CGL 3 - Persistent homology

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INRIA Sophia Antipolis-Méditerranée

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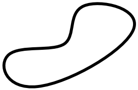
Topological Inference Problem



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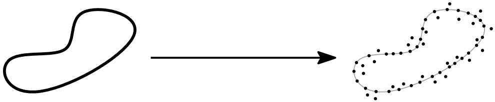

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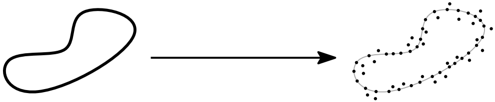

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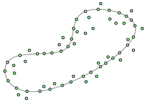

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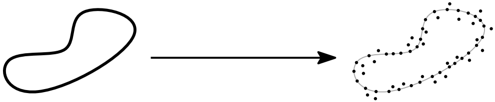

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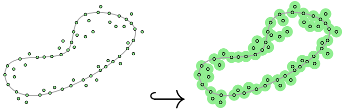

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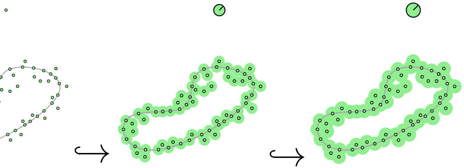

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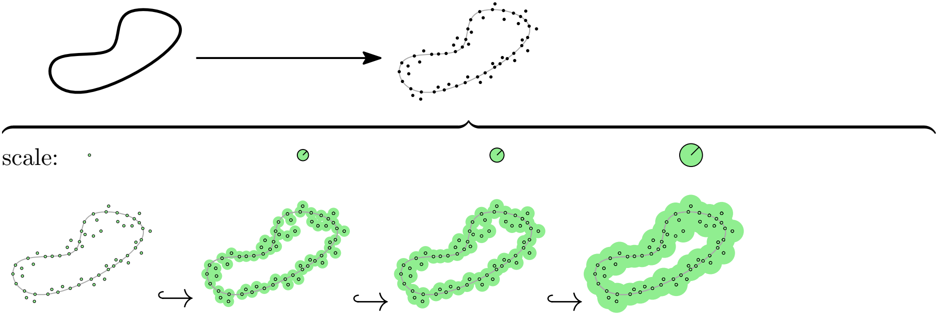

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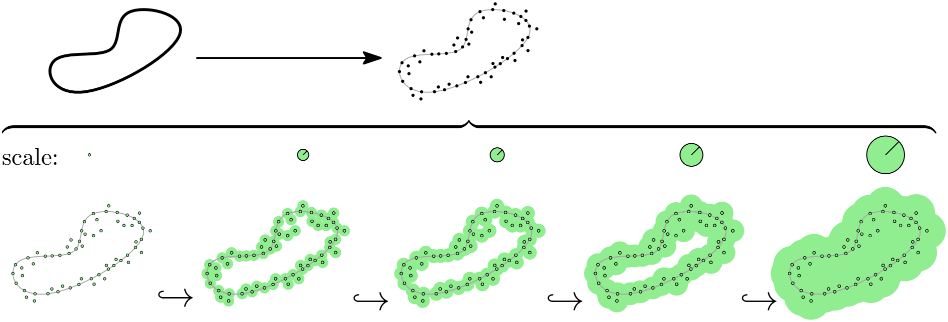

