3 - Persistent homology

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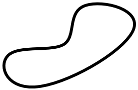
Topological Inference Problem



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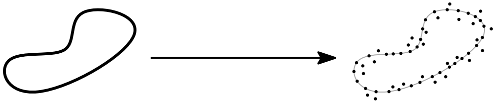

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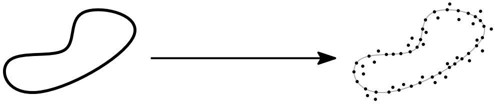

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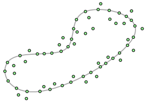

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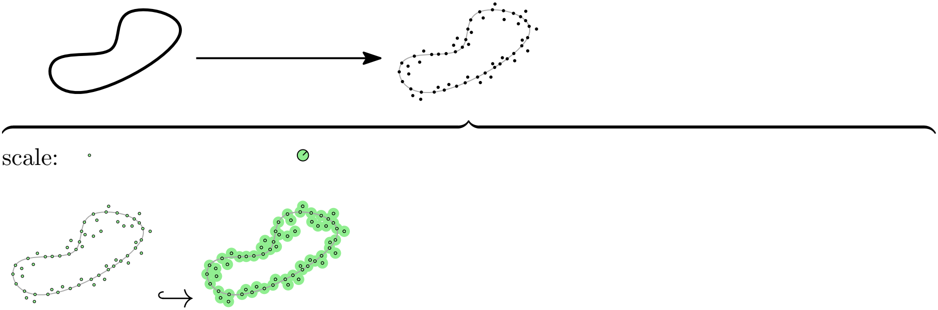

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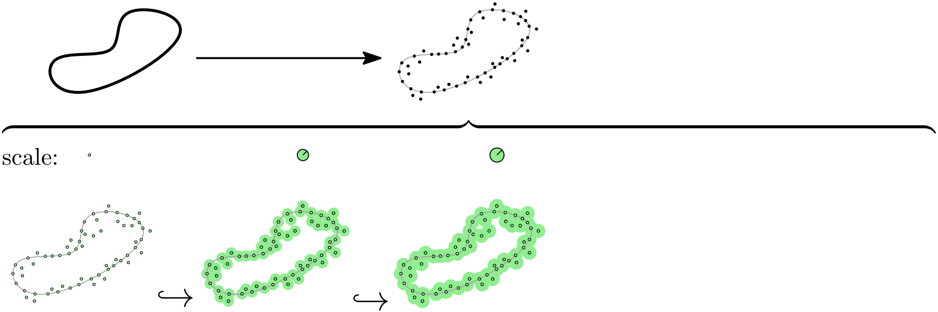

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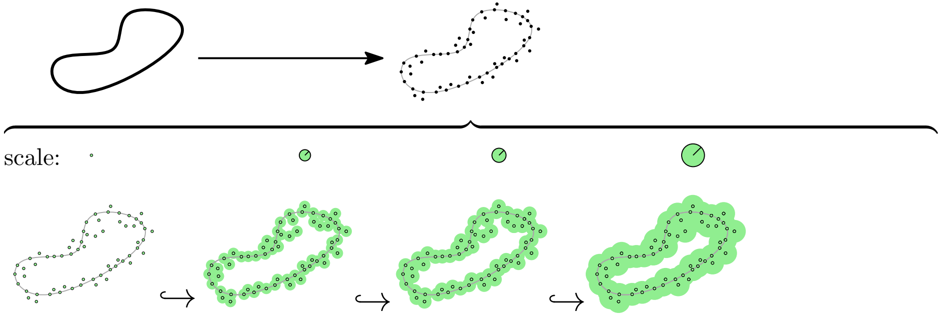

