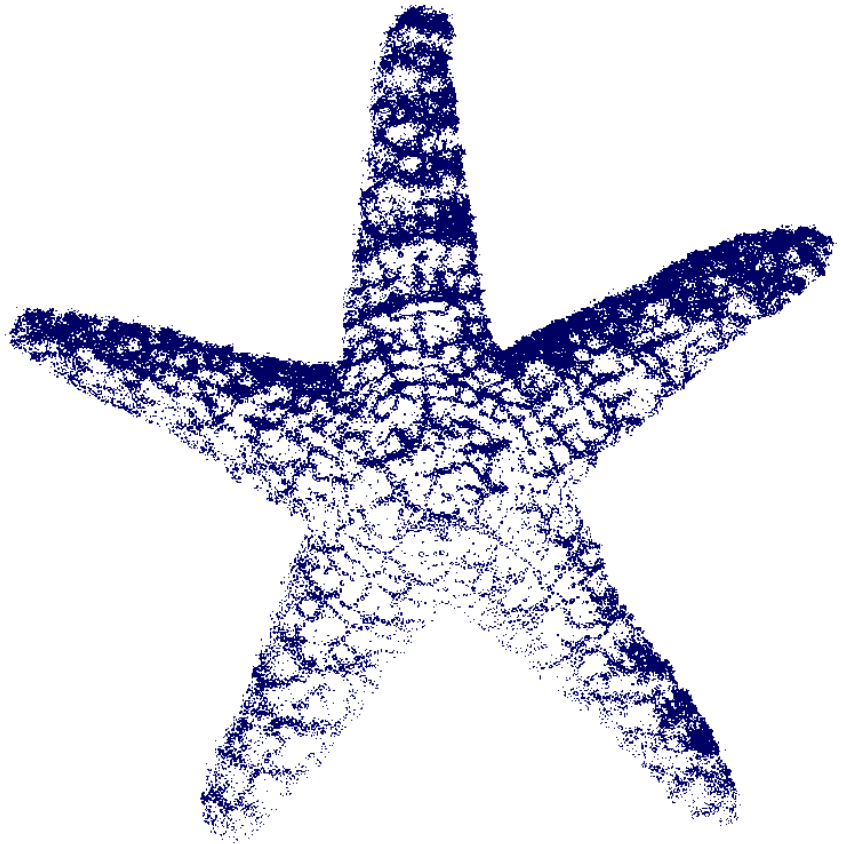

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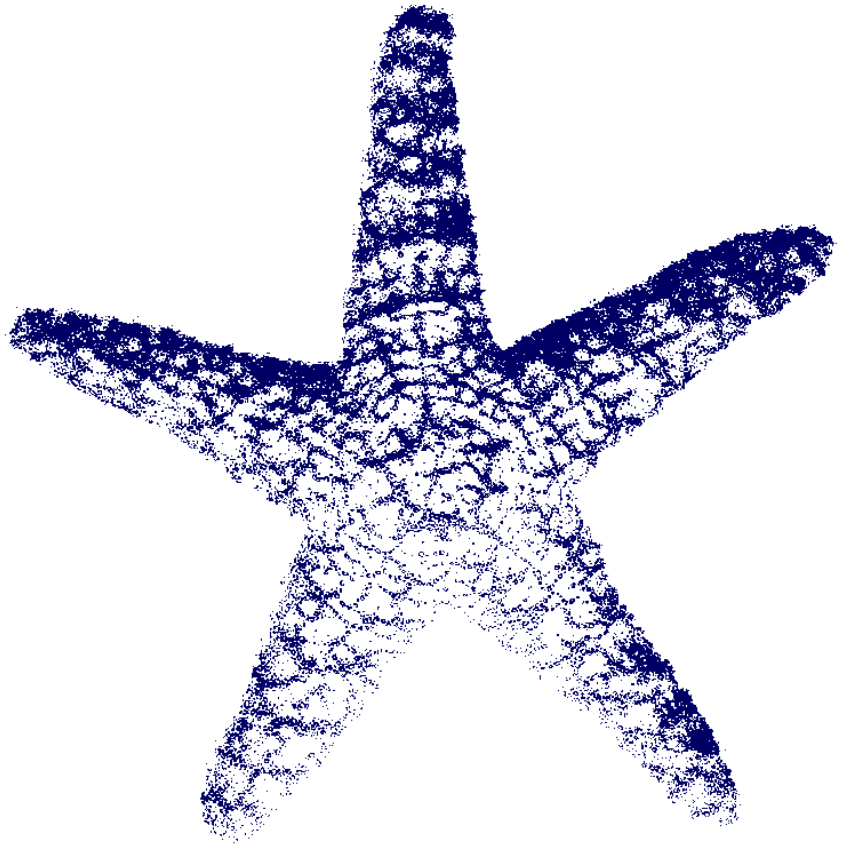
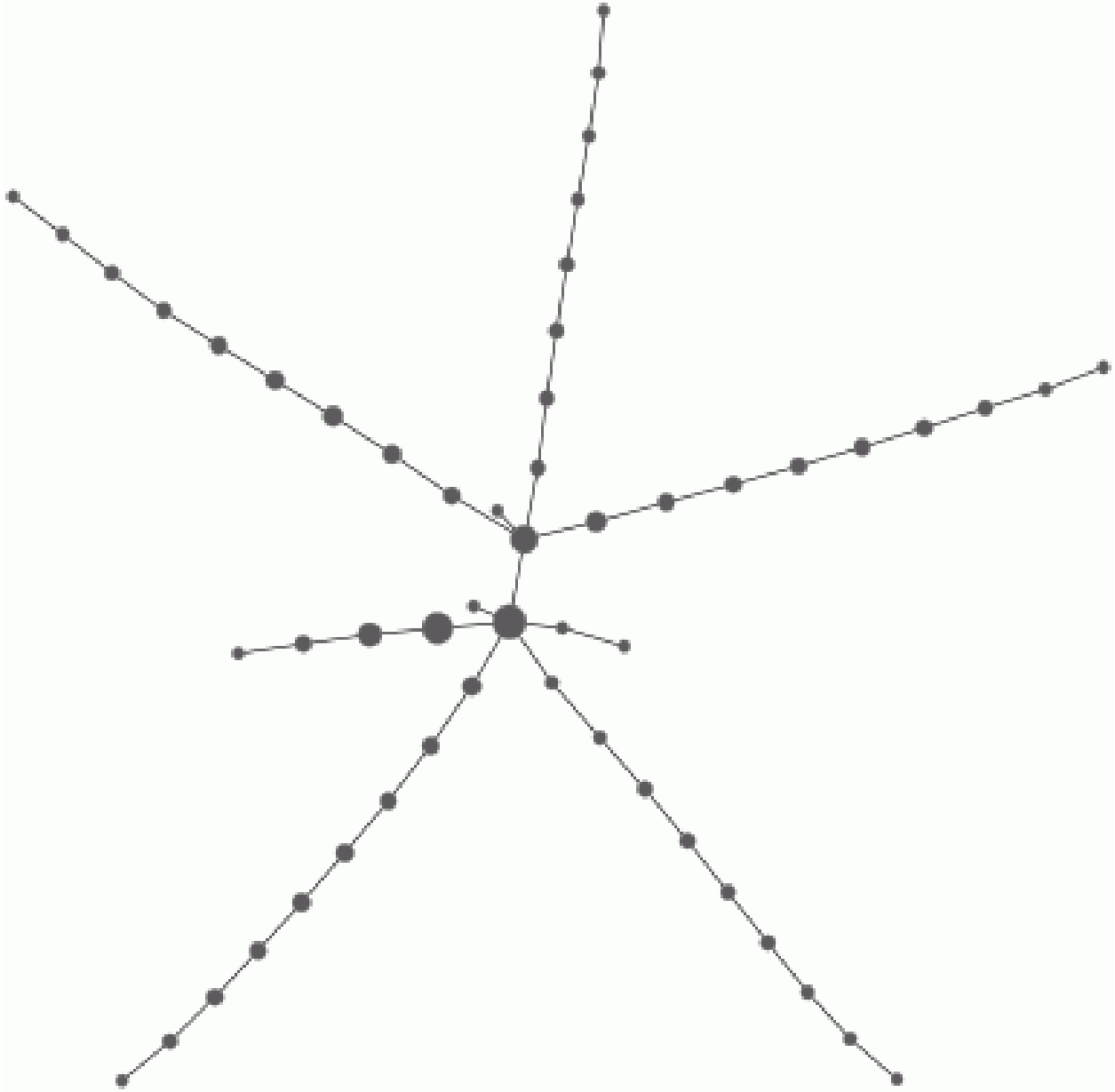