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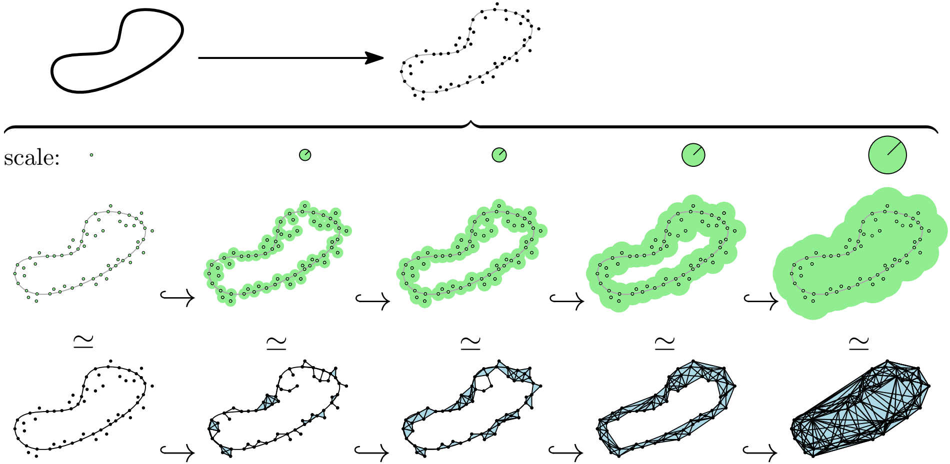

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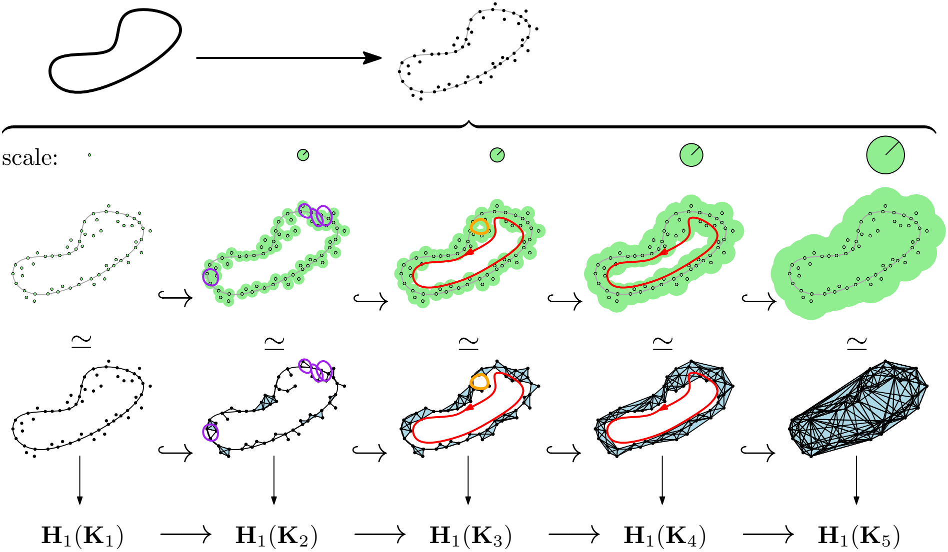

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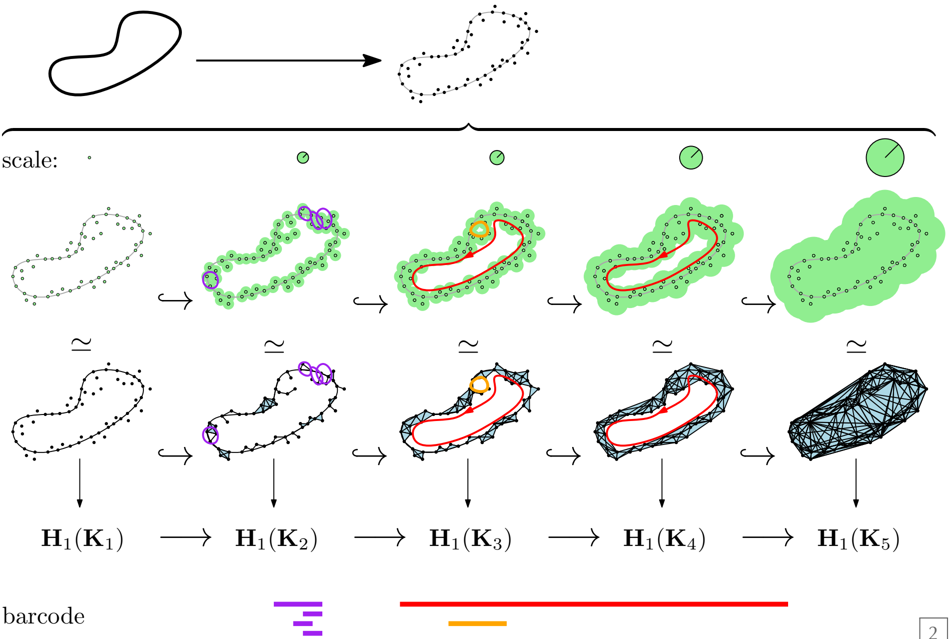
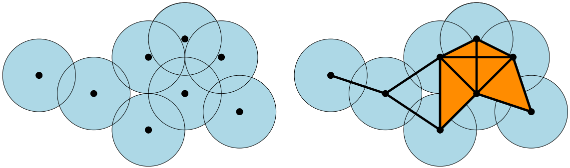