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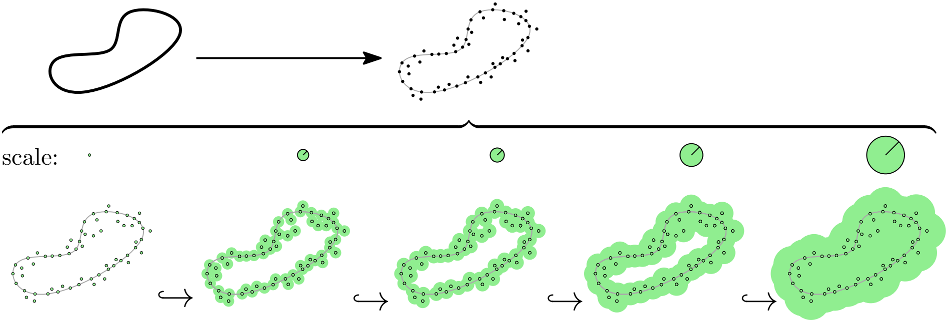

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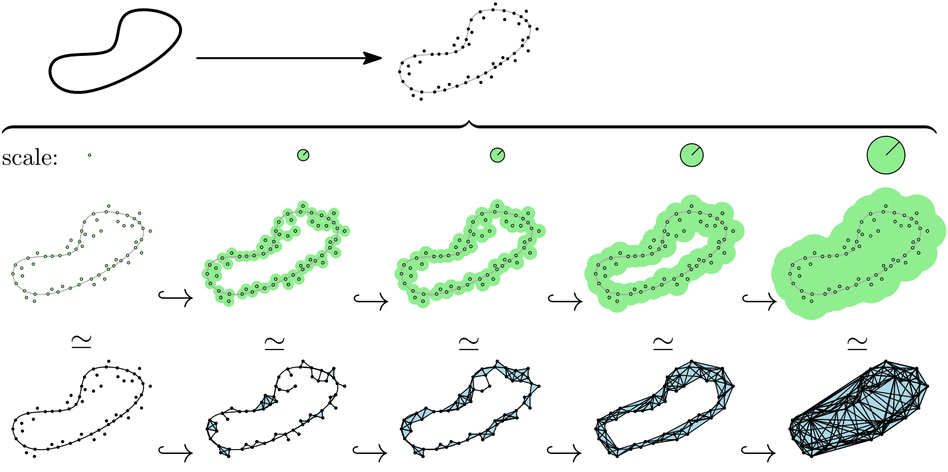

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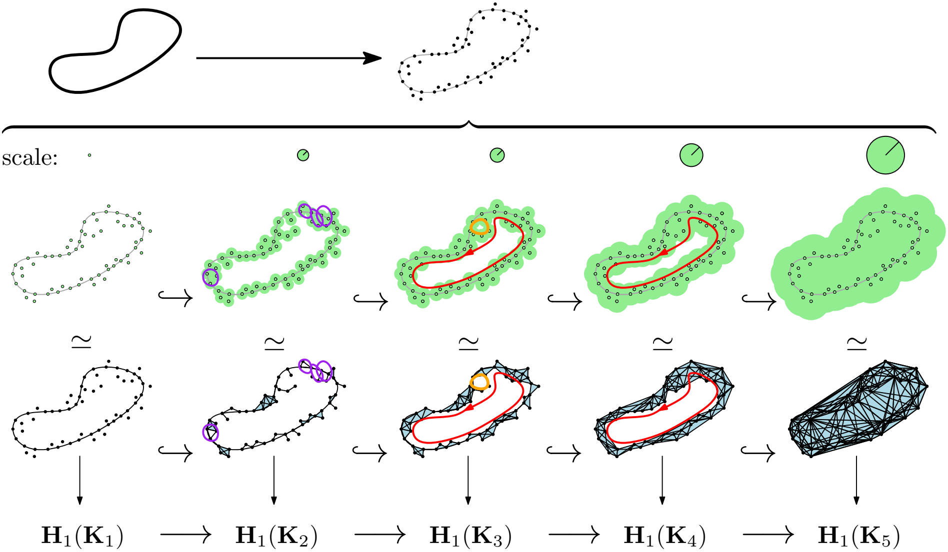