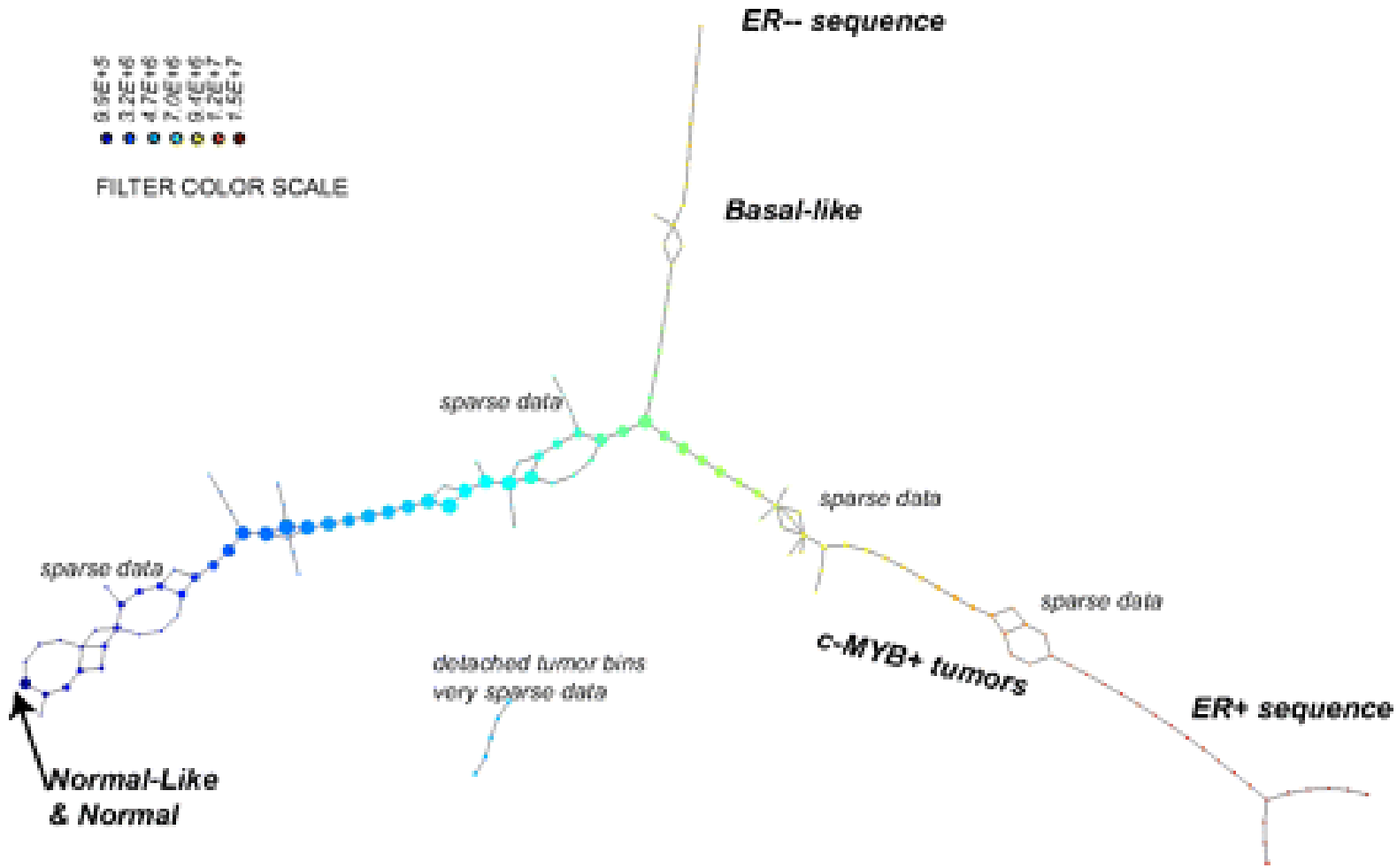
Choose $f : X \to [0, \infty), x \mapsto d(v_1, x)$

