Topological Data Analysis

Part I: Persistent homology

Ulrich Bauer

TUM

February 4, 2015

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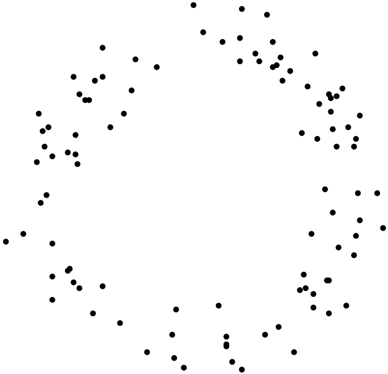
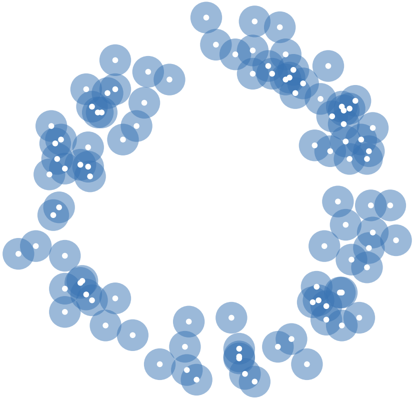
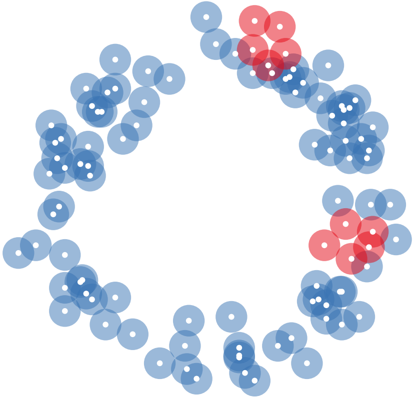
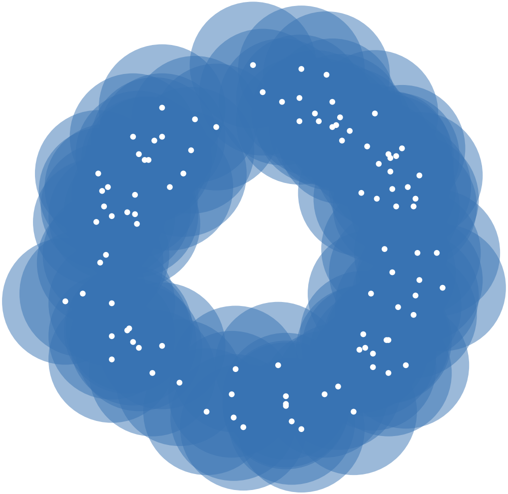
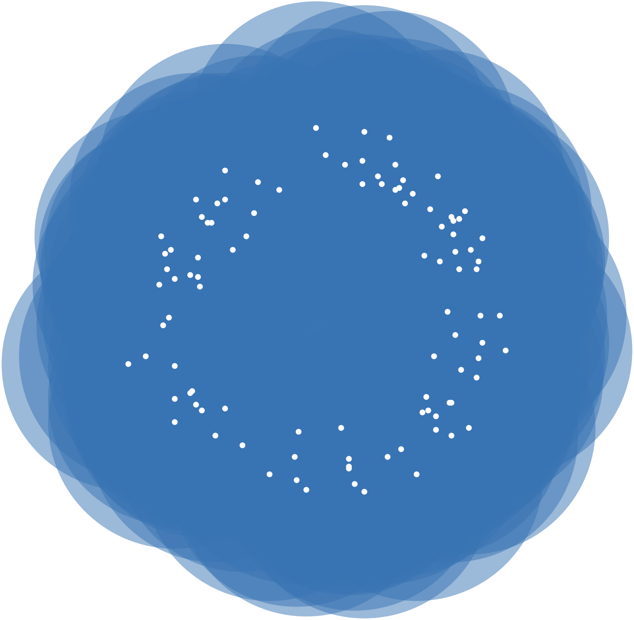
Persistent homology

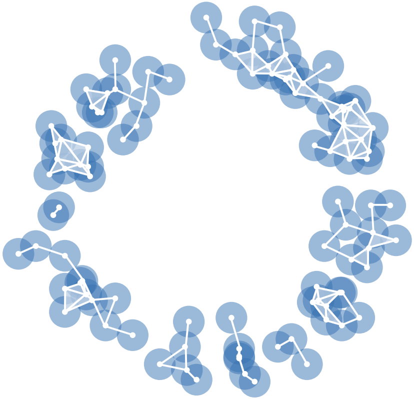


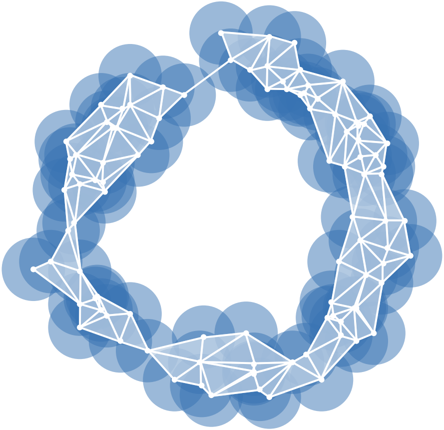


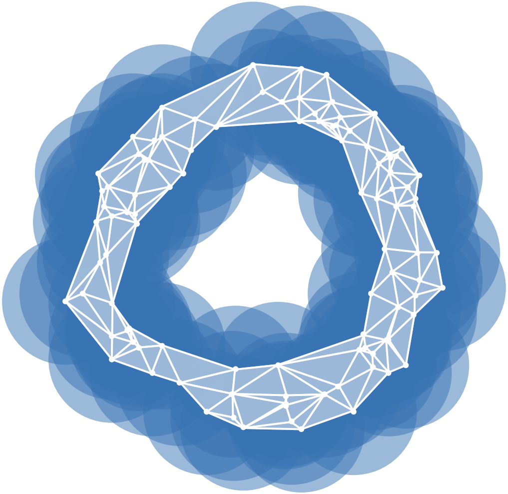


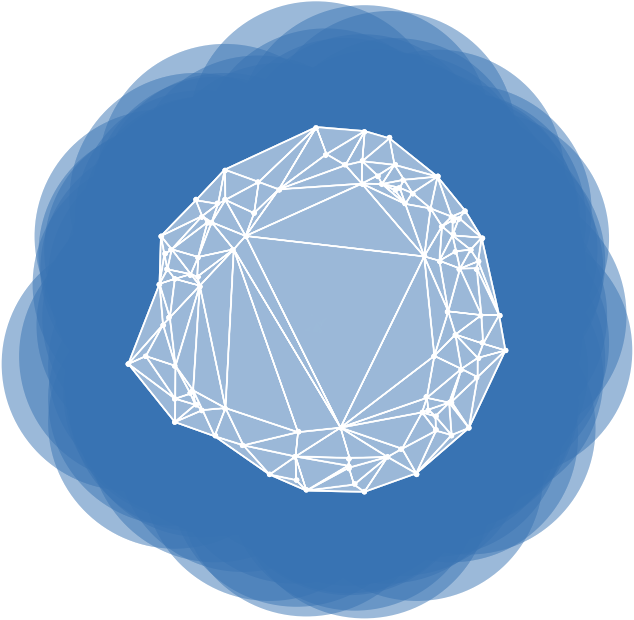












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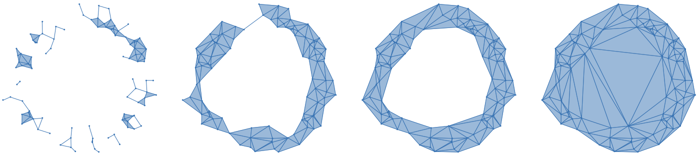