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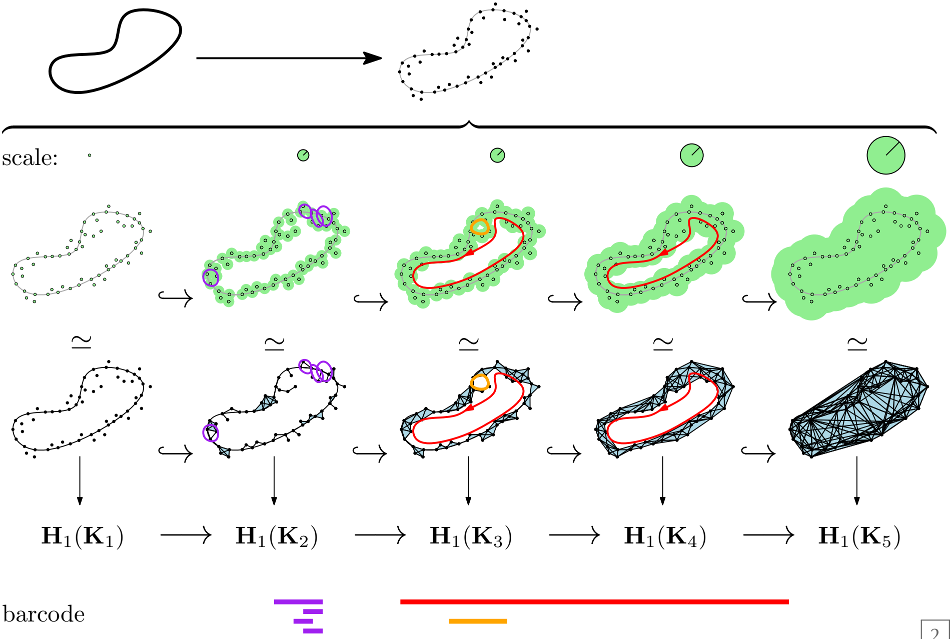
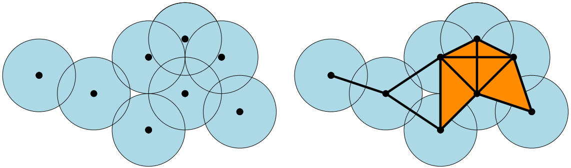


Čech complex and Nerve

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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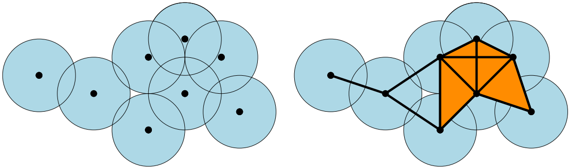

Lemma (Nerve)

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:

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

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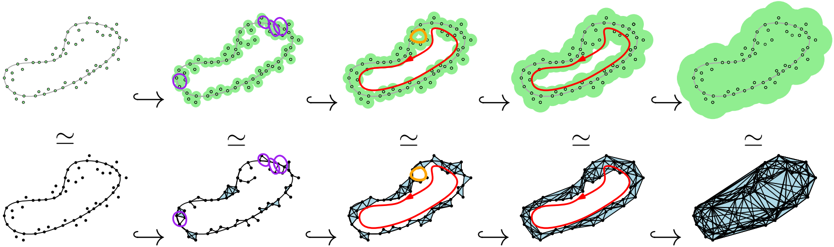

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For a fixed set of indices $\{1, \ldots, n\}$ (or real numbers $\alpha_1 < \ldots < \alpha_n$), a persistence module, denote by $\mathbb{V}$, is a collection $\{V_1, \ldots, V_n\}$ of finite dimensional $\mathbb{F}$-vector spaces, and linear maps $f_i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