and $\mathcal{U}$ an open cover of $Z = [0, \infty)$ with no triple overlaps

Mapper output for starfish sample



Mapper output for breast cancer microarray gene expression data



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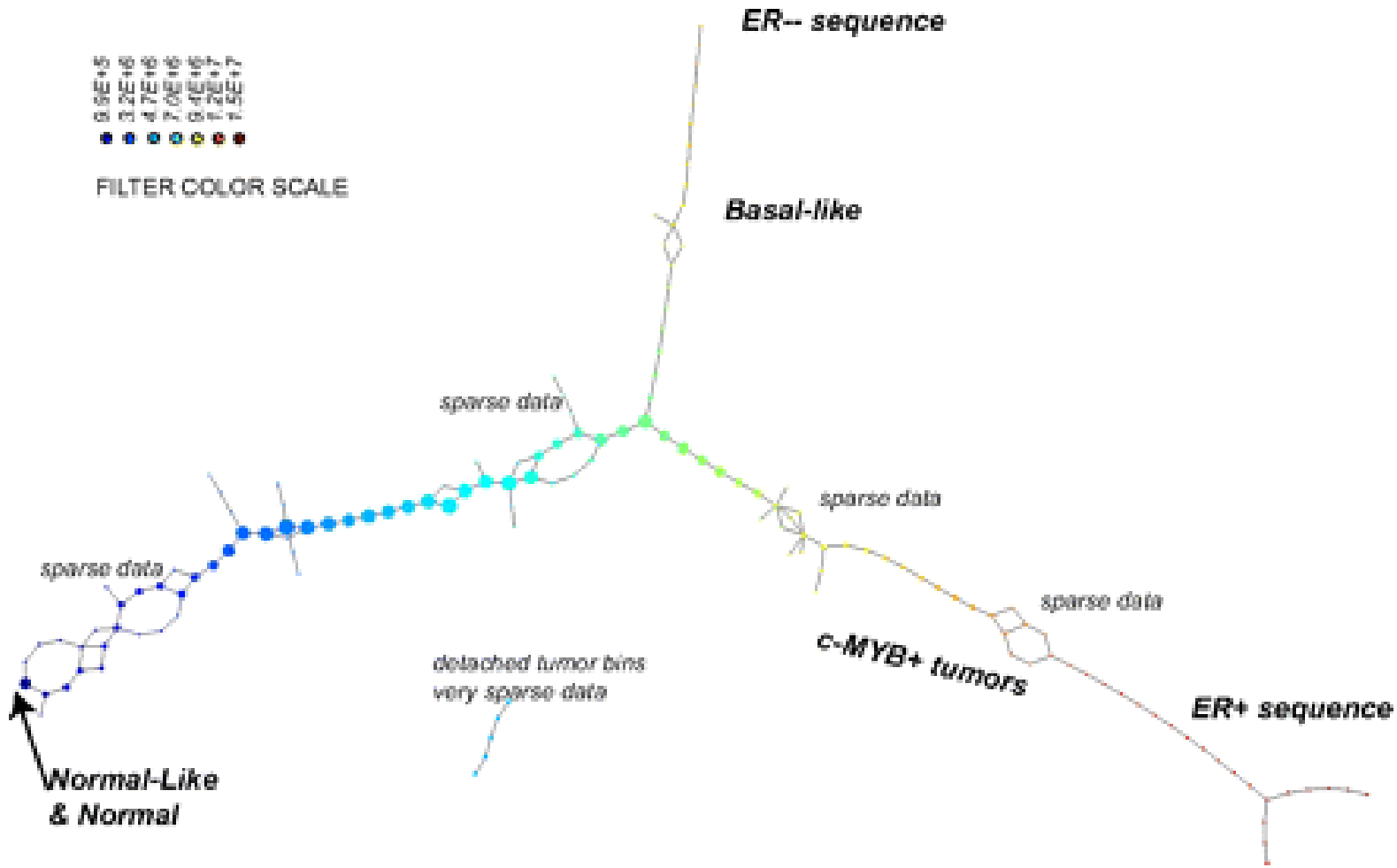

Nicolau, Levine, Carlsson (PNAS, 2011): identified a subgroup of ER+ breast cancers. These patients exhibit 100% survival.