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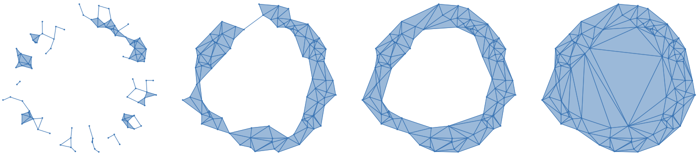

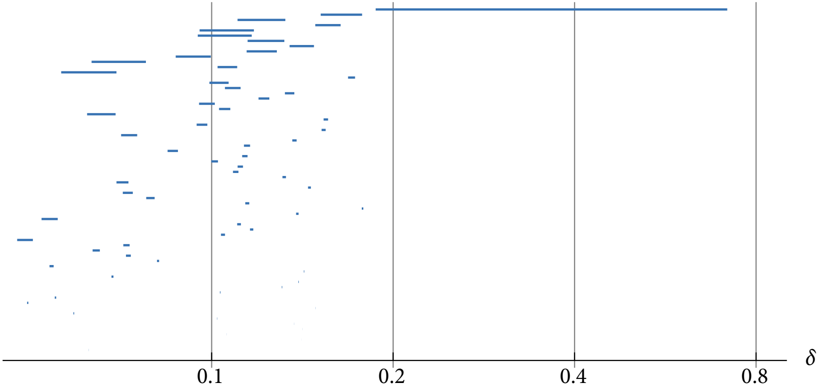

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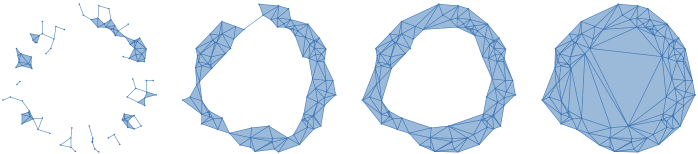

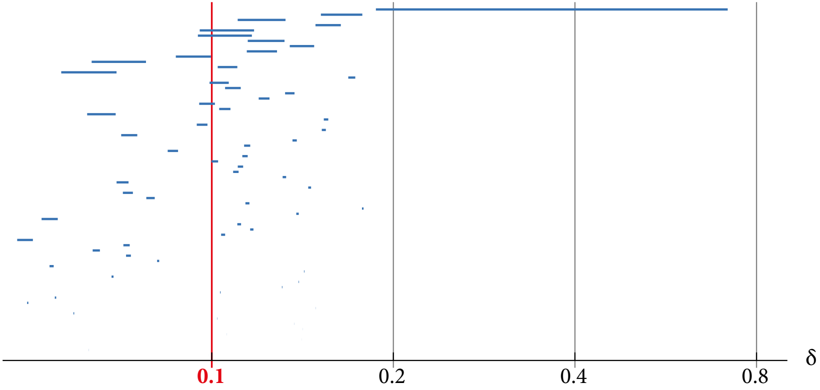

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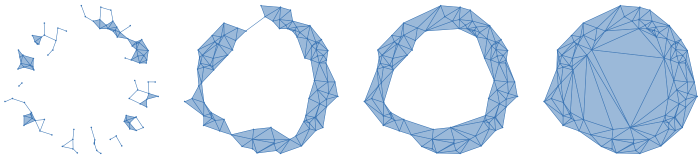

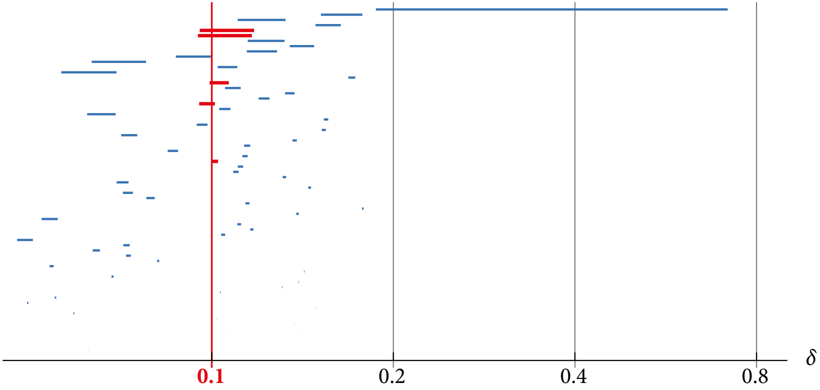

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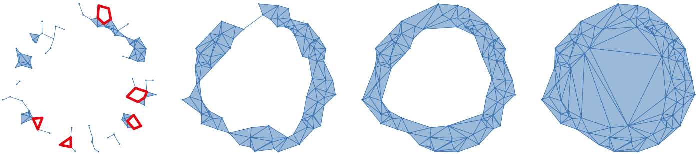

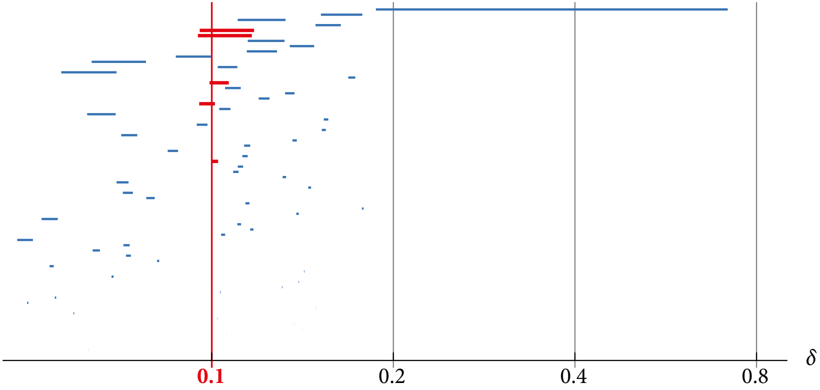

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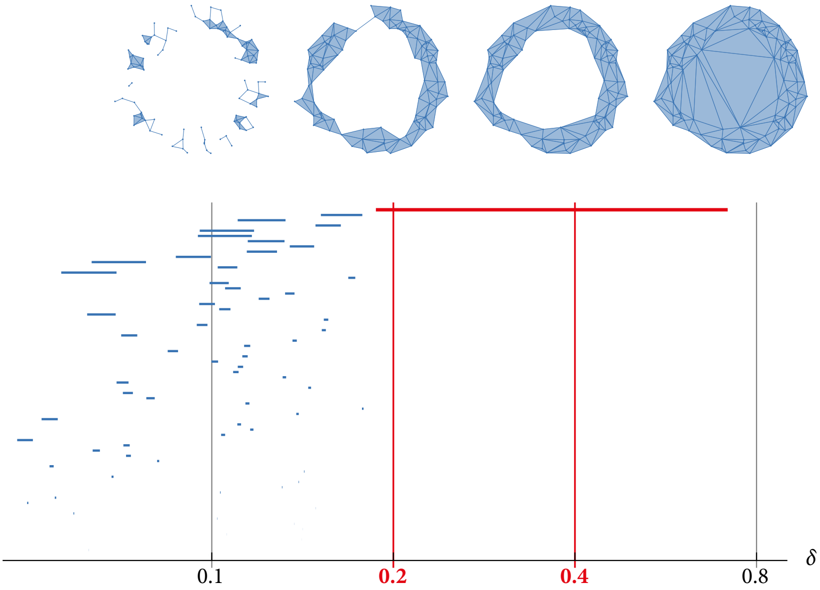