Čech complex and Nerve

Definition (Čech complex)

Let $P = \{p_1, \ldots, p_n\}$ be a set of points in $\mathbb{R}^D$, and denote by $\mathcal{B}_r(p)$ the closed ball of radius r centered at p. The Čech complex of parameter r on P is the simplicial complex $\check{\mathcal{C}}^r(P)$ statisfying:

$$\sigma = \{p_{i_0}, \ldots, p_{i_d}\} \in \check{\mathcal{C}}^r(P) \text{ iff } \bigcap_{j=0\ldots d} \mathcal{B}_r(p_{i_j}) \neq \emptyset$$



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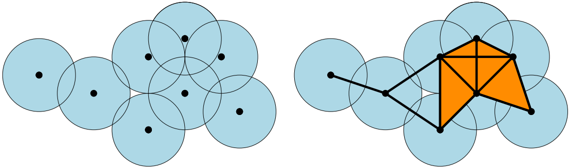


Lemma (Nerve)

The domains $\bigcup_{p_i \in P} \mathcal{B}_r(p_i)$ *and* $|\check{\mathcal{C}}^r(P)|$ *are* homotopy equivalent.

Čech complex and Nerve

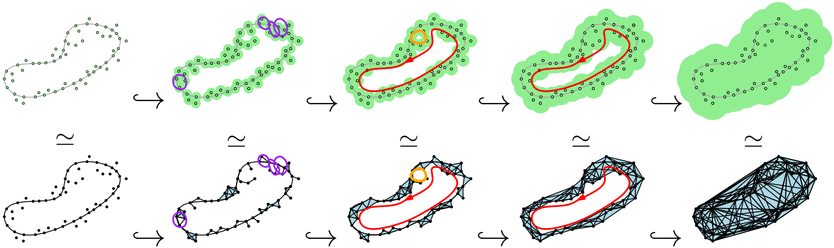
If P finite, $|\check{\mathcal{C}}^r(P)|$, $r \geq 0$, changes homotopy type a finite number of times for $r = r_1, \ldots, r_k$. Consider $\alpha_0, \ldots, \alpha_k$ such that:

$$0 < \alpha_0 < r_1 < \alpha_1 < \ldots < r_k < \alpha_k.$$

We study the sequence:

$$\check{\mathcal{C}}^{\alpha_0}(P) \longrightarrow \check{\mathcal{C}}^{\alpha_1}(P) \longrightarrow \check{\mathcal{C}}^{\alpha_2}(P) \longrightarrow \ldots \longrightarrow \check{\mathcal{C}}^{\alpha_k}(P)$$

$$\mathbf{H}_\bullet(\check{\mathcal{C}}^{\alpha_0}(P)) \longrightarrow \mathbf{H}_\bullet(\check{\mathcal{C}}^{\alpha_1}(P)) \longrightarrow \mathbf{H}_\bullet(\check{\mathcal{C}}^{\alpha_2}(P)) \longrightarrow \ldots \longrightarrow \mathbf{H}_\bullet(\check{\mathcal{C}}^{\alpha_k}(P))$$