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

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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 $\mathbb{W} = (W_i, g_i)$, $i = 1 \dots n$, is the persistence module:
$\mathbb{V} \oplus \mathbb{W} := (V_i \oplus W_i, f_i \oplus g_i)_{i=1,\dots,n}$, i.e.,:

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

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 into indecomposable persistence modules of the form:

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

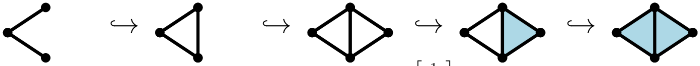
called interval modules, such that

$\mathbb{I}[b; d] :=$

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

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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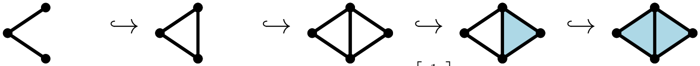

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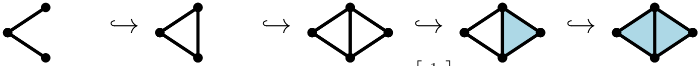

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barecode:

$\mathbb{I}[2;4] \oplus \mathbb{I}[3;3]$

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

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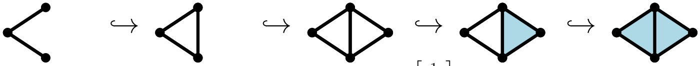

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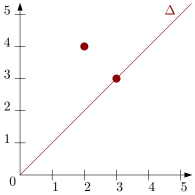

Algorithm for persistent homology

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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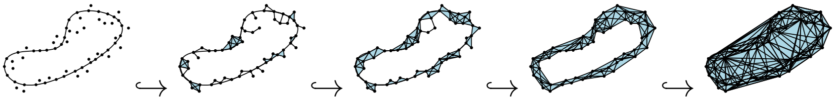

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Lemma (Elementary inclusion)

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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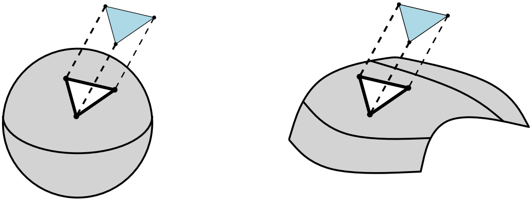

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Finally, we have:

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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:

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

Additionally,
$\mathbf{C}_d(\mathbf{K} \cup \{\sigma\}) = \mathbf{C}_d(\mathbf{K}) \oplus \langle \sigma \rangle \Rightarrow \dim \mathbf{C}_d(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{C}_d(\mathbf{K}) + 1$.

Finally, we have:

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

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

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:*

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

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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(i) σ creator. If $[\partial\sigma] = 0$ in $\mathbf{H}_{d-1}(\mathbf{K})$ then $\partial\sigma \in \mathbf{B}_{d-1}(\mathbf{K})$ and there exists a chain $a \in \mathbf{C}_d(\mathbf{K})$ such that $\partial\sigma = \partial a$.

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Hence $\dim \mathbf{Z}_d(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{Z}_d(\mathbf{K}) + 1$.

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Hence $\dim \mathbf{B}_{d-1}(\mathbf{K} \cup \{\sigma\}) = \dim \mathbf{B}_{d-1}(\mathbf{K}) + 1$.

Algorithm for persistent homology

Denote by $\mathbf{C}(\mathbf{K}) := \bigoplus_{d \geq 0} \mathbf{C}_d(\mathbf{K})$ and $\partial := \bigoplus_{d \geq 0} \partial_d \colon \mathbf{C}(\mathbf{K}) \to \mathbf{C}(\mathbf{K})$.

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We call this data a compatible basis for the filtration of $\mathbf{K}$.