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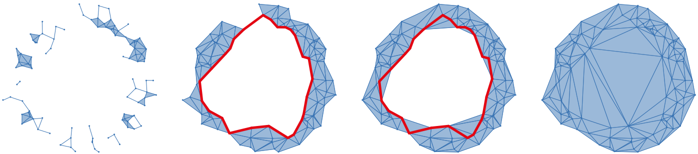

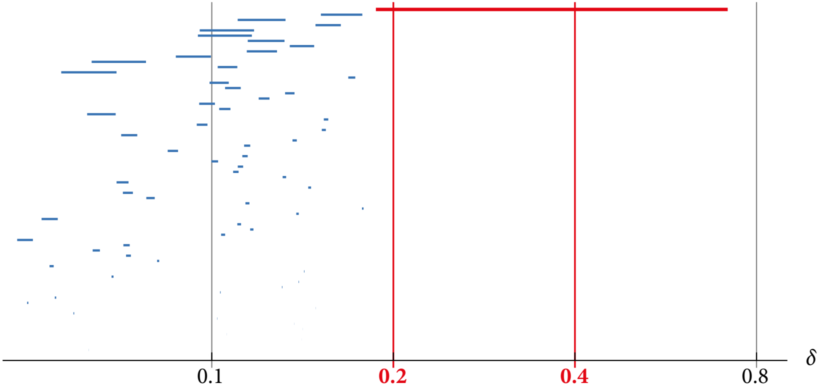

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- $\mathbf{R}$ is the poset category of $(\mathbb{R}, \le)$

The pipeline of topological data analysis

$$
\begin{tikzcd}
\text{Data} \arrow[d] & \text{point cloud} \arrow[d, "\text{distance}"] \\
\text{Geometry} \arrow[d] & \text{function} \arrow[d, "\text{sublevel sets}"] \\
\text{Topology} \arrow[d] & \text{topological spaces} \arrow[d, "\text{homology}"] \\
\text{Algebra} \arrow[d] & \text{vector spaces} \arrow[d, "\text{barcode}"] \\
\text{Combinatorics} & \text{intervals}
\end{tikzcd}
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Simplification & Reconstruction

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It is sometimes possible to recover the homology of Ω this way, but the assumptions are quite strong:

Homology reconstruction using union of balls

Theorem (Niyogi, Smale, Weinberger 2006)

Let M be a submanifold of $\mathbb{R}^d$. Let $P \subset M$ be such that $M \subseteq P^\delta$ for some $\delta < \sqrt{3/20}\,\mathrm{reach}(M)$. Then

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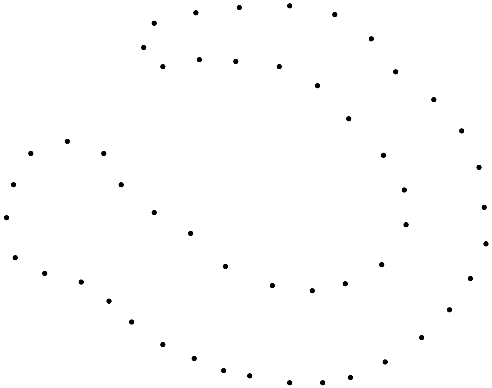
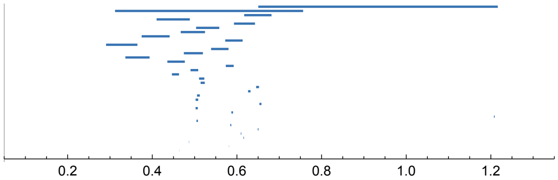
- The isomorphism is induced by the inclusion $M \hookrightarrow P^{2\delta}$.

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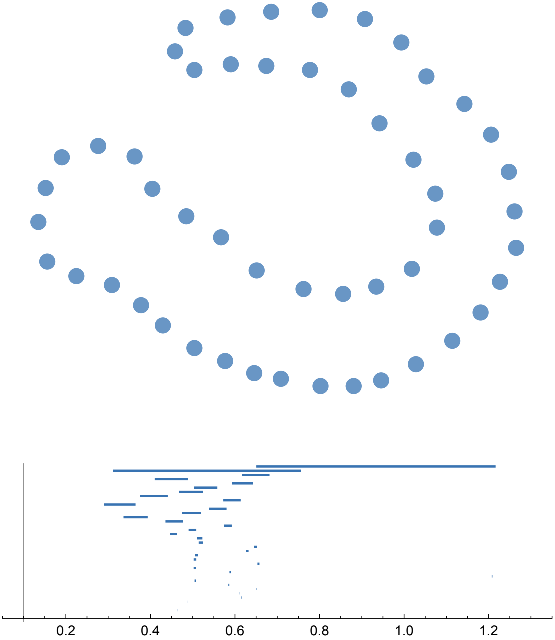
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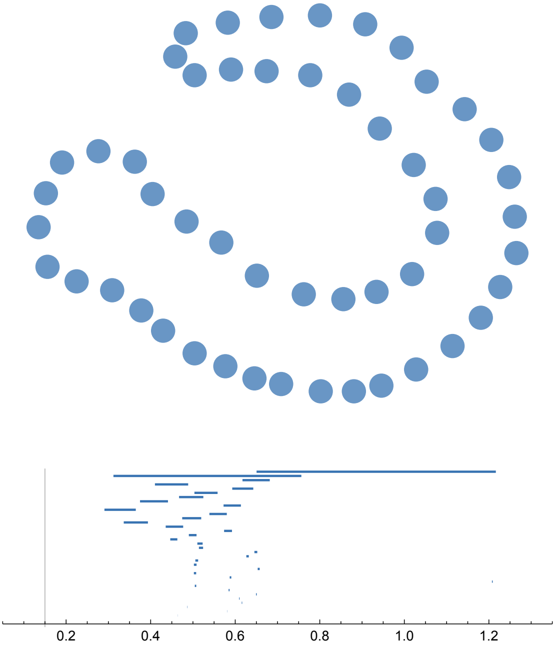
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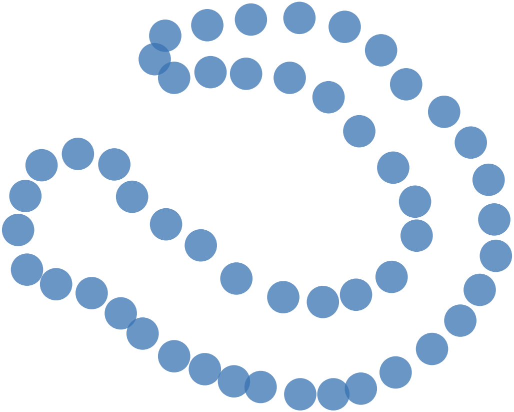

