Algorithmic Aspects of Topological Data Analysis

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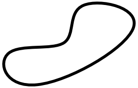
Collège de France
Geometry Understanding in Higher Dimensions



Topological Data Analysis

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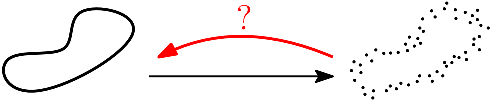

[Persistent homology '00]

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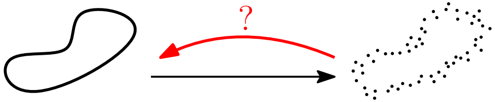

[Persistent homology ’00]

1. Geometry

- Cech/Vietoris-Rips complexes,
- sparsification,
- zigzag persistence.

2. Combinatorics

- discrete Morse theory,
- simplicial complex DS.

3. Algebra

- matrix optimisation,
- algebraic dualisation.

Focus on the topology inference problem.
$\longrightarrow$ using *persistent homology*.

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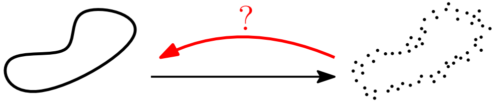

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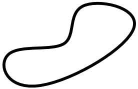
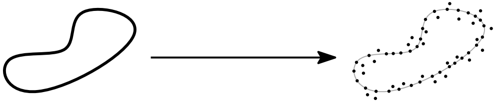
Focus on the topology inference problem.
$\longrightarrow$ using *persistent homology*.

Three (essentially) geometric constructions for persistent homology, with strong algorithmic consequences.

I/. Standard Persistent Homology



Persistent Homology and Topological Data Analysis



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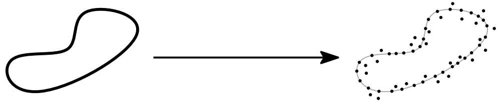
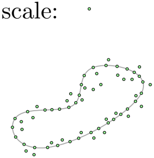


scale:



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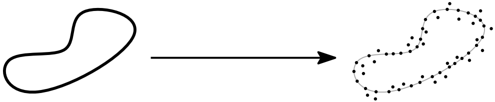

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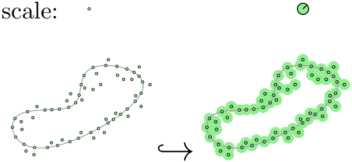

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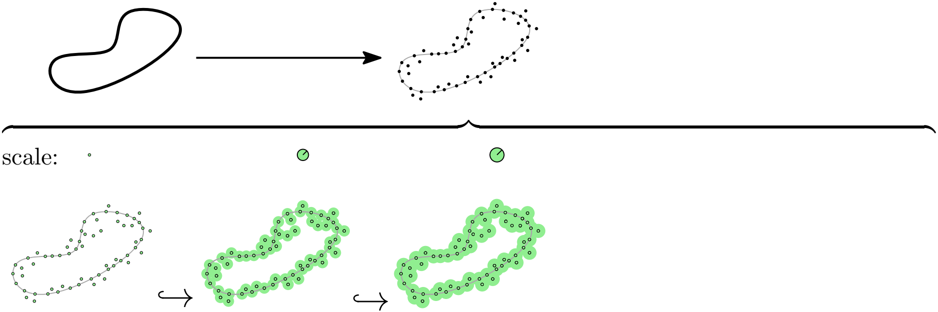

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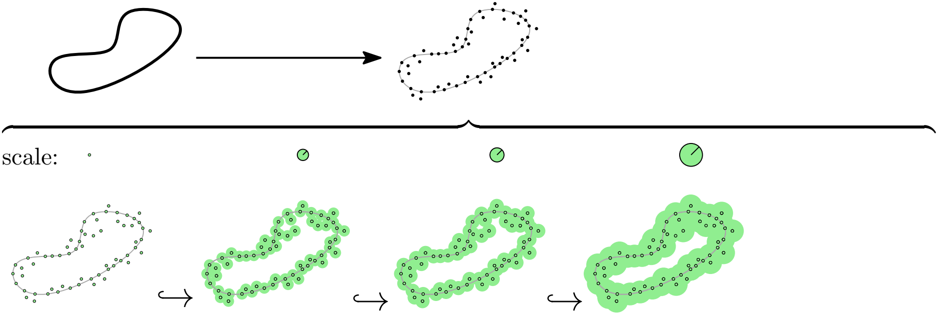

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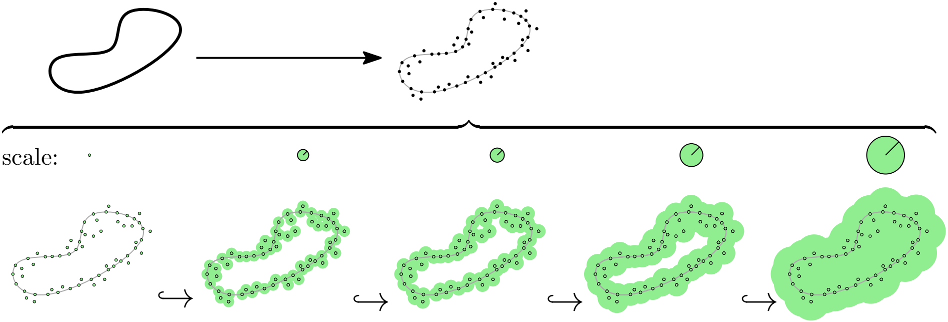

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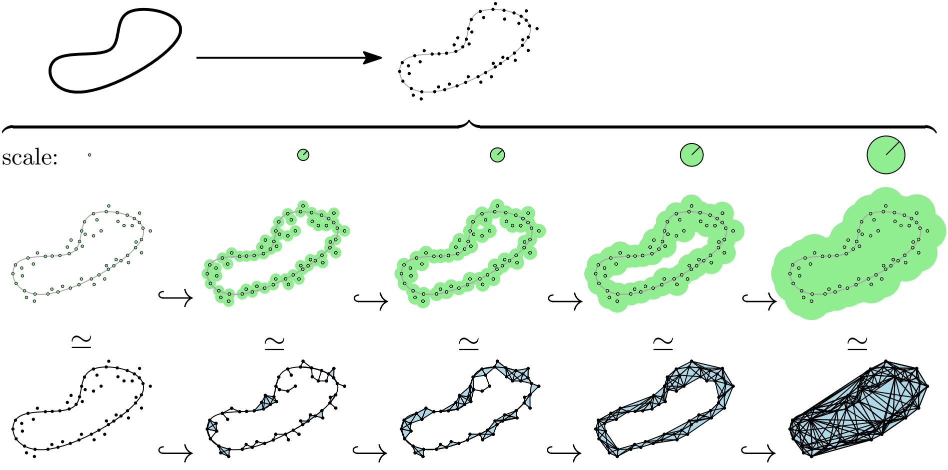