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For a fixed set of indices $\{1, \ldots, n\}$ (or real numbers $\alpha_1 < \ldots < \alpha_n$), a persistence module, denote by $\mathbb{V}$, is a collection $\{V_1, \ldots, V_n\}$ of finite dimensional $\mathbb{F}$-vector spaces, and linear maps $f_i \colon V_i \to V_{i+1}$, $1 \leq i < n$:

$$\mathbb{V} = \qquad V_1 \xrightarrow{f_1} V_2 \xrightarrow{f_2} V_3 \xrightarrow{f_3} \ldots \xrightarrow{f_{n-1}} V_n$$

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Definition (Morphism of persistence modules)

Let $\mathbb{V} = (V_i, f_i)$, $\mathbb{W} = (W_i, g_i)$, $i = 1 \ldots n$ be two persistence modules. A morphism of persistence modules $\varphi \colon \mathbb{V} \to \mathbb{W}$ is a collection of linear maps $\{\varphi_i \colon V_i \to W_i\}_{i=1\ldots n}$ such that each square:

$$\begin{array}{ccc} V_i & \xrightarrow{f_i} & V_{i+1} \\ \varphi_i \downarrow & \circlearrowleft & \downarrow \varphi_{i+1} \\ W_i & \xrightarrow[g_i]{} & W_{i+1} \end{array}$$

commutes for $i = 1 \ldots n-1$.

φ is an isomorphism of persistence modules if each φ_i is an isomorphism of vector spaces. We then denote $\mathbb{V} \cong \mathbb{W}$.

Decomposition of persistence modules

Definition (Direct sum of persistence modules)

A direct sum of two persistence modules $\mathbb{V} = (V_i, f_i)$ and $\mathbb{W} = (W_i, g_i)$, $i = 1 \ldots n$, is the persistence module $\mathbb{V} \oplus \mathbb{W} := (V_i \oplus W_i, f_i \oplus g_i)_{i=1,\ldots,n}$:

$$V_1 \oplus W_1 \xrightarrow{f_1 \oplus g_1} V_2 \oplus W_2 \xrightarrow{f_2 \oplus g_2} V_3 \oplus W_3 \xrightarrow{f_3 \oplus g_3} \ldots \xrightarrow{f_{n-1} \oplus g_{n-1}} V_n \oplus W_n$$

A persistence module $\mathbb{V}$ is indecomposable iff

$$\mathbb{V} \cong \mathbb{V}_1 \oplus \mathbb{V}_2 \implies \mathbb{V}_1 = 0 \text{ or } \mathbb{V}_2 = 0.$$

Decomposition

Theorem (Decomposition)

Every persistence module $\mathbb{V}$ *over the indices* $\{1, \ldots, n\}$ *admits a unique decomposition in indecomposable persistence modules*

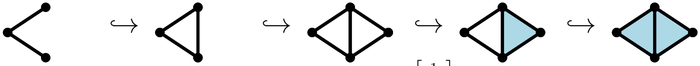
$$\mathbb{V} \cong \bigoplus_i \mathbb{I}[b_i; d_i], \qquad 1 \leq b_i \leq d_i \leq n,$$

called interval modules, such that $\quad \mathbb{I}[b; d] :=$

$$\underbrace{0 \xrightarrow{0} \cdots \xrightarrow{0} 0}_{\textit{indices: } [1;b-1]} \xrightarrow{0} \underbrace{\mathbb{F} \xrightarrow{\text{id}} \cdots \xrightarrow{\text{id}} \mathbb{F}}_{[b;d]} \xrightarrow{0} \underbrace{0 \xrightarrow{0} \cdots \xrightarrow{0} 0}_{[d+1;n]}$$