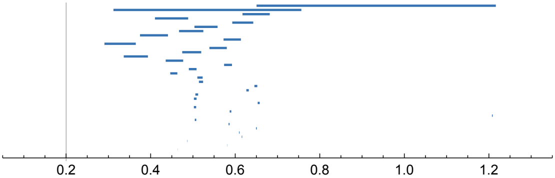
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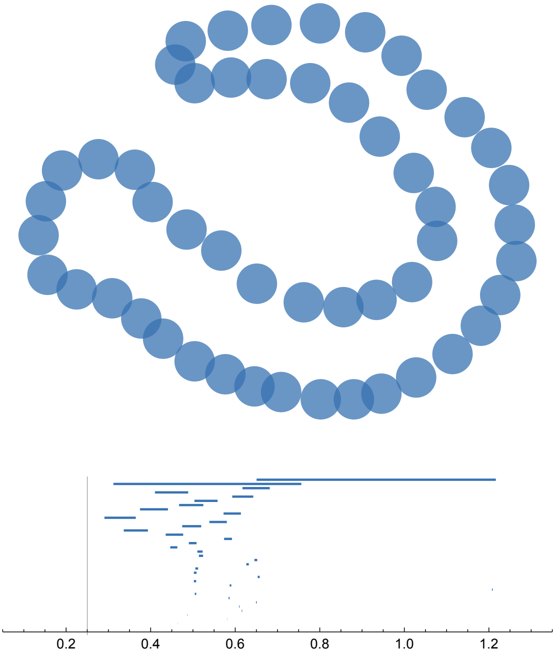
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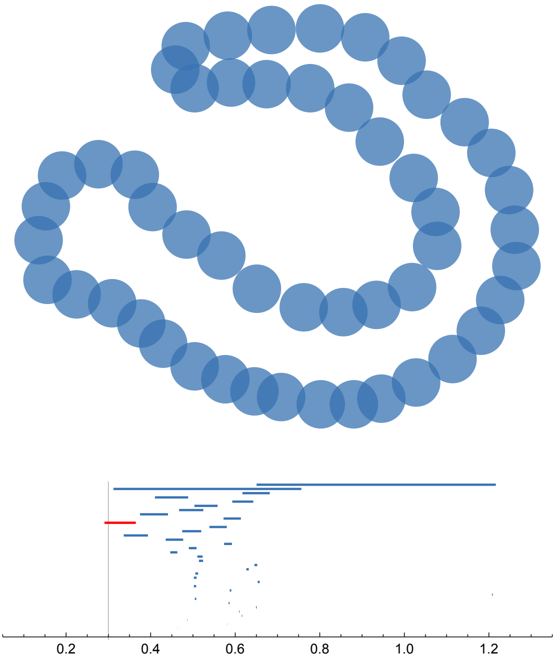
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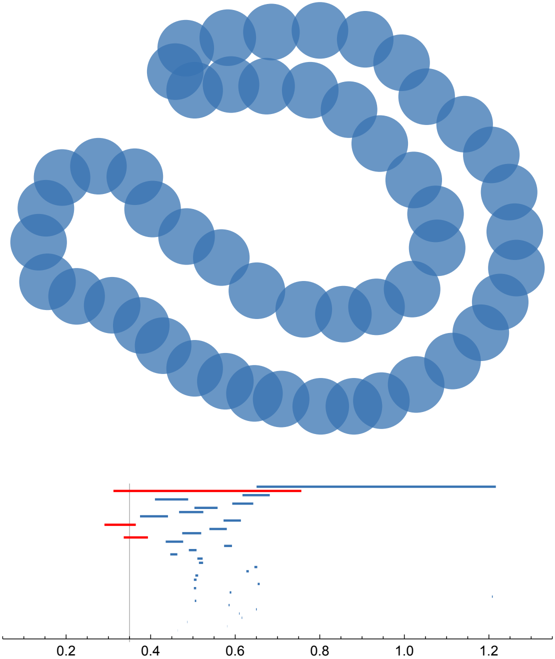
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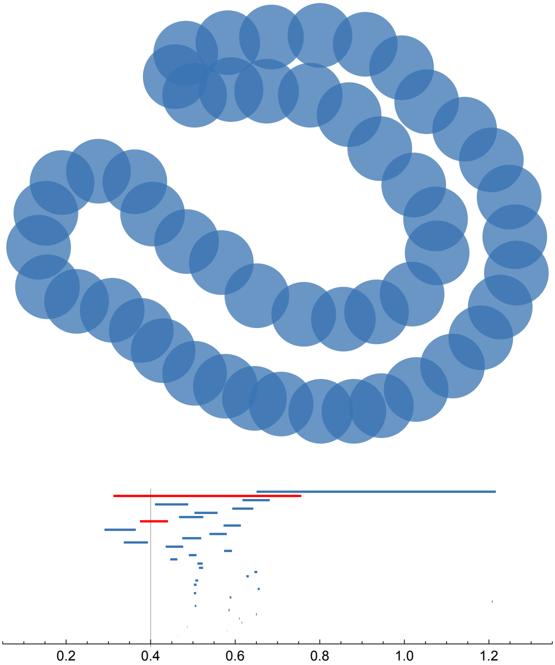
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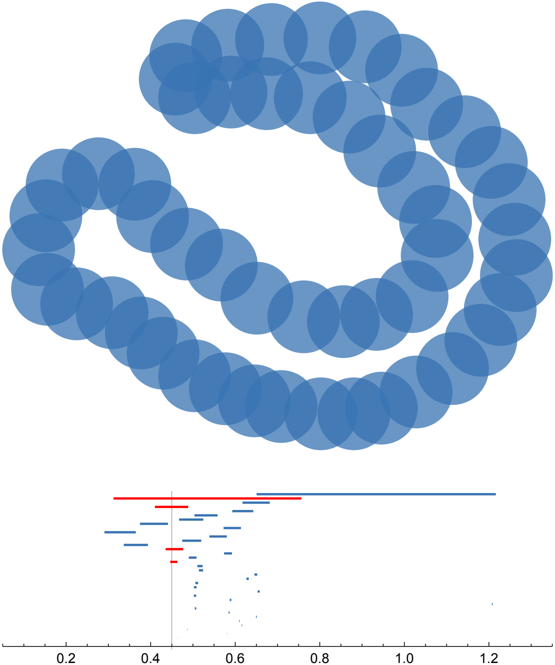
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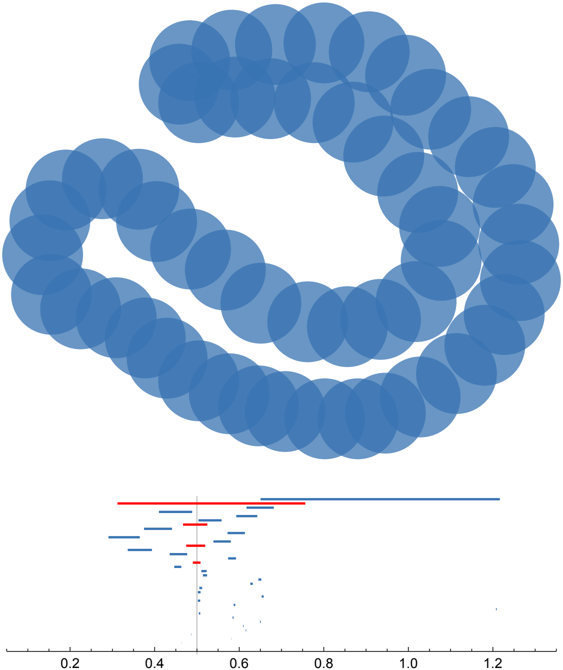
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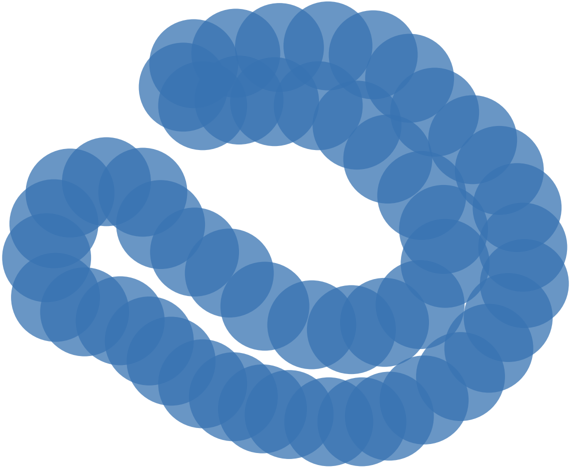