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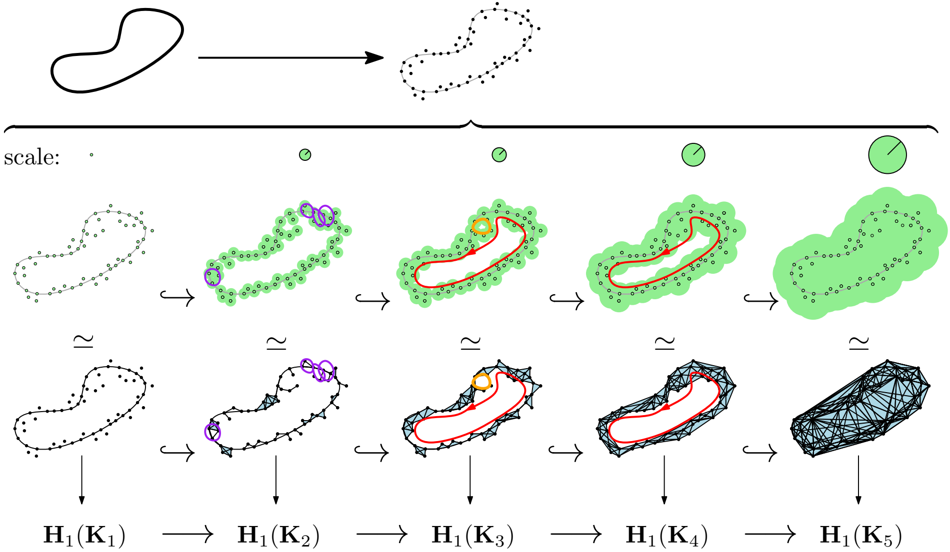

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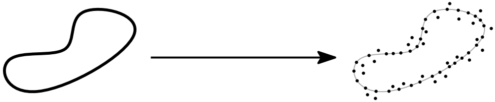

[Edelsbrunner, Letscher, Zomorodian '00]
[Carlsson, Zomorodian '04]
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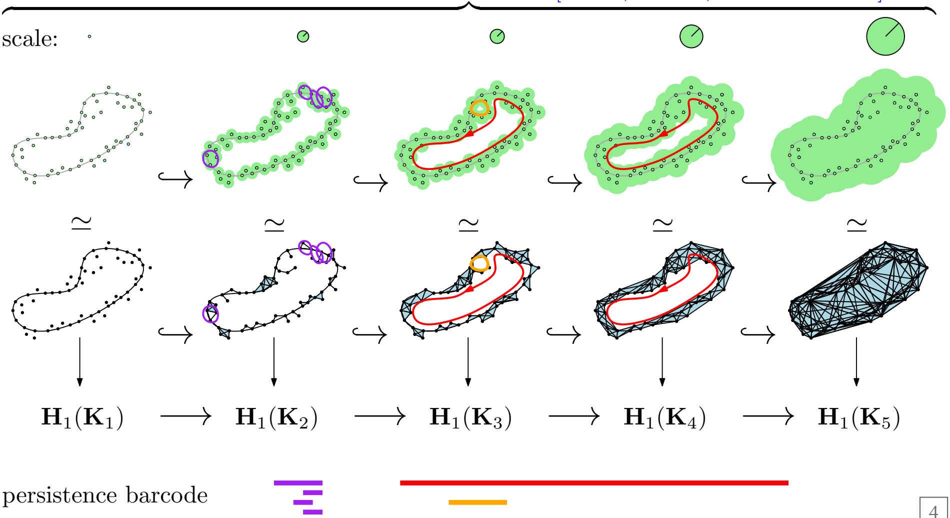
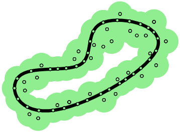


Topology Inference with Persistence



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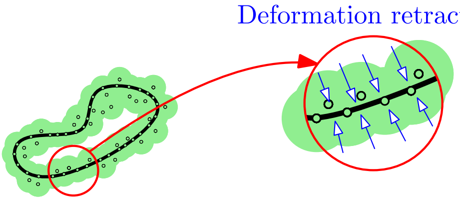

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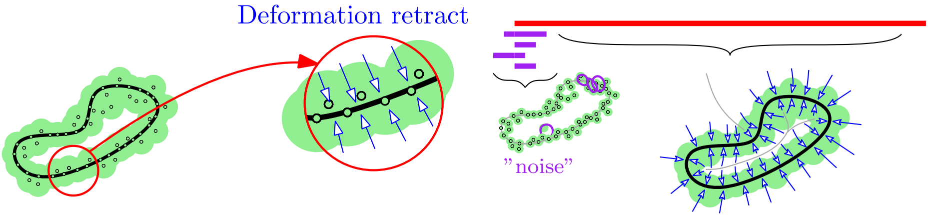

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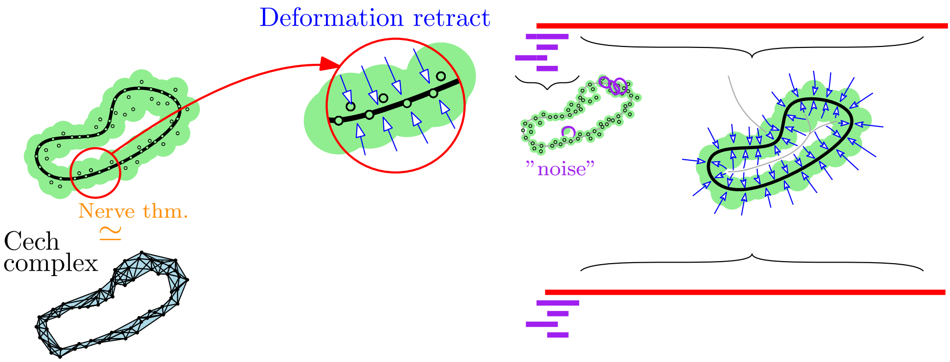

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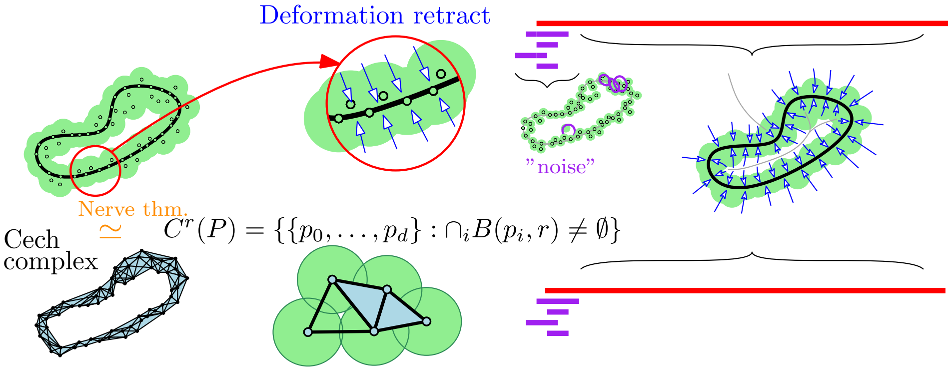
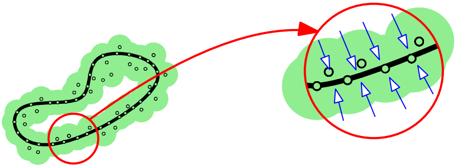
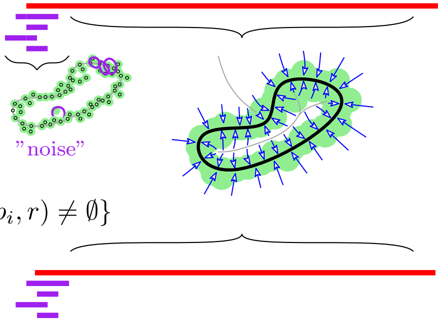


$$C^r(P) = \{\{p_0, \ldots, p_d\} : \cap_i B(p_i, r) \neq \emptyset\}$$

Topology Inference with Persistence

Deformation retract





Nerve thm.