Enhanced Mapper Cluster Analysis

E + Alokbi

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Mapper simplicial complex K with

- a simplicial space Y_σ for each $\sigma \in K$,
- an inclusion $Y_\sigma \hookrightarrow Y_\tau$ for each $\tau \subset \sigma$,
- $Y_\emptyset$ a model for X.

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Representation of output: For any functor

$$\Pi\colon \text{topology} \longrightarrow \text{algebra}$$

record $\Pi Y_\sigma \longrightarrow \Pi Y_\tau$.

Consider $S = \{v_1, \ldots, v_{500}\} \subset \mathrm{Im}\phi \subset \mathbb{R}^7$

$$\begin{array}{ccc} \phi\colon \mathbb{R}^3 & \longrightarrow & \mathbb{R}^7 \\ (x, y, z) & \mapsto & (\cos x, 2\sin x, \cos y, \sin y, -2\cos z, \sin z, \cos(x)\sin(y)). \end{array}$$

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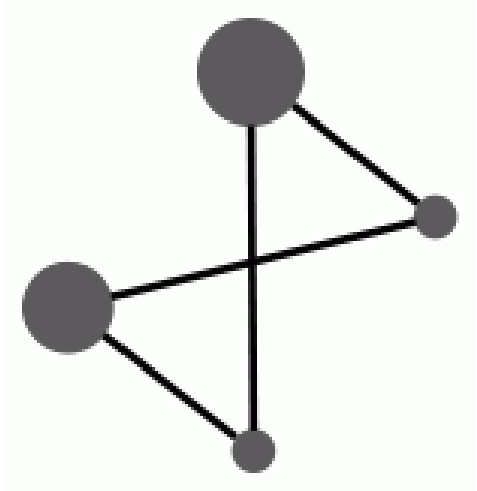
With Euclidean metric on $\mathbb{R}^7$, and filter function

$$\begin{array}{ccc} \mathbb{R}^7 & \xrightarrow{f} & \mathbb{R}^2, \\ (x_1, \ldots, x_7) & \mapsto & (x_1, x_2) \end{array}$$

and open cover $\{U_\alpha\}$ of $Z = \mathbb{R}^2$:

Basic Mapper output K



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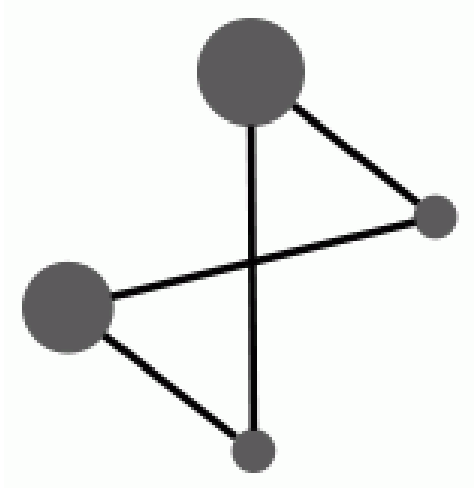

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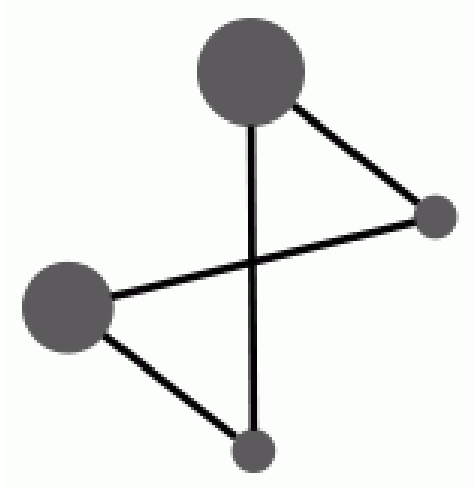

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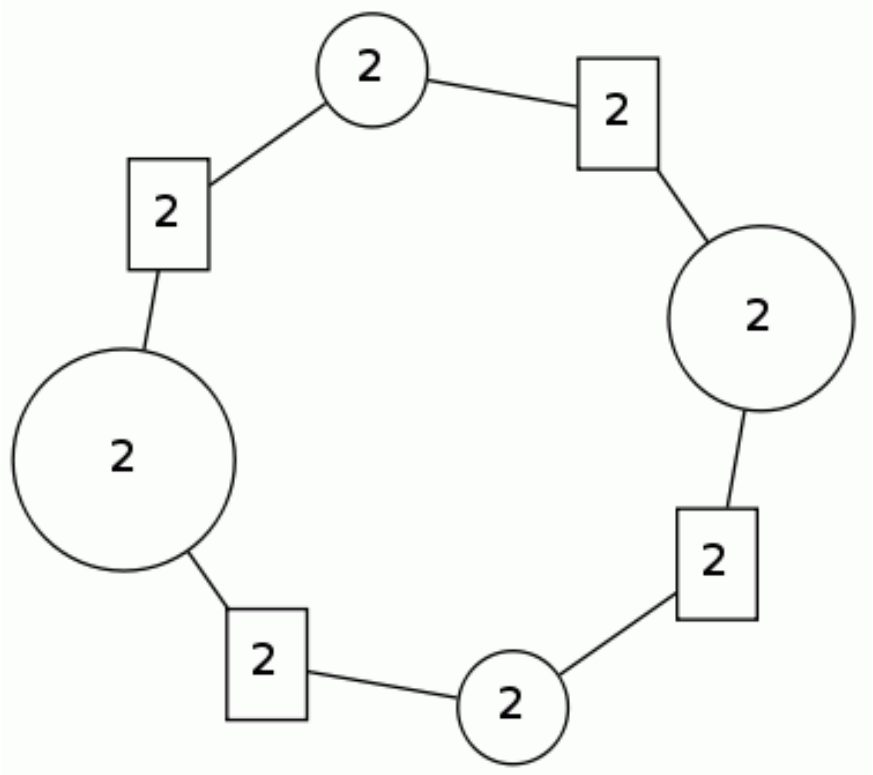
Associate to vertices of K the connected components of clique simplicial complexes $Y(W_\alpha, \epsilon)$, and to simplices $\sigma \in K$

$$Y_\sigma = \bigcap_{v \in \sigma} Y_v, \qquad Y_\emptyset = \bigcup_{v \in \sigma} Y_v.$$