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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* $\mathbf{K}$*:*

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

$$\mathbb{H}(\mathbf{K}) := 0 \longrightarrow \mathbf{H}(\mathbf{K}_1) \longrightarrow \mathbf{H}(\mathbf{K}_2) \longrightarrow \ldots \longrightarrow \mathbf{H}(\mathbf{K}_n)$$

then,

$$\mathbb{H}(\mathbf{K}) \cong \bigoplus_{g \leftrightarrow h} \mathbb{I}[g; h-1] \bigoplus_{f \in F} \mathbb{I}[f; n].$$

Claims (algorithmic proof):

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(a) A compatible basis exists, and $\{c_1, \dots, c_i\}$ basis for $\mathbf{C}(\mathbf{K}_i)$,

(b) $\{c_f \ : \ f \in F, \ f \leq i\} \cup \{c_g : g \in G, g \leq i\}$ basis for $\mathbf{Z}(\mathbf{K}_i)$,

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Claims (algorithmic proof):

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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 $\mathbf{K}$:

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

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Suppose we have a compatible basis for $\mathbf{K}_i$, claims (a), (b), (c) are satisfied for the filtration $\mathbf{K}_0 \longrightarrow \ldots \longrightarrow \mathbf{K}_i$. Next: $\mathbf{K}_i \xrightarrow{\sigma_{i+1}} \mathbf{K}_{i+1}$

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

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

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- Set $c_{f_0} \hookleftarrow \sum_{f \in F} \varepsilon_f c_f$, and $G \hookleftarrow G \cup \{f_0\}$, $F \hookleftarrow F - \{f_0\}$,

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$$\partial\sigma_{i+1} = \underbrace{\sum_{f\in F} \varepsilon_f c_f}_{\neq 0} + \underbrace{\sum_{g\in G} \varepsilon_g c_g}_{=\sum_{h\in H, g\leftrightarrow h} \varepsilon_g \partial c_h}$$

Let $f_0 = \max\{f \in F : \varepsilon_f \neq 0\}$. We have

$$\partial(\sigma_{i+1} - \sum_{h\in H, g\leftrightarrow h} \varepsilon_g c_h) = \sum_{f\in F} \varepsilon_f c_f.$$

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

- Set $c_{f_0} \hookleftarrow \sum_{f\in F} \varepsilon_f c_f$, and $G \hookleftarrow G \cup \{f_0\}$, $F \hookleftarrow F - \{f_0\}$,
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Algebraic algorithm for persistent homology

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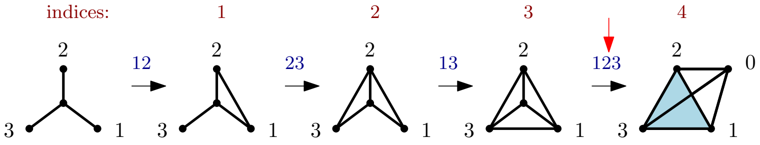
Note that (a) is maintained by the choice of f_0 as max. **exercise**

Algorithm for persistent homology

Example:



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

Algorithm for persistent homology

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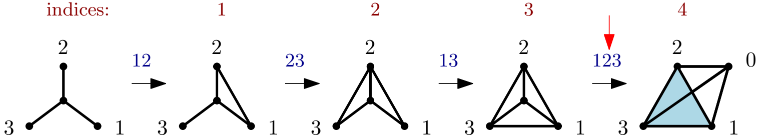

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$\partial(123) = 12 + 23 + 13 = c_1 + c_2 + c_3$

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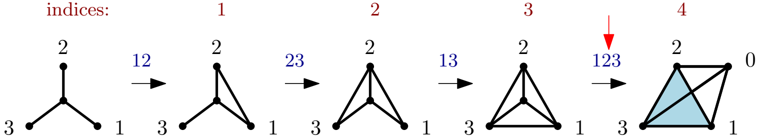

$$c_1 = 01 + 02 + 12$$
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Algorithm for persistent homology