$\simeq$

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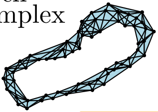
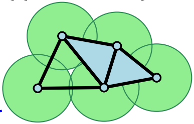
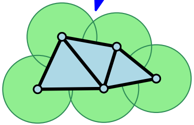
Cech complex





Relaxation

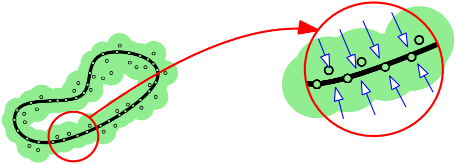
Rips complex

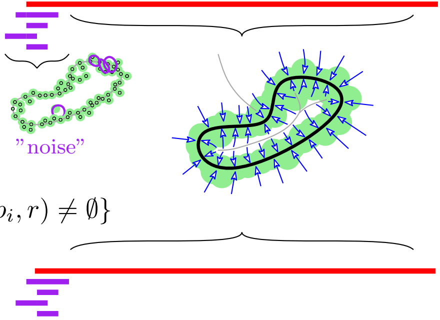


Only distance computations.

Topology Inference with Persistence

Deformation retract





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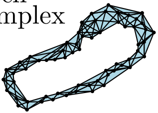

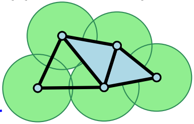

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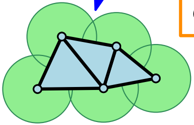
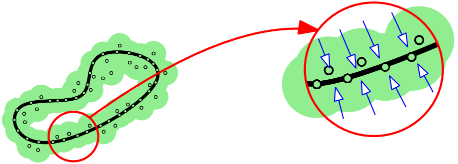


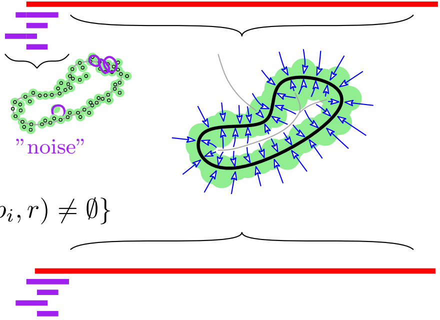
$C^r(P) \subseteq R^r(P)$

Only distance computations.

Topology Inference with Persistence

Deformation retract





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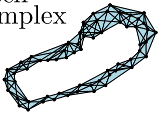

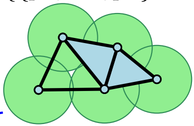

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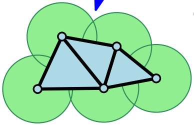
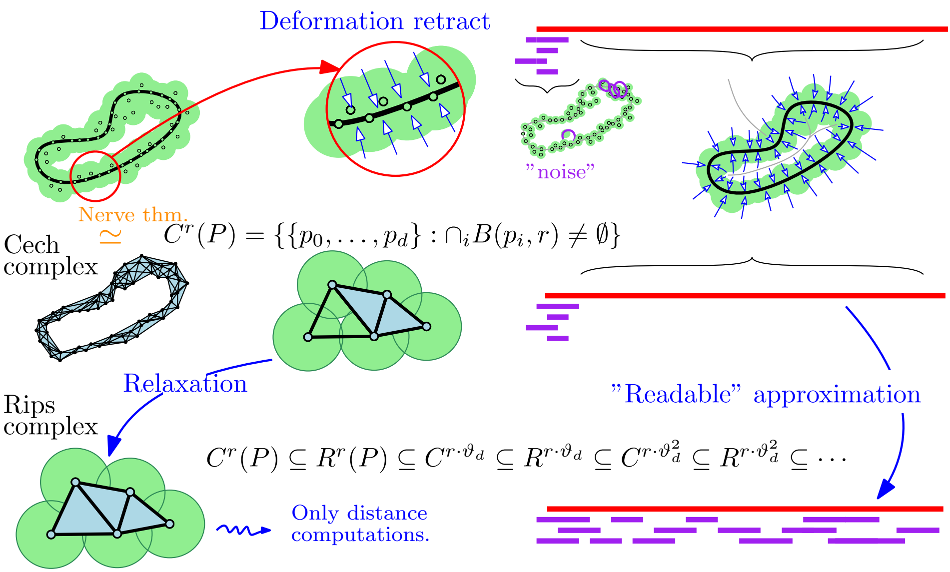


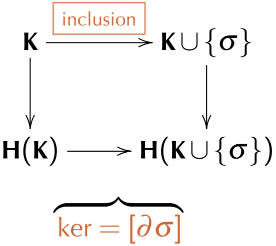
$$C^r(P) \subseteq R^r(P) \subseteq C^{r\cdot\vartheta_d} \subseteq R^{r\cdot\vartheta_d} \subseteq C^{r\cdot\vartheta_d^2} \subseteq R^{r\cdot\vartheta_d^2} \subseteq \cdots$$

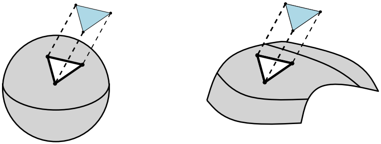
Only distance computations.

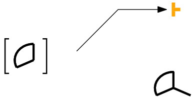
Topology Inference with Persistence



Algorithm for Persistent Homology via Inclusions







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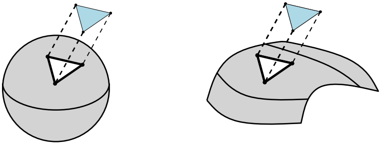
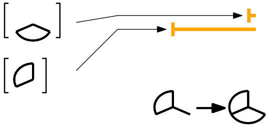
$$\begin{array}{ccc} \mathbf{K} & \xrightarrow{\text{inclusion}} & \mathbf{K} \cup \{\sigma\} \\ \downarrow & & \downarrow \\ \mathbf{H}(\mathbf{K}) & \longrightarrow & \mathbf{H}(\mathbf{K} \cup \{\sigma\}) \end{array}$$

$$\underbrace{\qquad\qquad\qquad}_{\ker = [\partial\sigma]}$$





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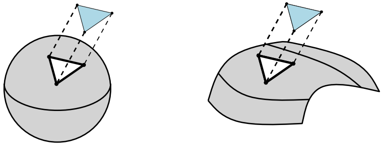

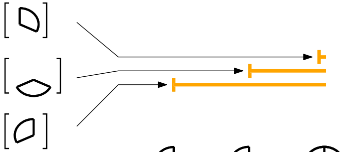

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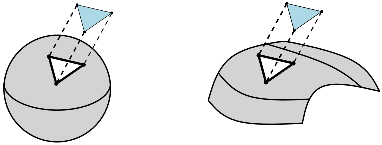