Mapper output enhanced with $\dim H_1(Y_\sigma, \mathbb{Q})$



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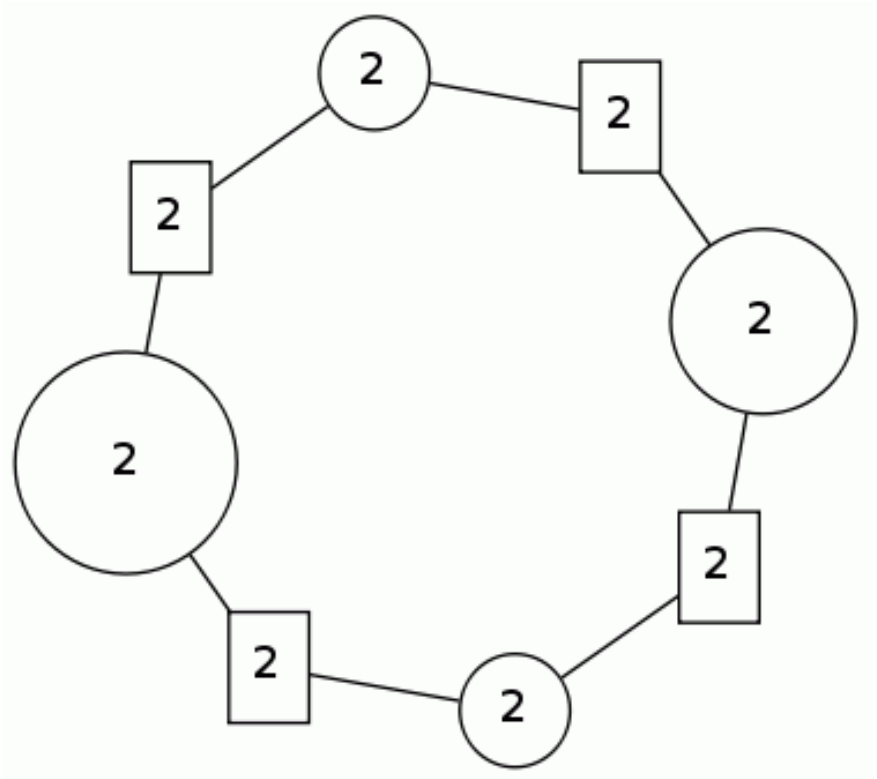
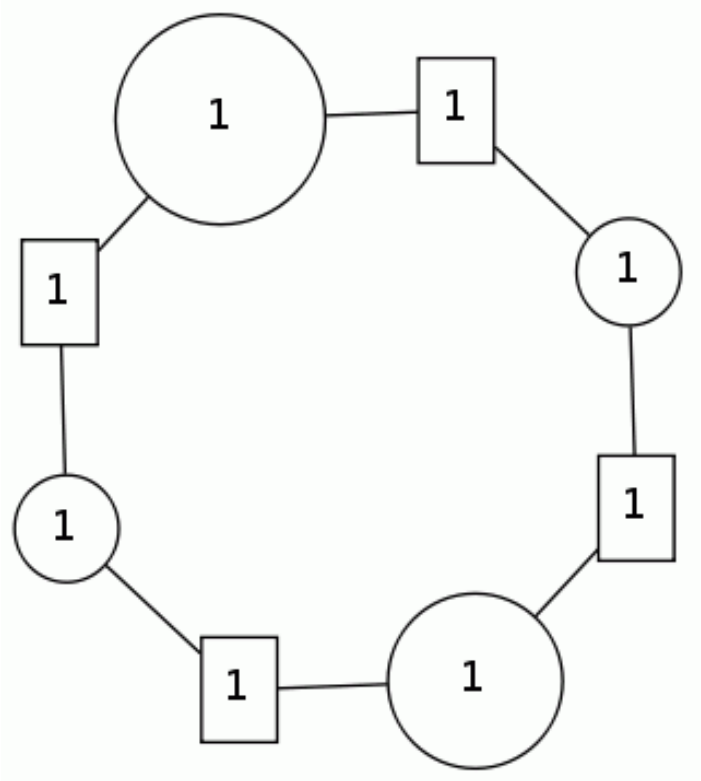


$$H_1(Y_\emptyset, \mathbb{Q}) = \mathbb{Q} \oplus \mathbb{Q}$$

Mapper output enhanced with $\dim H_2(Y_\sigma, \mathbb{Q})$



$$H_2(Y_\emptyset, \mathbb{Q}) = \mathbb{Q}$$

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Need functors

$$\Pi\colon \text{topology} \longrightarrow \text{algebra}$$

that distinguish between such spaces.

Fundamental group presentations

A finite presentation for

$$\pi_1(Y, y_0) = \{p\colon [0,1] \longrightarrow Y \ : \ p(0) = p(1) = y_0\}/\simeq$$

is implemented in GAP for **small** cellular spaces Y.

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$$H^1(Y, \mathbb{Z}) \times H^1(Y, \mathbb{Z}) \longrightarrow H^2(Y, \mathbb{Z}), (\alpha, \beta) \mapsto \alpha \cup \beta$$

induced by

$$Y \longrightarrow Y \times Y, x \mapsto (x, x).$$

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$\alpha \cup \beta$ is non-trivial for $Y = S^1 \times S^1 \times S^1$ and trivial for $Y = S^1 \vee S^1 \vee S^1 \vee S^2 \vee S^2 \vee S^2 \vee S^3$.