Representation of interval decompositions

Indices: 1 2 3 4 5



$$\mathbf{H}_1 : \quad 0 \xrightarrow{0} \mathbb{F} \xrightarrow{[1 \ \ 0]} \mathbb{F} \oplus \mathbb{F} \xrightarrow{\begin{bmatrix} 1 \\ 0 \end{bmatrix}} \mathbb{F} \xrightarrow{0} 0$$

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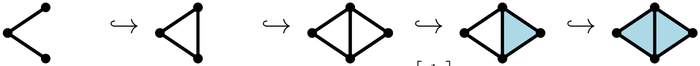

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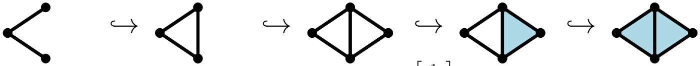

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Let $\mathbb{V} \cong \bigoplus_{i \in I} \mathbb{I}[b_i; d_i]$. The persistence barecode of $\mathbb{V}$ is the drawing of the collection of horizontal intervals $[b_i; d_i]$.

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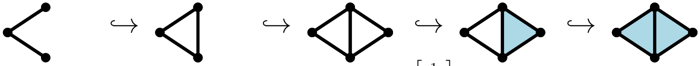

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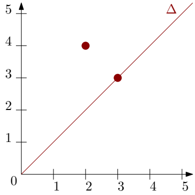

Algorithm for persistent homology

Definition (Filtration)

A filtration of a simplicial complex $\mathbf{K}$ is an ordering $(\sigma_1, \ldots, \sigma_n)$ of its simplices such that $\mathbf{K}_i := \{\sigma_1, \ldots, \sigma_i\}$ is a simplicial complex for all $i = 1, \ldots, n$. We represent it by the sequence of elementary inclusions:

$$\emptyset := \mathbf{K}_0 \xrightarrow{\sigma_1} \mathbf{K}_1 \xrightarrow{\sigma_2} \mathbf{K}_2 \xrightarrow{\sigma_3} \ldots \xrightarrow{\sigma_n} \mathbf{K}_n = \mathbf{K}$$

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Example: Filtration induced by scale in the Čech complex, where each inclusion is *decomposed* further into inclusions of one simplex at a time:

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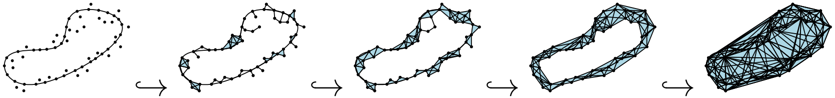

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Lemma (Elementary inclusion)

Let $\mathbf{K} \to \mathbf{K} \cup \{\sigma\}$ *be an elementary inclusion, with* $\dim \sigma = d$. *Then:*

- *either* $\dim \mathbf{H}_{d-1}(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{H}_{d-1}(\mathbf{K}) - 1$,
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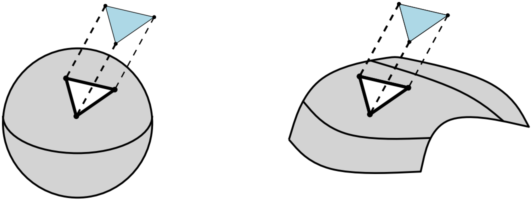

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Finally, we have:

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$$\dim \mathbf{C}_d(\mathbf{K} \cup \{\sigma\}) = \overbrace{\dim \mathbf{Z}_d(\mathbf{K} \cup \{\sigma\})}^{\dim \ker \partial_d} + \overbrace{\dim \mathbf{B}_{d-1}(\mathbf{K} \cup \{\sigma\})}^{\dim \operatorname{im} \partial_d},$$ so:

- either $\dim \mathbf{B}_{d-1}(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{B}_{d-1}(\mathbf{K}) + 1$,
- or $\quad \dim \mathbf{Z}_{d}(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{Z}_{d}(\mathbf{K}) + 1$.