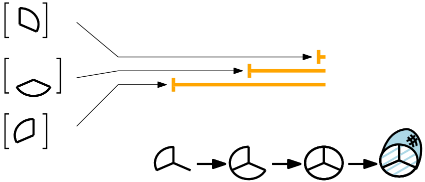

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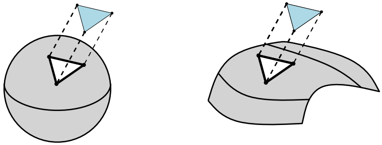

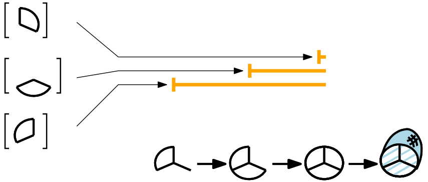

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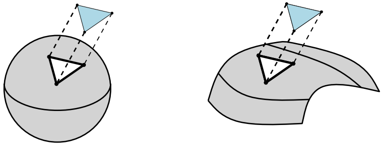

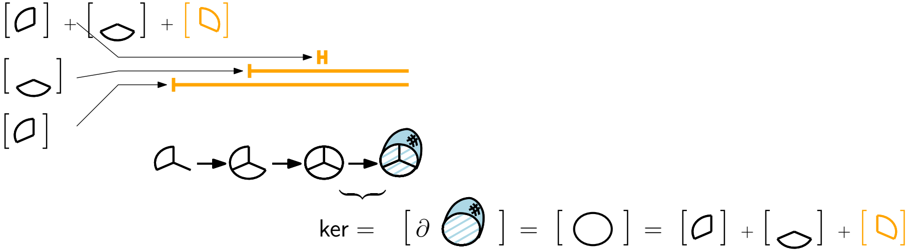

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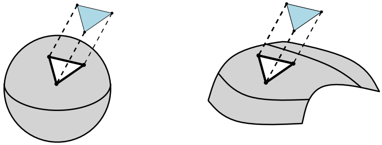
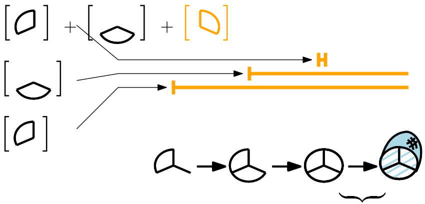
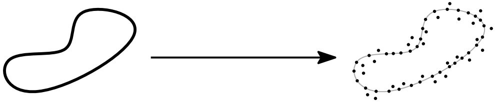


Only one bar modified per inclusion.



Persistent Homology and Topological Data Analysis



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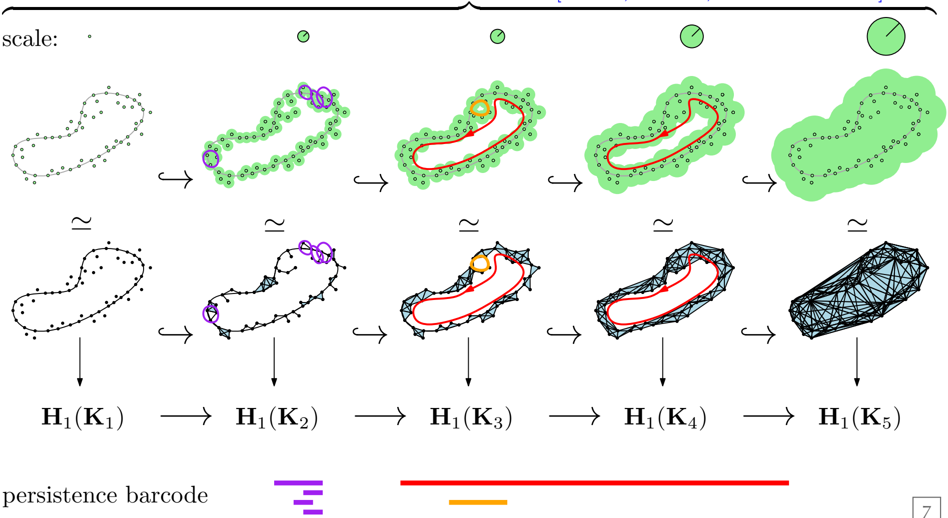
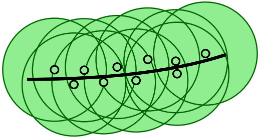


II/. Sparsification in Persistence

Sparsification

[Sheehy '12]



Sparsification

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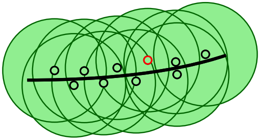

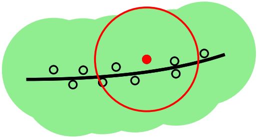

Sparsification

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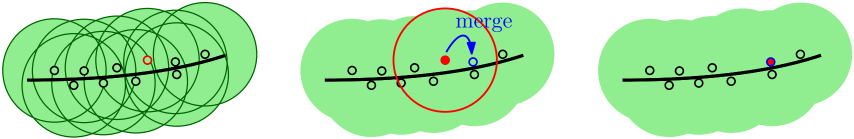

Sparsification

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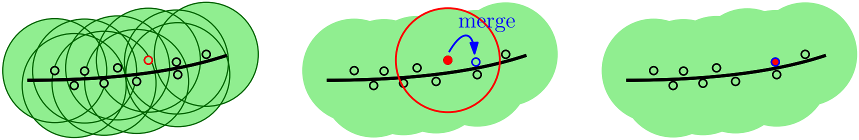
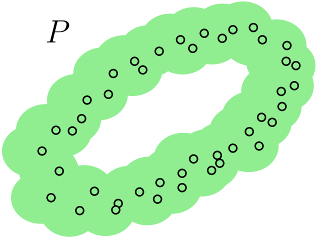
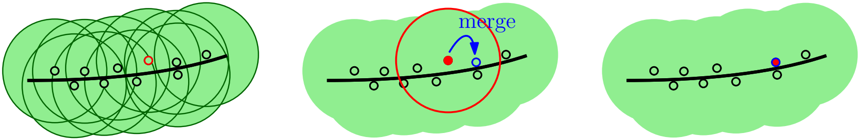
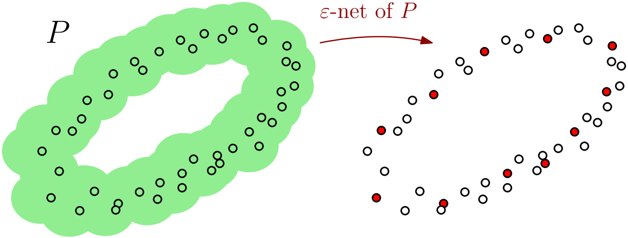




Sparsification

[Sheehy '12]