Parallel computation of $\pi_1 Y$?

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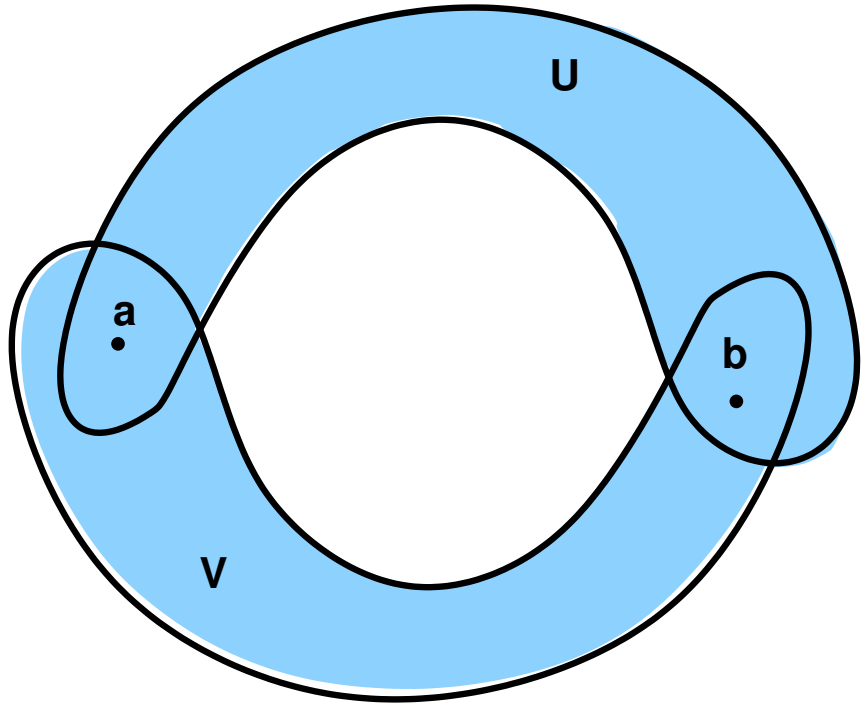
$Y =$



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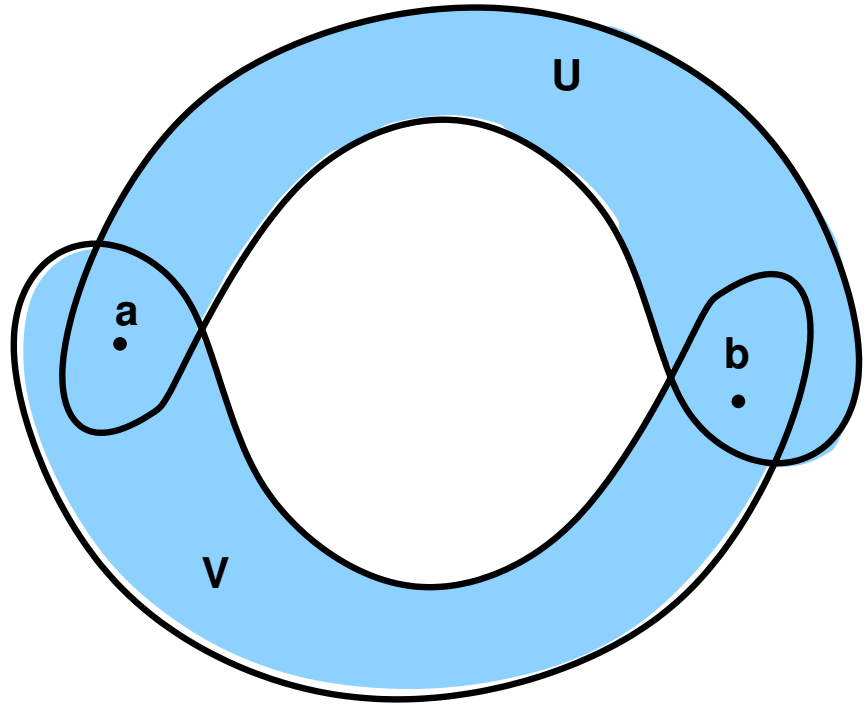

Enter groupoids

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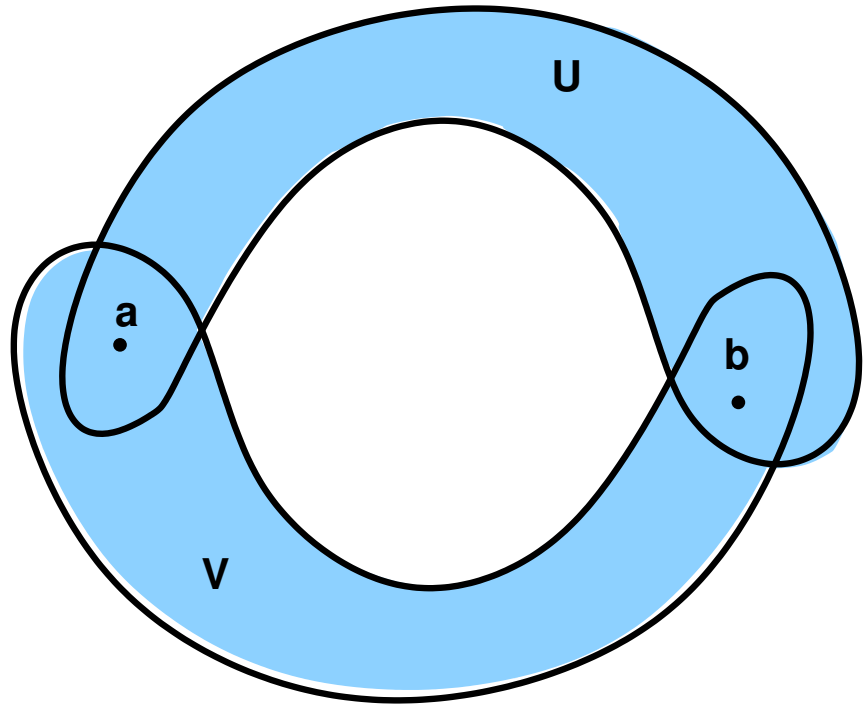
$Y =$ 