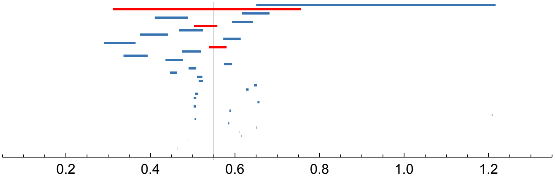

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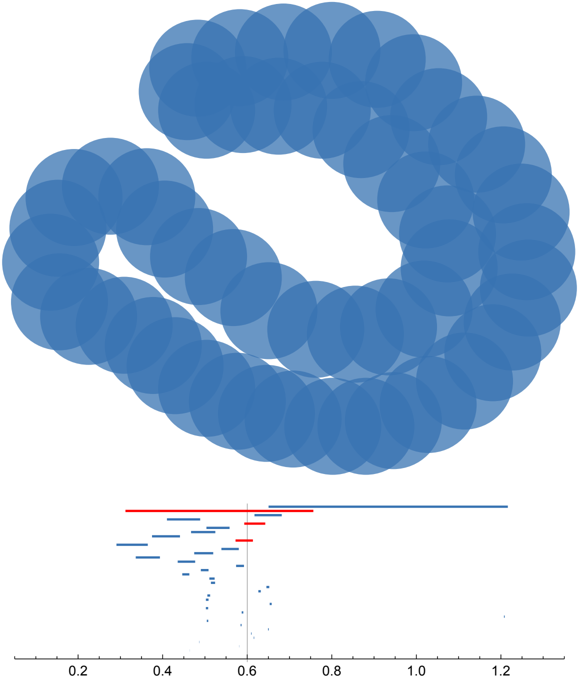
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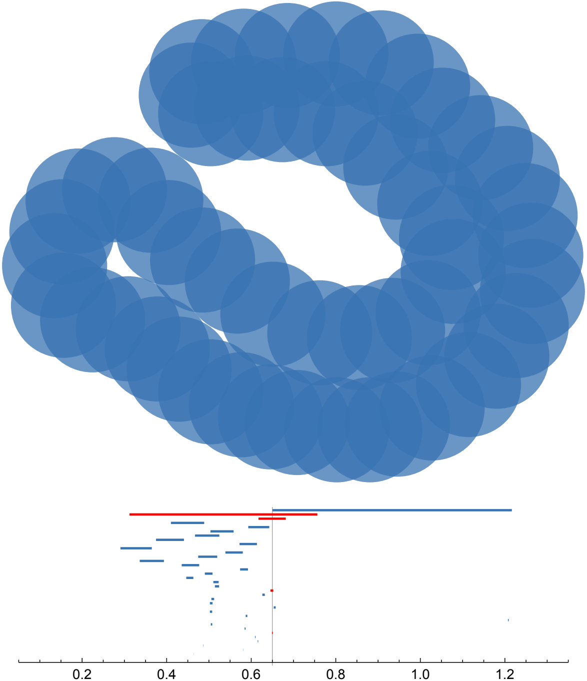

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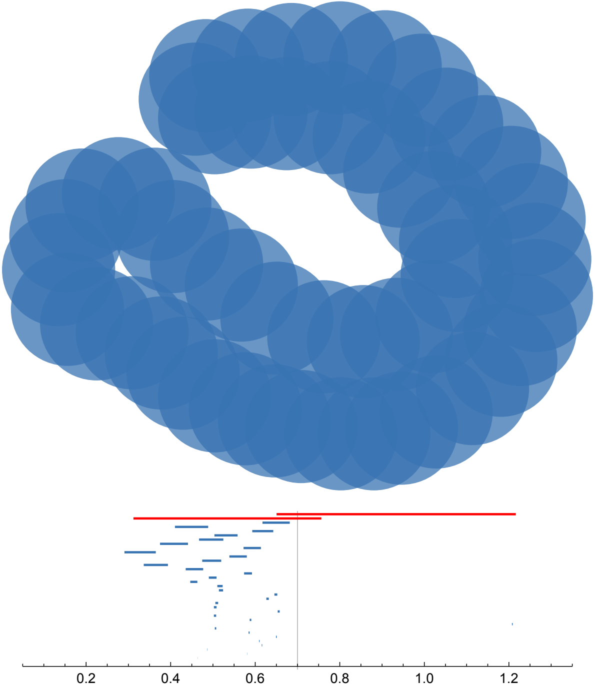