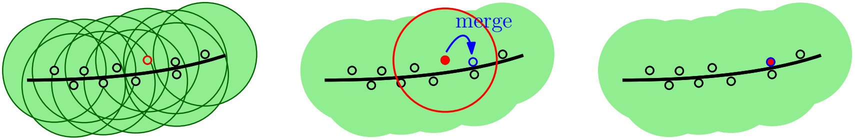


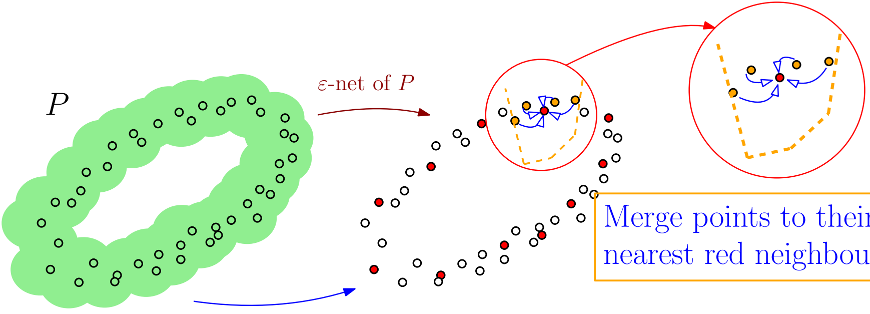


Select an ε-net of P

Sparsification

[Sheehy '12]



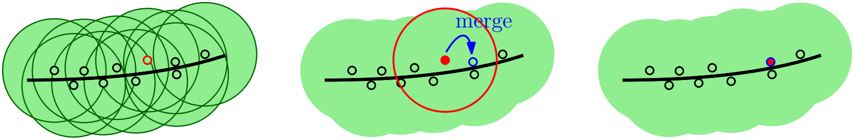


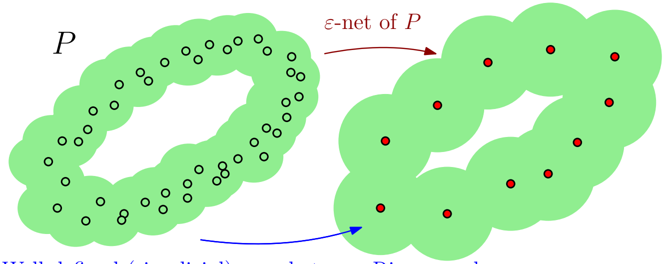
Merge points to their nearest red neighbour

Well-defined (simplicial) map between Rips complexes

Sparsification

[Sheehy '12]



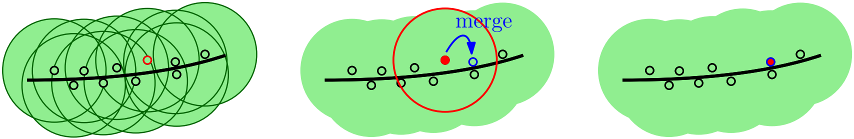


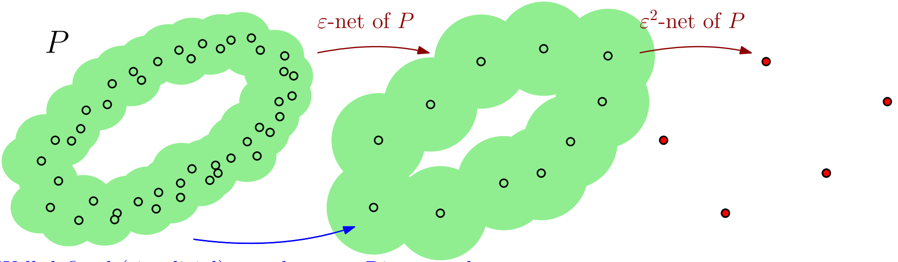
Increase scale

Well-defined (simplicial) map between Rips complexes

Sparsification

[Sheehy '12]



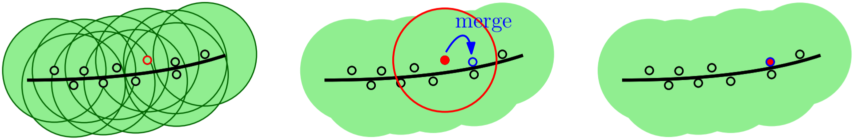


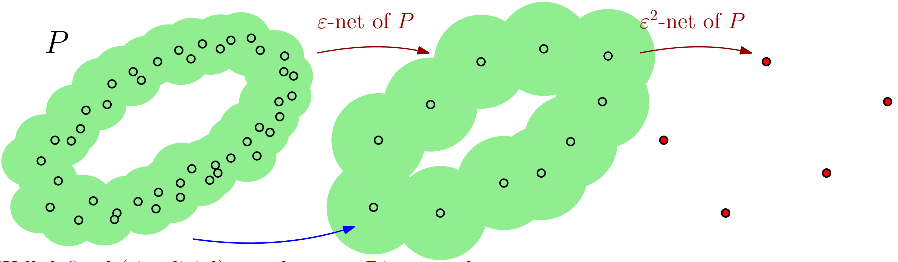
Well-defined (simplicial) map between Rips complexes

[Dey, Fan, Wang '14]

Sparsification

[Sheehy '12]





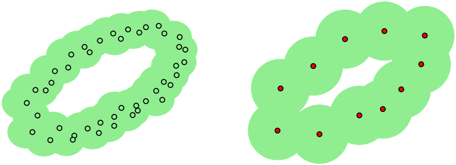
Well-defined (simplicial) map between Rips complexes

[Dey, Fan, Wang '14]

[Kerber, Sharathkumar '13] [Botnan, Spreeman '14] [Dey, Shi, Wang '16]

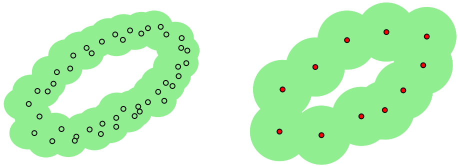
[Aruni, Kerber, Raghvendra '16] ...

Algorithm for Persistent Homology via Contractions



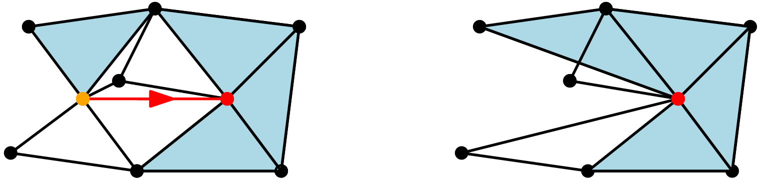
Increase scale $\longrightarrow$ inclusions $\mathbf{K} \xrightarrow{\text{inclusion}} \mathbf{K} \cup \{\sigma\}$

Algorithm for Persistent Homology via Contractions

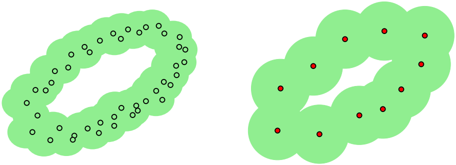


Increase scale $\longrightarrow$ inclusions $\mathbf{K} \xrightarrow{\text{inclusion}} \mathbf{K} \cup \{\sigma\}$

Merge points $\longrightarrow$ edge contraction:



Algorithm for Persistent Homology via Contractions



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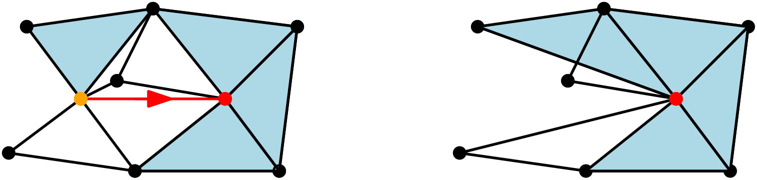
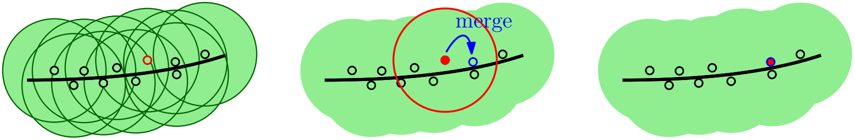


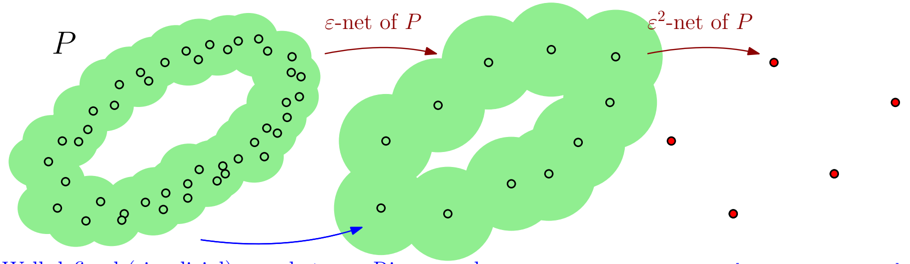
Several bars get 'destroyed' in the persistence barcode.

$\longrightarrow$ directed by the combinatorics/geometry.

Sparsification

[Sheehy '12]





Well-defined (simplicial) map between Rips complexes

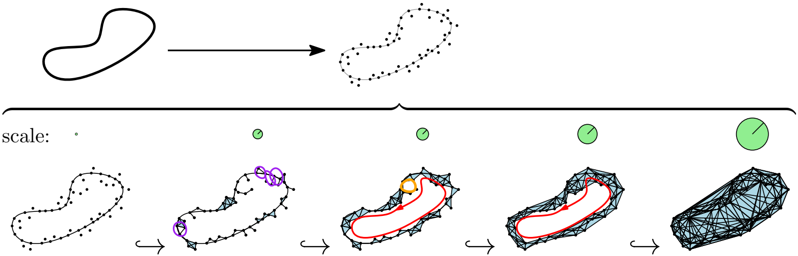
[Dey, Fan, Wang '14]

[Kerber, Sharathkumar '13] [Botnan, Spreeman '14] [Dey, Shi, Wang '16]

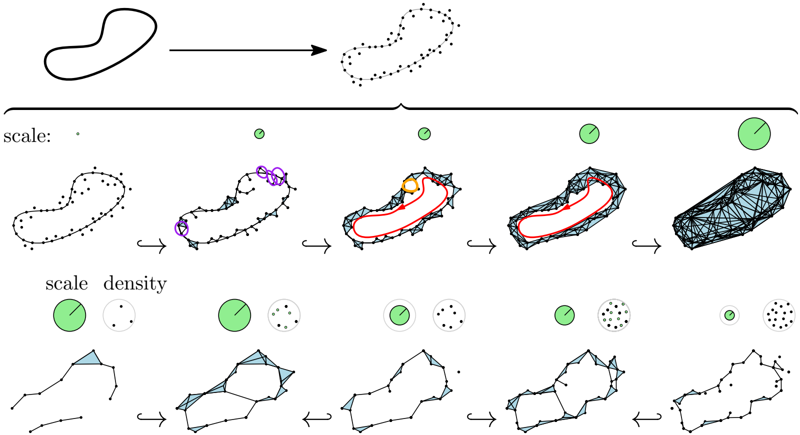
[Aruni, Kerber, Raghvendra '16] ...

III/. Zigzag Persistent Homology

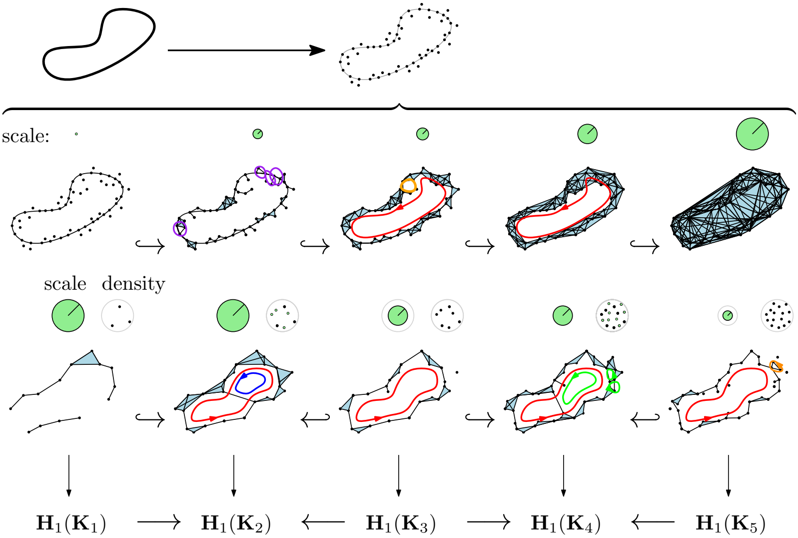
Zigzag Persistence for Topological Data Analysis



Zigzag Persistence for Topological Data Analysis

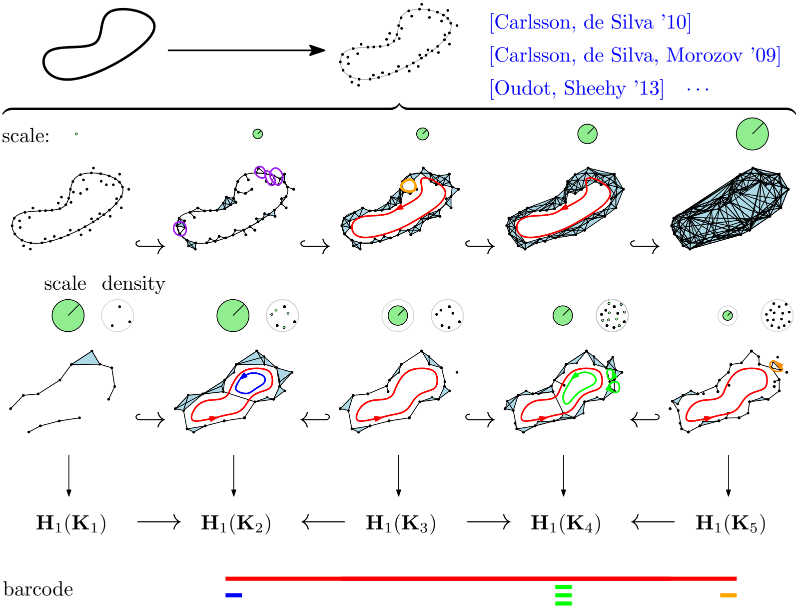


Zigzag Persistence for Topological Data Analysis



Zigzag Persistence for Topological Data Analysis

[Carlsson, de Silva '10]
[Carlsson, de Silva, Morozov '09]
[Oudot, Sheehy '13] ...