Algorithm for persistent homology

Lemma (Elementary inclusion)

Let $\mathbf{K} \to \mathbf{K} \cup \{\sigma\}$ *be an elementary inclusion, with* $\dim \sigma = d$*. Then:*

- *either* $\dim \mathbf{H}_{d-1}(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{H}_{d-1}(\mathbf{K}) - 1$,
- *or* $\dim \mathbf{H}_d(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{H}_d(\mathbf{K}) + 1$

First, note that for all dimensions d we have:

- $\mathbf{Z}_d(\mathbf{K}) \subset \mathbf{Z}_d(\mathbf{K} \cup \{\sigma\}) \Rightarrow \dim \mathbf{Z}_d(\mathbf{K}) \leq \dim \mathbf{Z}_d(\mathbf{K} \cup \{\sigma\})$,
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We conclude with $\dim \mathbf{H}_d = \dim \mathbf{Z}_d - \dim \mathbf{B}_d$.

Algorithm for persistent homology

Lemma

Let $\mathbf{K} \to \mathbf{K} \cup \{\sigma\}$ *and* $\dim \sigma = d$*. We have:*

$$\dim \mathbf{H}_d(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{H}_d(\mathbf{K}) + 1 \quad \textit{iff} \quad [\partial\sigma] = 0 \ \textit{ in } \ \mathbf{H}_d(\mathbf{K}).$$

In which case σ *is a creator. Otherwise, we have:*

$$\dim \mathbf{H}_{d-1}(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{H}_{d-1}(\mathbf{K}) - 1 \ \textit{ and } \ [\partial\sigma] \neq 0 \ \textit{ in } \ \mathbf{H}_d(\mathbf{K}),$$

and σ *is a destructor.*

Note that $\partial\sigma \in \mathbf{C}_{d-1}(\mathbf{K})$ *because all subfaces of* σ *are in* $\mathbf{K}$.

Algorithm for persistent homology

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Algorithm for persistent homology

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NB: c_i is a chain in $\mathbf{K}$. Talking about "c_i in $\mathbf{K}_i$" means the *restriction of c_i in $\mathbf{K}_i$*.

Algorithm for persistent homology

Theorem (Correctness)

Let $\{c_1, \ldots, c_n\}$, $F \sqcup G \sqcup H$ and $G \leftrightarrow H$ be a compatible basis for $\mathbf{K}$. Denote by $\mathbb{H}(\mathbf{K})$ the persistence module induced by the filtration of $\mathbf{K}$:

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Theorem (Correctness)

Let $\{c_1, \ldots, c_n\}$, $F \sqcup G \sqcup H$ and $G \leftrightarrow H$ be a compatible basis for $\mathbf{K}$. Denote by $\mathbb{H}(\mathbf{K})$ the persistence module induced by the filtration of $\mathbf{K}$:

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$\Rightarrow \sigma_{i+1}$ *creates* a new homology class $[\sigma_{i+1} - \sum \varepsilon_g c_h] \neq 0$:

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- set $c_{i+1} = \sigma_{i+1} - \sum \varepsilon_g c_h$, and $F \leftarrow F \cup \{i+1\}$.

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This is a compatible basis for $\mathbf{K}_0 \longrightarrow \ldots \longrightarrow \mathbf{K}_{i+1}$, satisfying (i),(ii),(iii). **exercise**

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$\Rightarrow$ σ_{i+1} *destroys* the non-trivial homology class $\sum_{f\in F} \varepsilon_f [c_f]$.

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$\Rightarrow \sigma_{i+1}$ *destroys* the non-trivial homology class $\sum_{f \in F} \varepsilon_f [c_f]$.