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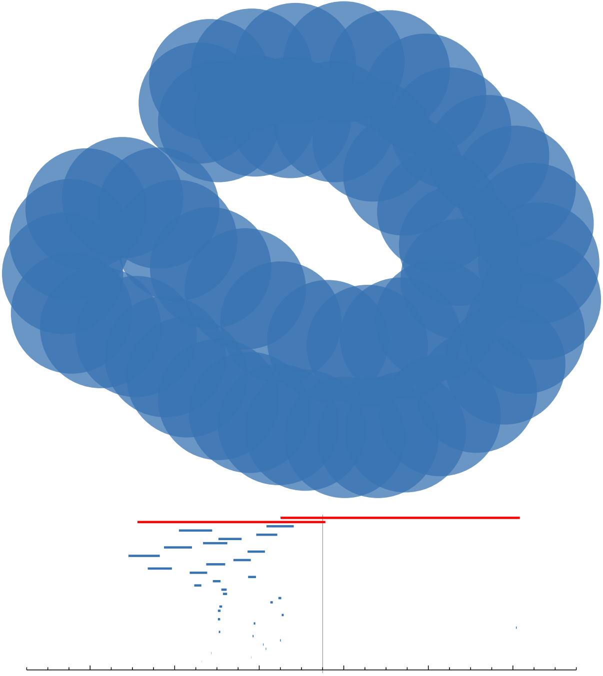
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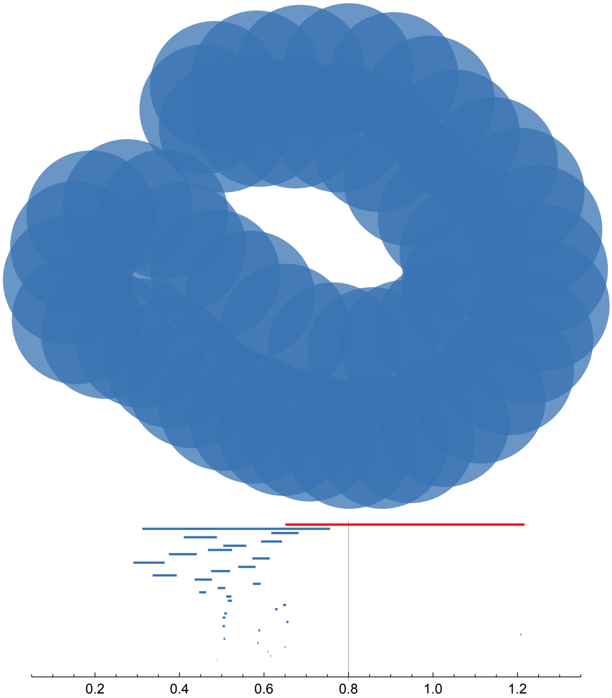
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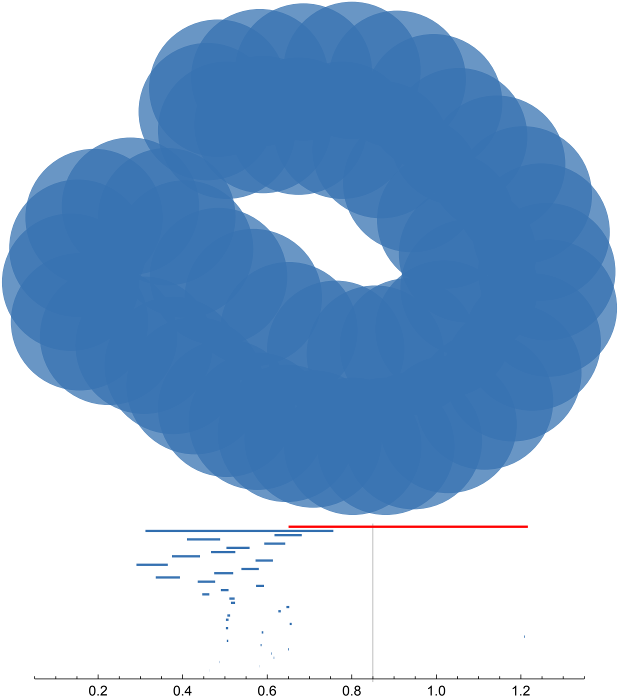
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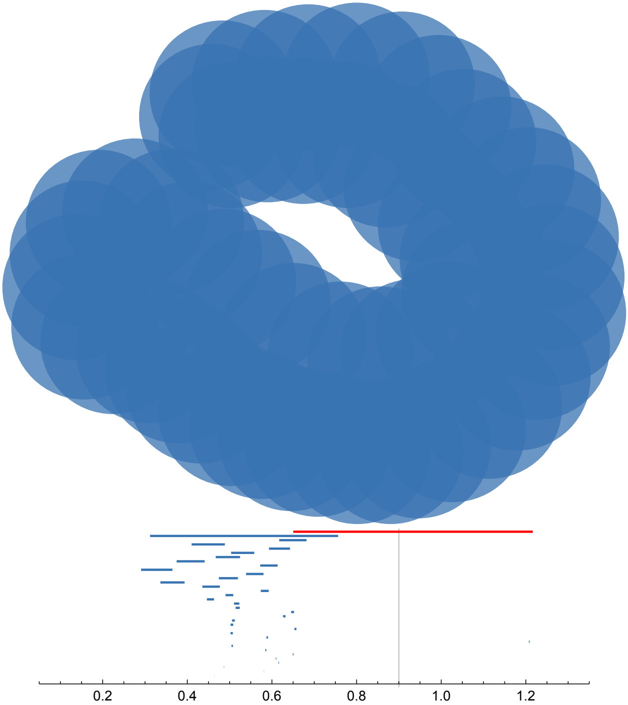
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$P_\delta = B_\delta(P)$: δ-neighborhood (union of balls) around P

Theorem (Cohen-Steiner, Edelsbrunner, Harer 2005)

Let $\Omega \subset \mathbb{R}^d$. Let $P \subset \Omega$ be such that

- $\Omega \subseteq P_\delta$ *for some* $\delta > 0$ *and*
- *both* $H_*(\Omega \hookrightarrow \Omega_\delta)$ *and* $H_*(\Omega_\delta \hookrightarrow \Omega_{2\delta})$ *are isomorphisms.*

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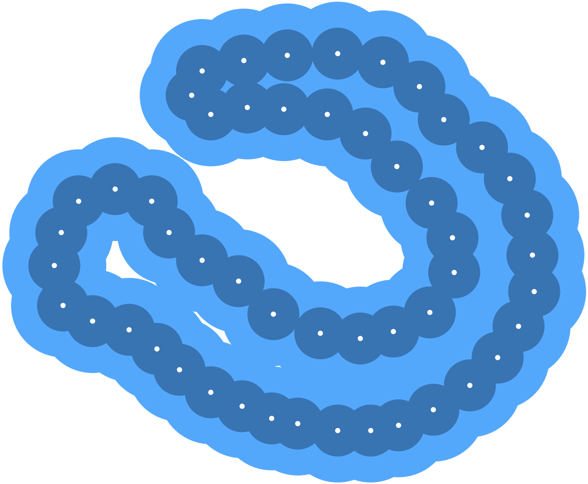

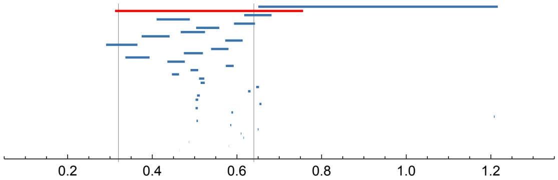

0.2
0.4
0.6
0.8
1.0
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Proof.

$$\begin{tikzcd}[column sep=small]
\Omega \arrow[dr, hook] & & \Omega_{\delta+\epsilon} \arrow[dr, hook] & & \Omega_{2(\delta+\epsilon)} \\
& P_\delta \arrow[ur, hook] & & P_{2\delta+\epsilon} \arrow[ur, hook] &
\end{tikzcd}$$