Zigzag Persistence Algorithm

We compute the persistent homology of:

$$\mathbf{K}_1 \longleftrightarrow \mathbf{K}_2 \longleftrightarrow \cdots \longleftrightarrow \mathbf{K}_i \overset{\sigma}{\longleftrightarrow} \mathbf{K}_{i+1} \longleftrightarrow \cdots \longleftrightarrow \mathbf{K}_{n-1} \longleftrightarrow \mathbf{K}_n$$

Zigzag Persistence Algorithm

We compute the persistent homology of:

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by maintaining a compatible homology basis for [M., Oudot '15 '16]

$$\underbrace{\mathbf{K}_1 \longleftrightarrow \cdots \longleftrightarrow \mathbf{K}_i = \mathbf{K}'_m}_{\mathbb{K}[1;i]} \xleftarrow{\tau_m} \mathbf{K}'_{m-1} \xleftarrow{\tau_{m-1}} \mathbf{K}'_{m-2} \xleftarrow{\tau_{m-2}} \cdots \xleftarrow{\tau_1} \emptyset$$

Zigzag Persistence Algorithm

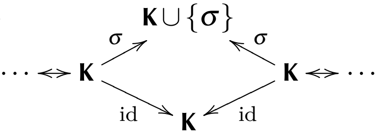
We compute the persistent homology of:

$$\mathbf{K}_1 \longleftrightarrow \mathbf{K}_2 \longleftrightarrow \cdots \longleftrightarrow \mathbf{K}_i \overset{\sigma}{\longleftrightarrow} \mathbf{K}_{i+1} \longleftrightarrow \cdots \longleftrightarrow \mathbf{K}_{n-1} \longleftrightarrow \mathbf{K}_n$$

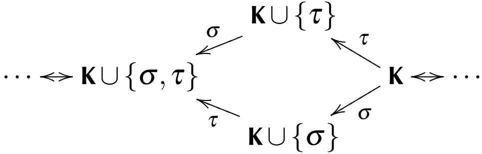
by maintaining a compatible homology basis for [M., Oudot '15 '16]

$$\underbrace{\mathbf{K}_1 \longleftrightarrow \cdots \longleftrightarrow \mathbf{K}_i = \mathbf{K}'_m}_{\mathbb{K}[1;i]} \xleftarrow{\tau_m} \mathbf{K}'_{m-1} \xleftarrow{\tau_{m-1}} \mathbf{K}'_{m-2} \xleftarrow{\tau_{m-2}} \cdots \xleftarrow{\tau_1} \emptyset$$

under

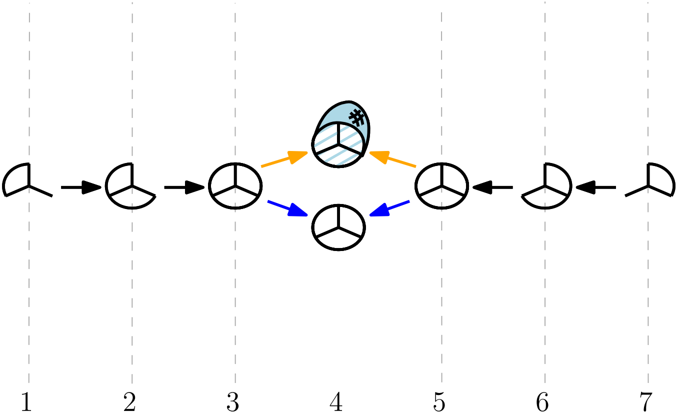


Arrow reflections if $\mathbf{K}_{\overline{k}} \xrightarrow{\sigma} \mathbf{K}_{\overline{k+1}}$ is forward.

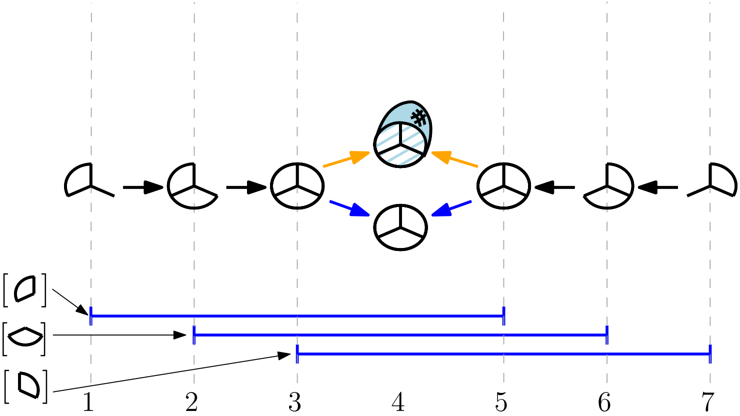


Arrow transpositions in sequence if $\mathbf{K}_{\overline{k}} \xleftarrow{\sigma} \mathbf{K}_{\overline{k+1}}$ is backward.