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Algebraic algorithm for persistent homology

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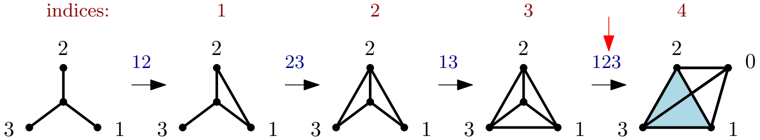
Note that (i) is maintained by the choice of f_0 as max. **exercise**

Algorithm for persistent homology

Example:



$$c_1 = 01 + 02 + 12$$
$$c_2 = 02 + 03 + 23$$
$$c_3 = 01 + 03 + 13$$
$$\left. \right\} \in F$$

Algorithm for persistent homology

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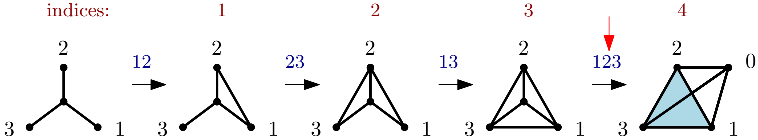

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$$\partial(123) = 12 + 23 + 13 = c_1 + c_2 + c_3$$

Algorithm for persistent homology

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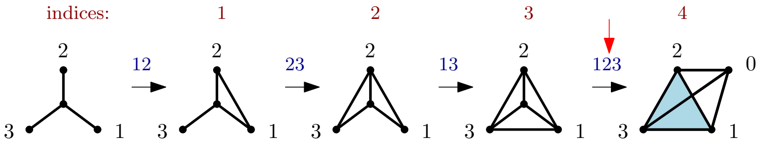

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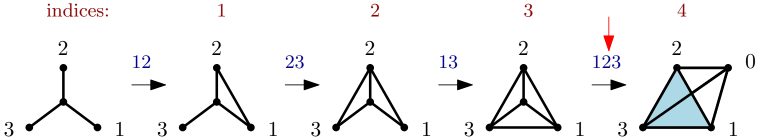

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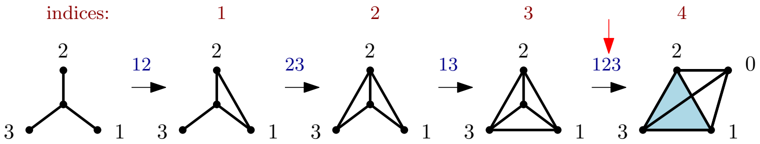

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$\quad = 12 + 23 + 13$

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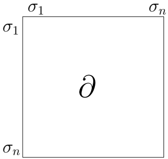
Matrix implementation

define low_i = index of lowest 1 in *i*-th column.
Undefined if column = 0.



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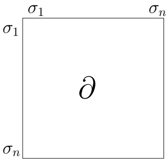

- **For** $i = 1 \ldots n$,
  - **While** $\exists j < i$ s.t. $\mathrm{low}_j = \mathrm{low}_i$,
    - $\mathrm{col}_i \leftarrow col_j + \mathrm{col}_i$ (in $\mathbb{Z}/2\mathbb{Z}$)
  - **if** $\mathrm{col}_i \neq 0$ add $[\mathrm{low}_i; i-1]$ to the barecode
- add all $[i; n]$ to barecode s.t. $\mathrm{col}_i = 0$ and no column j satisfies $\mathrm{low}_j = i$.

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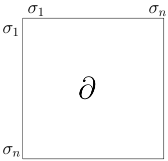

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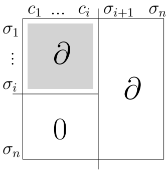

Invariant: at the end of step i, we have:

- if $\text{low}_h = g$, $g < h \leq i$ then $g \leftrightarrow h$ in partition.
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i.e., there is a compatible basis $c_1, \dots c_i$ for $\mathbf{K}_i$ such that $\text{col}_k = \partial c_k, 1 \leq k \leq i$.