Proof.

$$
\begin{tikzcd}[column sep=small]
H_*(\Omega) \arrow[dr] & & H_*(\Omega_{\delta+\epsilon}) \arrow[dr] & & H_*(\Omega_{2(\delta+\epsilon)}) \\
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□

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This motivates the *homological realization problem*:

Problem

Given a simplicial pair $L \subseteq K$*, find* X *with* $L \subseteq X \subseteq K$ *such that*

$$H_*(X) = \operatorname{im} H_*(L \hookrightarrow K).$$

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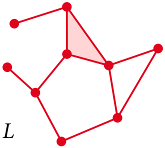

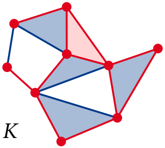

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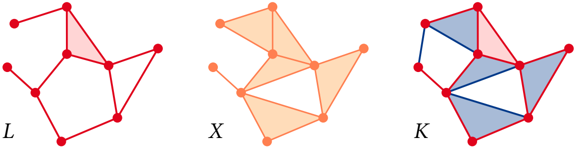

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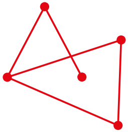

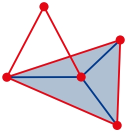

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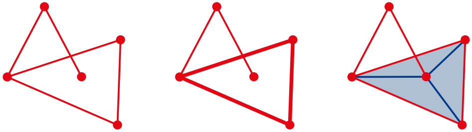

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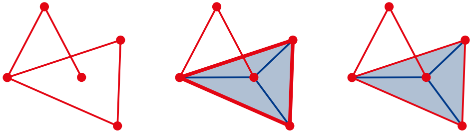

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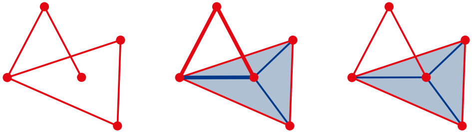

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- Provides homological reconstruction under much weaker assumptions
- Even though the pair $P_\delta \subseteq P_{2\delta}$ has the reconstruction Ω_δ, the pair $\mathrm{Del}_\delta(P) \subseteq \mathrm{Del}_{2\delta}(P)$ might not have a reconstruction

Computation

Persistent homology of sublevel sets

$$\begin{tikzcd}
\text{Data} \arrow[d] & \text{point cloud} \arrow[d, "\text{distance}"] \\
\text{Geometry} \arrow[d] & \text{function} \arrow[d, "\text{sublevel sets}"] \\
\text{Topology} \arrow[d] & \text{topological spaces} \arrow[d, "\text{homology}"] \\
\text{Algebra} \arrow[d] & \text{vector spaces} \arrow[d, "\text{barcode}"] \\
\text{Combinatorics} & \text{intervals}
\end{tikzcd}$$

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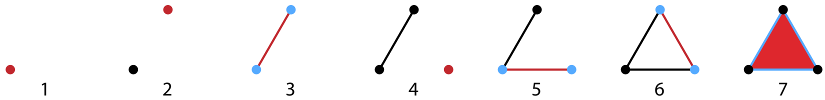
Example: filtration and boundary matrix



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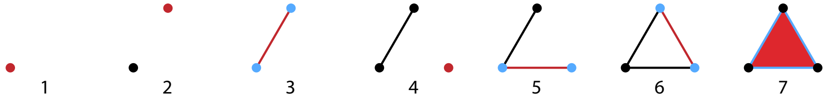
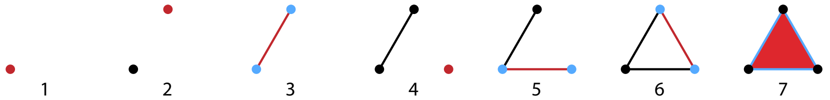


$D =$

	1	2	3	4	5	6	7
1			1		1		
2			1			1	
3							1
4					1	1	
5							1
6							1
7							

Matrix reduction



	1	2	3	4	5	6	7
1			1		1		
2			1			1	
3							1
4					1	1	
5							1
6							1
7							

$= D \cdot$

	1	2	3	4	5	6	7
1	1						
2		1					
3			1				
4				1			
5					1		
6						1	
7							1

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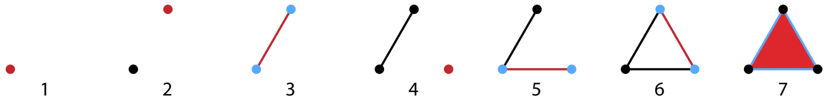

$$
\begin{array}{c|ccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
\hline
1 & & & 1 & & 1 & & \\
2 & & & 1 & & & 1 & \\
3 & & & & & & & 1 \\
4 & & & & & 1 & 1 & \\
5 & & & & & & & 1 \\
6 & & & & & & & 1 \\
7 & & & & & & &
\end{array}
= D \cdot
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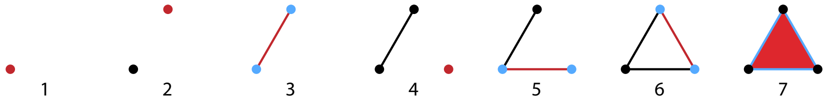
3 & & & 1 & & & & \\
4 & & & & 1 & & & \\
5 & & & & & 1 & & \\
6 & & & & & & 1 & \\
7 & & & & & & & 1
\end{array}
$$

Pivot of column m_j:

- largest index with nonzero entry

Matrix reduction



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2			1			1	
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6							1
7							

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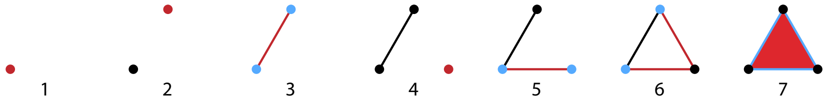
2		1					
3			1				
4				1			
5					1		
6						1	
7							1

Matrix reduction algorithm:

- while there are $i < j$ with $\operatorname{pivot} m_i = \operatorname{pivot} m_j$
  - add m_i to m_j

Matrix reduction



	1	2	3	4	5	6	7
1			1		1	1	
2			1			1	
3							1
4					1	0	
5							1
6							1
7							

$= D \cdot$

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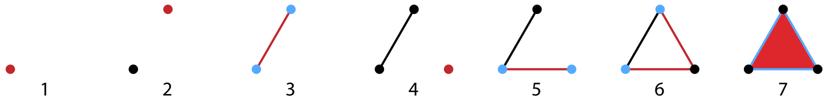

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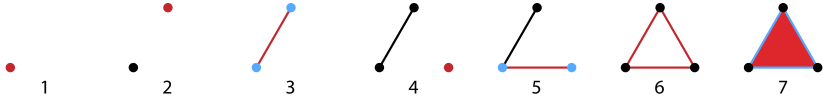
\hline
1 & 1 & & & & & & \\
2 & & 1 & & & & & \\
3 & & & 1 & & & & \\
4 & & & & 1 & & & \\
5 & & & & & 1 & 1 & \\
6 & & & & & & 1 & \\
7 & & & & & & & 1
\end{array}
$$