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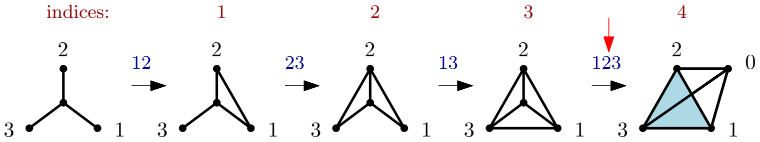

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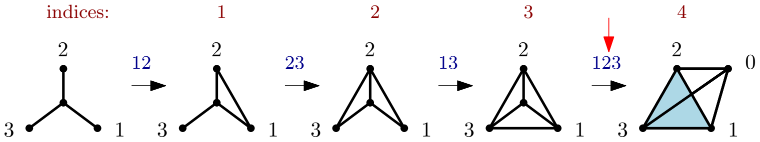

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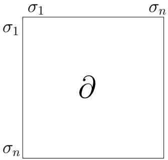
Matrix implementation

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



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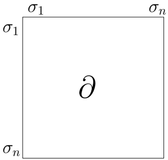

define low_i = index of lowest 1 in i-th column. Undefined if column = 0.

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

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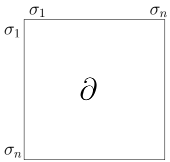

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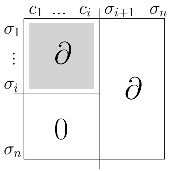

Invariant: at the end of step i, we have:

- 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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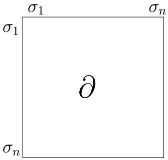

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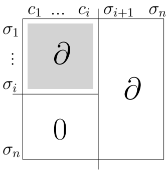

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$O(n^3)$

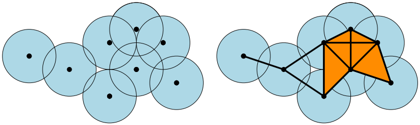
Comparing geometric diagrams

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:

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

Geometric filtration:

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



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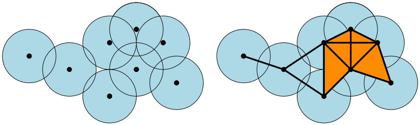

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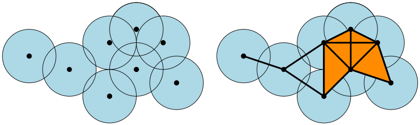

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$\longrightarrow$ use points (α_b, α_d) instead of (b, d) to get the geometric persistence diagram.

Comparing persistence diagrams

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

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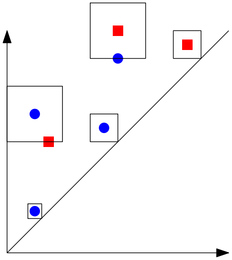
The bottleneck distance $\mathrm{d}_B(\mathrm{D}, \mathrm{D}')$ between D and D′ is:

$$\mathrm{d}_B(\mathrm{D}, \mathrm{D}') := \inf_{\substack{\Phi:\mathrm{D}\to\mathrm{D}' \\ \text{bijection}}} \sup_{p\in\mathrm{D}} ||p - \Phi(p)||_\infty$$



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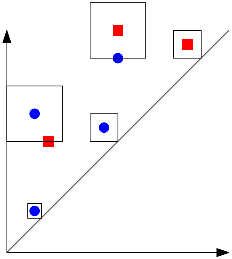
Defined even when $|I| \neq |J|$ by sending points to the diagonal.



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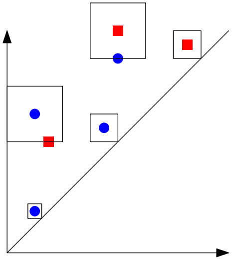

Theorem (Stability on a simplicial complex)

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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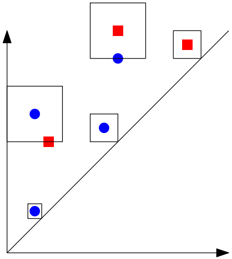

Theorem (Stability on general space)

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