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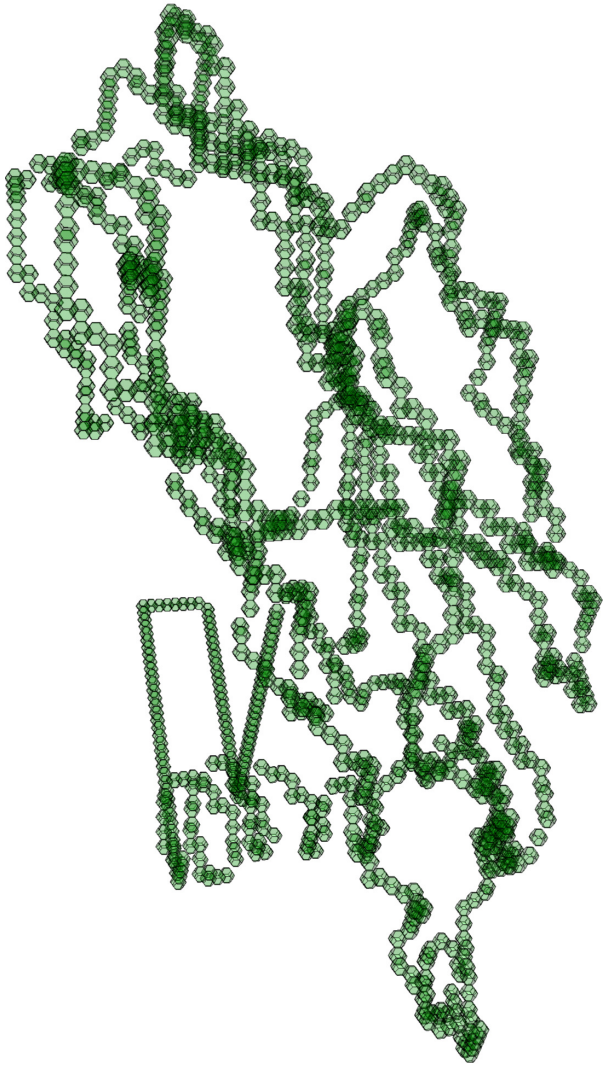
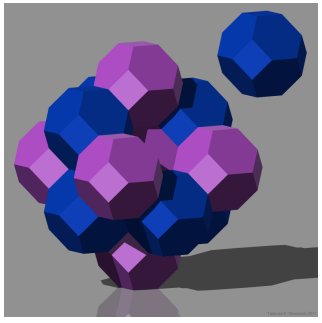
$$\pi_1(U \cup V, \{a,b\}) \cong \pi_1(U, \{a,b\}) *_{\pi_1(U \cap V, \{a,b\})} \pi_1(V, \{a,b\})$$

1V2X protein backbone





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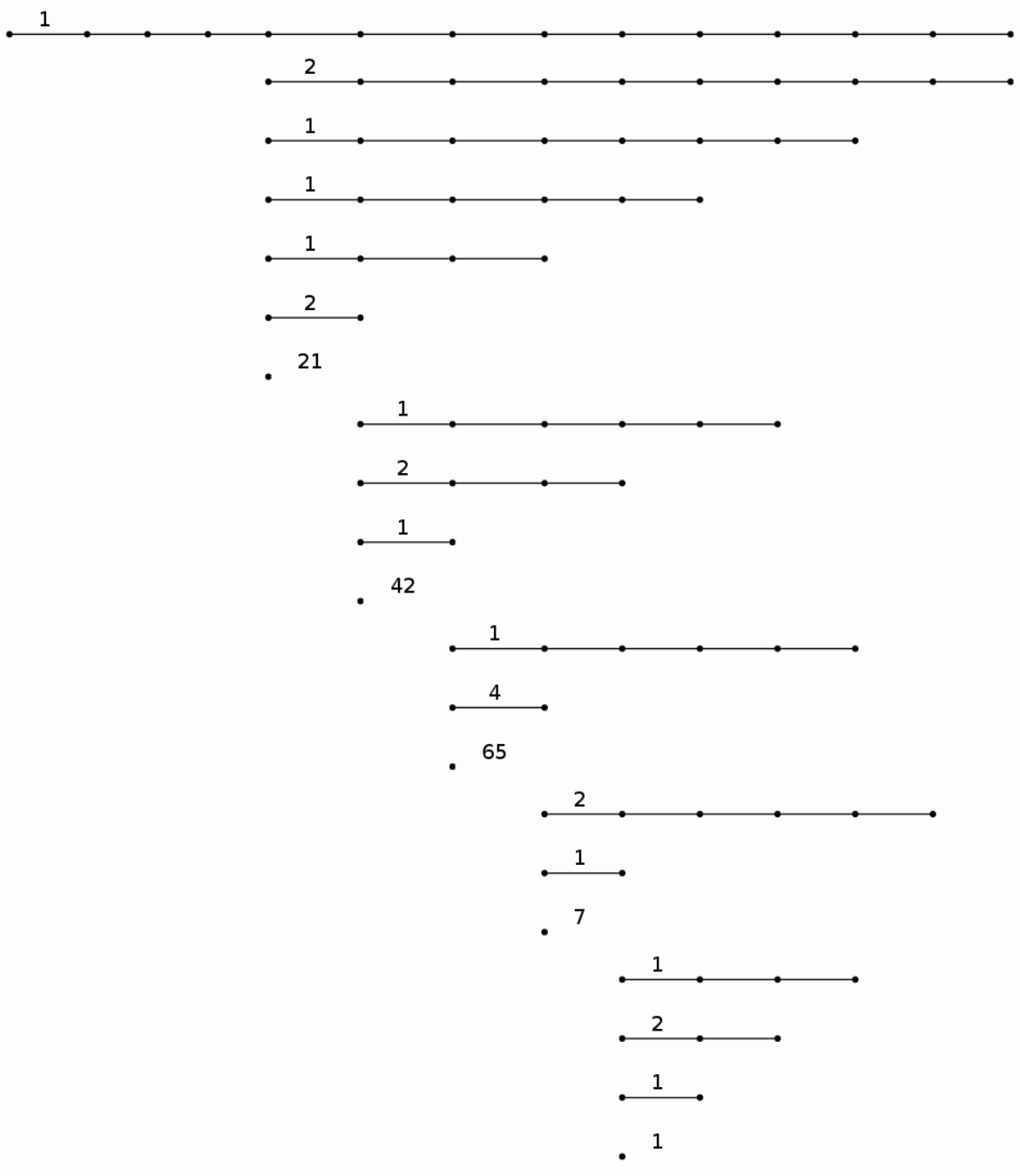
Persistent β_1