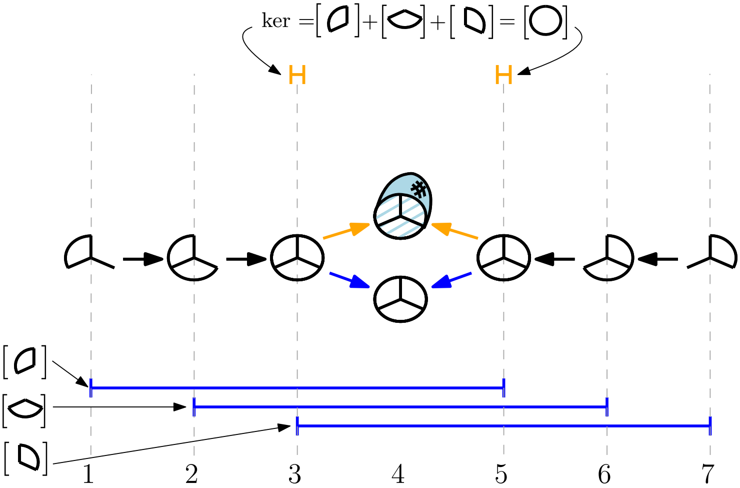
Zigzag Persistence Algorithm



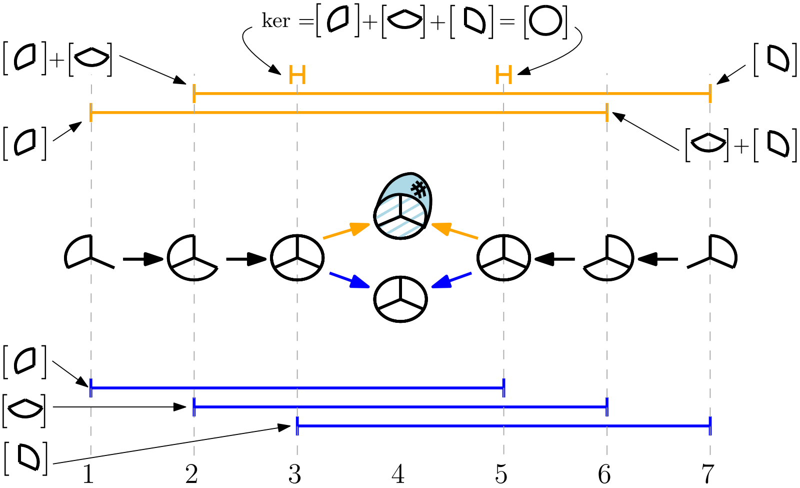
Zigzag Persistence Algorithm



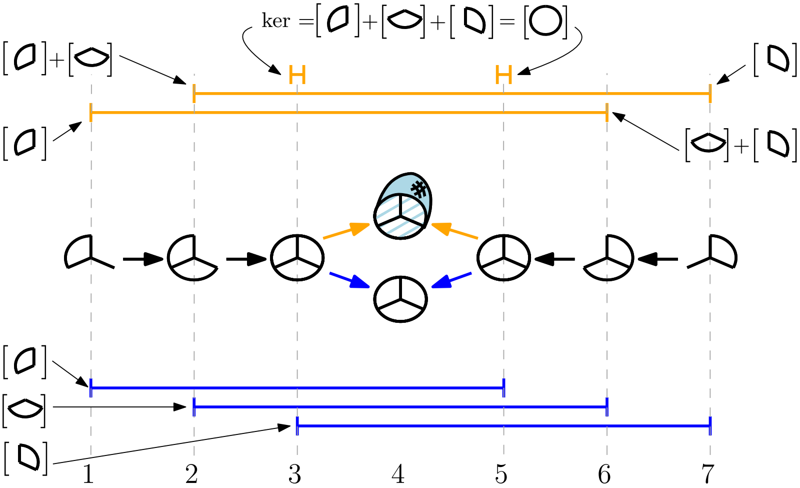
Zigzag Persistence Algorithm



Zigzag Persistence Algorithm



Zigzag Persistence Algorithm



An arbitrary number of bars change

⟶ directed by the topology/algebra.

Concluding Remarks

In Practice, a Toy Example

Standard persistence		Sparse persistence		Zigzag Persistence		
#$\mathbf{K}_{max}$	T	#$\mathbf{K}_{max}$	T	# arrows	#$\mathbf{K}_{max}$	T
$230 \cdot 10^6$	3147 sec.	7474	24 sec.	$2.4 \cdot 10^6$	50840	285 sec.

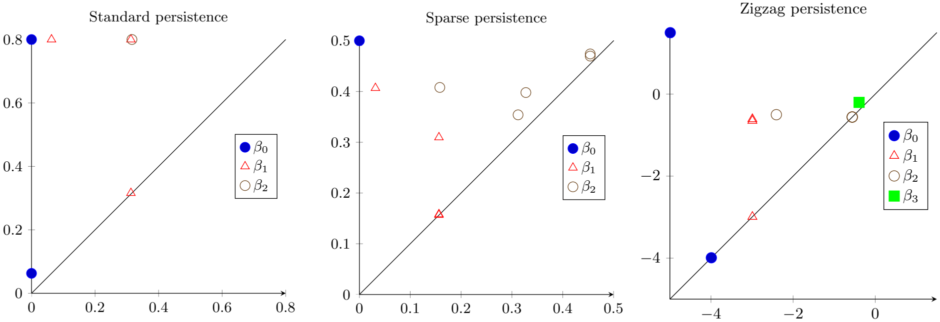


Figure: Best possible persistence diagrams obtained by the different methods on 2000 points sampling a torus wrapped around a (poorly sampled) 3-sphere in $\mathbb{R}^4$.

Conclusion & Perspectives

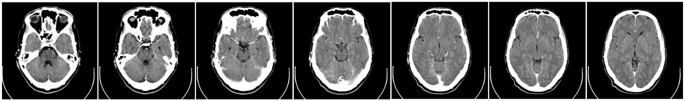
Three technologies to solve the inference problem:

$$\mathbf{K}_1 \hookrightarrow \mathbf{K}_2 \hookrightarrow \cdots \hookrightarrow \mathbf{K}_i \hookrightarrow \mathbf{K}_{i+1} \hookrightarrow \cdots \qquad \text{inclusions.}$$

$$\mathbf{K}_1 \longmapsto \mathbf{K}_2 \longmapsto \cdots \longmapsto \mathbf{K}_i \longmapsto \mathbf{K}_{i+1} \longmapsto \cdots \qquad \text{incl. \& contractions.}$$

$$\mathbf{K}_1 \longleftarrow \mathbf{K}_2 \longrightarrow \cdots \longleftarrow \mathbf{K}_i \longrightarrow \mathbf{K}_{i+1} \longleftarrow \cdots \qquad \text{incl. \& removals.}$$

Conclusion & Perspectives

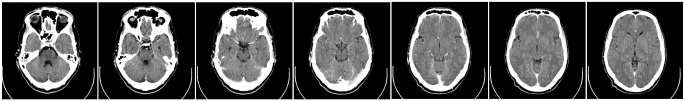


$\mathbf{K}_1 \hookrightarrow \mathbf{K}_2 \hookrightarrow \cdots \hookrightarrow \mathbf{K}_i \hookrightarrow \mathbf{K}_{i+1} \hookrightarrow \cdots$ inclusions.

$\mathbf{K}_1 \longmapsto \mathbf{K}_2 \longmapsto \cdots \longmapsto \mathbf{K}_i \longmapsto \mathbf{K}_{i+1} \longmapsto \cdots$ incl. & contractions.

$\mathbf{K}_1 \longleftarrow \mathbf{K}_2 \longrightarrow \cdots \longleftarrow \mathbf{K}_i \longrightarrow \mathbf{K}_{i+1} \longleftarrow \cdots$ incl. & removals.

Conclusion & Perspectives



$\mathbf{K}_1 \hookrightarrow \mathbf{K}_2 \hookrightarrow \cdots \hookrightarrow \mathbf{K}_i \hookrightarrow \mathbf{K}_{i+1} \hookrightarrow \cdots$ inclusions.

 $\overset{?}{\hookrightarrow}$ 

$\mathbf{K}_1 \longmapsto \mathbf{K}_2 \longmapsto \cdots \longmapsto \mathbf{K}_i \longmapsto \mathbf{K}_{i+1} \longmapsto \cdots$ incl. & contractions.

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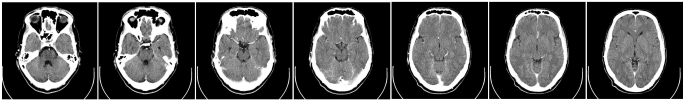
Conclusion & Perspectives



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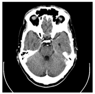 $\overset{\text{deformation}}{\longmapsto}$ 

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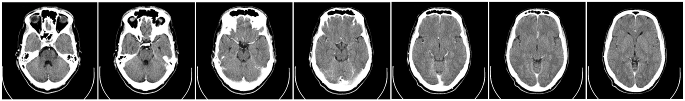
Conclusion & Perspectives



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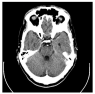 $\overset{\text{deformation}}{\longmapsto}$ 

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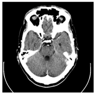
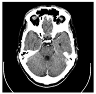
 $\overset{\text{incl.}}{\longrightarrow}$  $\cup$  $\overset{\text{incl.}}{\longleftarrow}$