Matrix reduction algorithm:

- while there are $i < j$ with pivot m_i = pivot m_j
    - add m_i to m_j

Matrix reduction



	1	2	3	4	5	6	7
1			1		1	0	
2			1			0	
3							1
4					1		
5							1
6							1
7							

$= D \cdot$

	1	2	3	4	5	6	7
1	1						
2		1					
3			1			1	
4				1			
5					1	1	
6						1	
7							1

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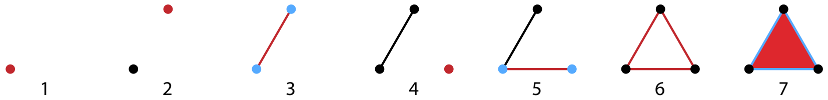
Matrix reduction



	1	2	3	4	5	6	7
1			1		1		
2			1				
3							1
4					1		
5							1
6							1
7							

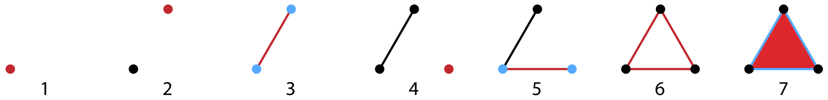
$= D \cdot$

	1	2	3	4	5	6	7
1	1						
2		1					
3			1			1	
4				1			
5					1	1	
6						1	
7							1

Column m_j is *reduced:*

- pivot of col m_j minimal under left-to-right column additions

Matrix reduction

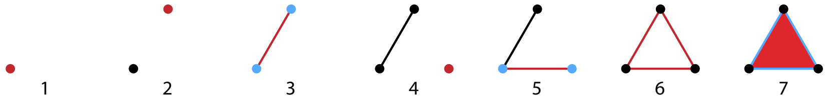


$$
\begin{array}{c|ccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
\hline
1 & & & 1 & & 1 & & \\
2 & & & 1 & & & & \\
3 & & & & & & & 1 \\
4 & & & & & 1 & & \\
5 & & & & & & & 1 \\
6 & & & & & & & 1 \\
7 & & & & & & &
\end{array}
= D \cdot
\begin{array}{c|ccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
\hline
1 & 1 & & & & & & \\
2 & & 1 & & & & & \\
3 & & & 1 & & & 1 & \\
4 & & & & 1 & & & \\
5 & & & & & 1 & 1 & \\
6 & & & & & & 1 & \\
7 & & & & & & & 1
\end{array}
$$

Matrix M is *reduced:*

- all columns are reduced (equivalently: pivots are unique)

Matrix reduction



	1	2	3	4	5	6	7
1			1		1		
2			1				
3							1
4					1		
5							1
6							1
7							

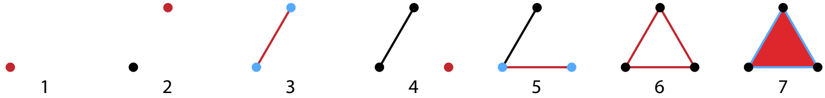
$= D \cdot$

	1	2	3	4	5	6	7
1	1						
2		1					
3			1			1	
4				1			
5					1	1	
6						1	
7							1

Matrix M is *reduced at index* (i, j) :

- submatrix with rows $\geq i$ and cols $\leq j$ (lower left) is reduced

Matrix reduction



	1	2	3	4	5	6	7
1			1		1		
2			1				
3							1
4					1		
5							1
6							1
7							

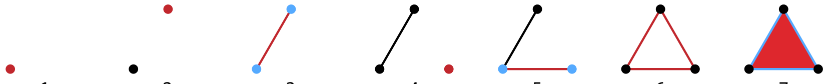
$= D \cdot$

	1	2	3	4	5	6	7
1	1						
2		1					
3			1			1	
4				1			
5					1	1	
6						1	
7							1

i = pivot m_j and M is reduced at index $(i, j) \Rightarrow$

- column m_j is reduced
- (i, j) is a *persistence pair:*
  homology is created at step i and killed at step j

Matrix reduction



	1	2	3	4	5	6	7
1			1		1		
2			1				
3							1
4					1		
5							1
6							1
7							

$= D \cdot$

	1	2	3	4	5	6	7
1	1						
2		1					
3			1			1	
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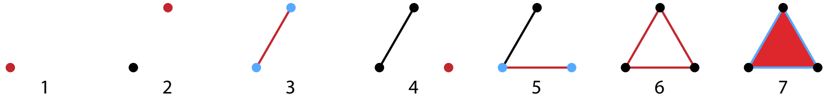

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1			1		1		
2			1				
3							1
4					1		
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1	1						
2		1					
3			1			1	
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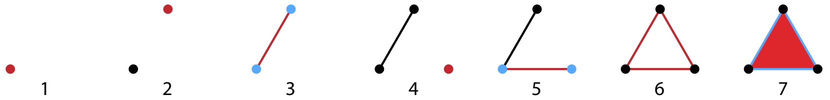

$$
\begin{array}{c|ccccccc}
 & 1 & 2 & \color{red}{3} & 4 & \color{red}{5} & 6 & \color{red}{7} \\
\hline
1 & & & 1 & & 1 & & \\
\color{red}{2} & & & \color{red}{1} & & & & \\
3 & & & & & & & 1 \\
\color{red}{4} & & & & & \color{red}{1} & & \\
5 & & & & & & & 1 \\
\color{red}{6} & & & & & & & \color{red}{1} \\
7 & & & & & & &
\end{array}
= D \cdot
\begin{array}{c|ccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
\hline
1 & 1 & & & & & & \\
2 & & 1 & & & & & \\
3 & & & 1 & & & 1 & \\
4 & & & & 1 & & & \\
5 & & & & & 1 & 1 & \\
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\end{array}
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Matrix reduction

Theorem

Let D be the boundary matrix of a filtered chain complex $C_{n\in\mathbb{N}}$ (with coefficients in a field $\mathbb{K}$, indices in filtration order).

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Then the persistence barcode of $H_*(C_n)$ consists of

$$\{[i,j) : i = \operatorname{pivot} r_j\} \cup \{[i,\infty) : r_i = 0, i \neq \operatorname{pivot} r_j \textit{ for any } j\},$$

where r_j is the jth column of R.

Proof.

Let v_i denote the ith column of V and r_j the jth column of R.

For each k:

- Basis for cycles of C_k: $\quad b_Z = \{v_i : r_i = 0, i \leq k\}$

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- Extend this basis to another basis for cycles:

$$\tilde{b}_Z = \{r_j \neq 0 : \text{pivot}\, r_j \leq k\} \cup \{v_i : r_i = 0, i \leq k, i \neq \text{pivot}\, r_j \text{ for all } j\}$$

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- The additional cycles generate a basis for homology:

$$b_H = \tilde{b}_Z \setminus b_B = \{r_j \neq 0 : i \leq k < j, i = \operatorname{pivot} r_j\} \cup \\ \{v_i : r_i = 0, i \leq k, i \neq \operatorname{pivot} r_j \text{ for all } j\}$$

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$\square$