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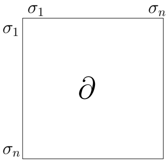

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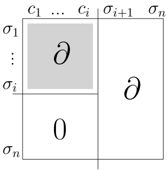

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$O(n^3)$

Comparing geometric diagrams

If P finite, $|\check{\mathcal{C}}^r(P)|$, $r \geq 0$, changes homotopy type a finite number of times for $r = r_1, \ldots, r_k$. Consider $\alpha_0, \ldots, \alpha_k$ such that:

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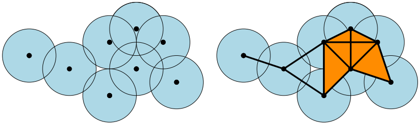
$$\check{\mathcal{C}}^{\alpha_0}(P) \longrightarrow \check{\mathcal{C}}^{\alpha_1}(P) \longrightarrow \check{\mathcal{C}}^{\alpha_2}(P) \longrightarrow \ldots \longrightarrow \check{\mathcal{C}}^{\alpha_k}(P)$$



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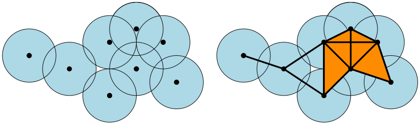

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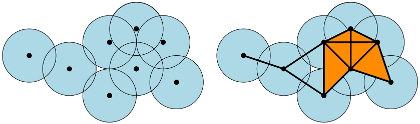

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$\longrightarrow$ use points (α_b, α_d) instead of (b, d) to get the geometric persistence diagram.

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Let $D = \{(b_i, d_i)\}_{i \in I} \cup \{x = y\}$ and $D' = \{(b'_j, d'_j)\}_{j \in J} \cup \{x = y\}$ be two persistence diagrams, $b, d \in \mathbb{R}$.

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The bottleneck distance $\mathrm{d}_B(\mathrm{D}, \mathrm{D}')$ between D and D′ is:

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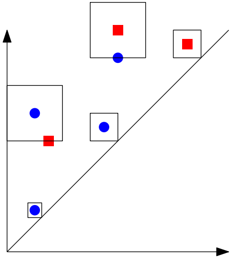

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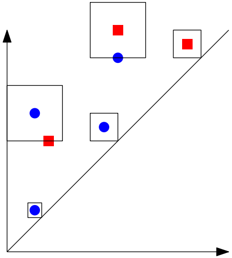

Defined even when $|I| \neq |J|$ by sending points to the diagonal.

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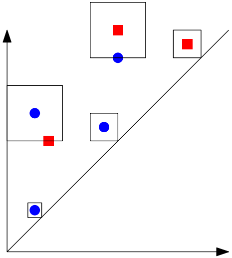

Theorem (Stability on a simplicial complex)

Let $f, g \colon \mathbf{K} \to \mathbb{R}$ be two functions on a same simplicial complex $\mathbf{K}$, inducing filtrations $\mathbf{K}_\alpha = f^{-1}((-\infty; \alpha])$ and $\mathbf{K}'_\gamma = g^{-1}((-\infty; \gamma])$. Then

$$\mathrm{d}_B(\mathrm{D}(f), \mathrm{D}(g)) \leq ||f - g||_\infty.$$

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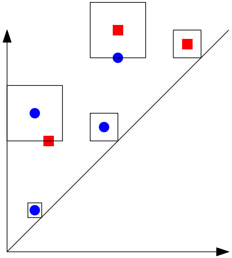

Theorem (Stability on general space)

Let $f, g\colon M \to \mathbb{R}$ be two functions on a same metric space M, satisfying some "tameness" conditions. If $\exists \varepsilon \geq 0$ s.t. $\forall r \in \mathbb{R}$ $f^{-1}(-\infty; r] \subseteq g^{-1}(-\infty; r+\varepsilon]$ and $g^{-1}(-\infty; r] \subseteq f^{-1}(-\infty; r+\varepsilon]$,

then $\mathrm{d}_B(\mathrm{D}(f), \mathrm{D}(g)) \leq \varepsilon$.