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But what good is this presentation of the fundamental group?

An isomorphism invariant of finitely presented groups

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$I_n(\pi_1(\mathbb{R}^3 \setminus K))$ tested on 1701935 **prime knots** ≤ 14 **crossings**

min value of n to distinguish between knots on c crossings

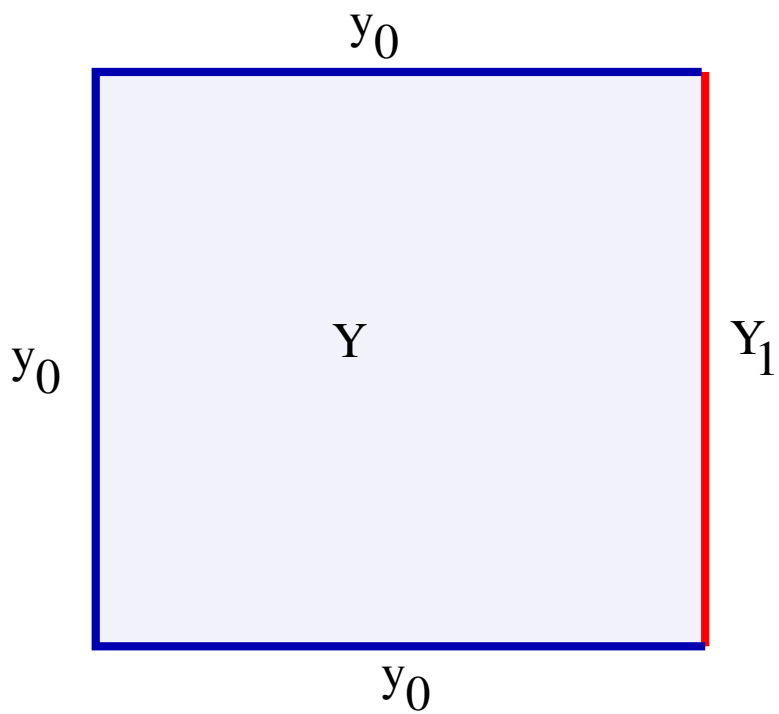
c	3	4	5	6	7	8	9	10	11	12	13	14
n	2	2	3	3	3	3	5	5	6	6	7	7

Brendel, E., Juda, Mrozek

Crossed modules

For $y_0 \in Y_1 \subset Y$ we consider

$$\pi_2(Y, Y_1) = \{p\colon [0,1]^2 \to Y \ : \begin{array}{ll} p(x,y) = y_0 & \text{if } x = 0, \\ p(x,y) = y_0 & \text{if } y = 0 \text{ or } 1 \\ p(x,y) \in Y_1 & \text{if } x = 1\} \end{array} \}/\simeq$$



$G = \pi_1(Y_1)$ acts on $M = \pi_2(Y, Y_1)$ and the group homomorphism

$$\partial \colon M \to G$$

satisfies

- $\partial({}^{g}m) = gmg^{-1}$,
- ${}^{\partial m}m' = mm'm^{-1}$.

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The crossed module $\Pi(Y^2, Y^1)$ is **freely presented** and, given any **finite** crossed module C, the set of homotopy classes of morphisms

$$[\Pi(Y, Y^1), C] = \{\Pi(Y, Y^1) \to C\}/\simeq$$

can be computed and is a homotopy invariant of Y.

The **order** of homotopy 2-type X is the least value of $m = |M||G|$ for a representative crossed module $M \xrightarrow{\partial} G$.

Proposition (E, Le)

The homotopy 2-types of order m are classified up to homotopy for $m \leq 127$, $m \neq 32, 64, 81, 96$ and are distributed with GAP.

$\partial\colon Q \to Aut(Q)$

```
gap> G2:=AutoCrossedModule(DihedralGroup(216));;

gap> Size(G2);
839808

gap> IdQuasiCrossedModule(G2);
[ 72, 68 ]
```

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Crossed module
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Crossed module


gap> Homology(G,5);
[ 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 18 ]
```