Une introduction à la topologie et à la géométrie des données

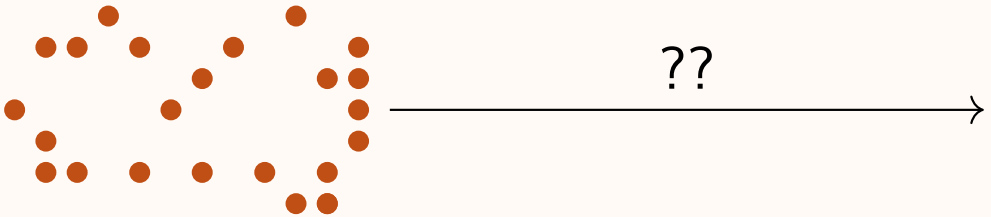
Dina Razafindralandy

Laboratoire des Sciences de l'Ingénieur pour l'Environnement
La Rochelle Université – UMR CNRS 7356

GDR Géométrie Différentielle et Mécanique
La Rochelle, Juillet 2020

But

Data



Properties

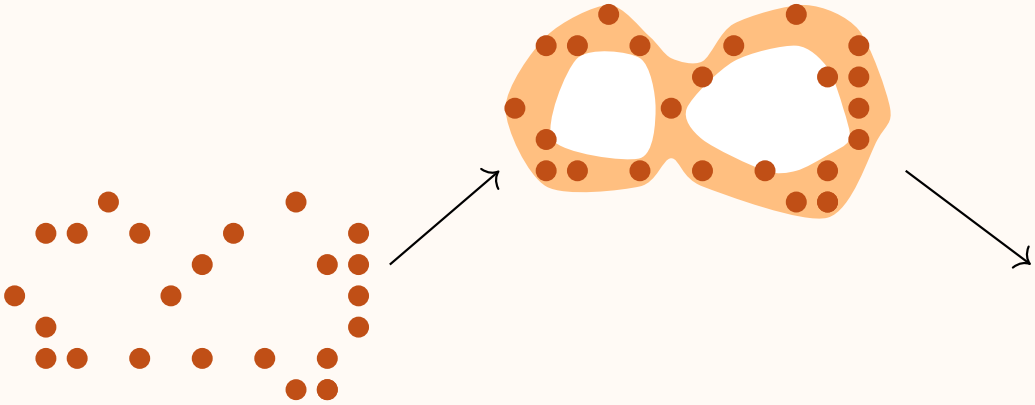
- Topological: connexity, holes, ...
- Geometrical: curvature, interpolation, ...

Differential calculus on manifold

(discrete exterior calculus, ...)

But

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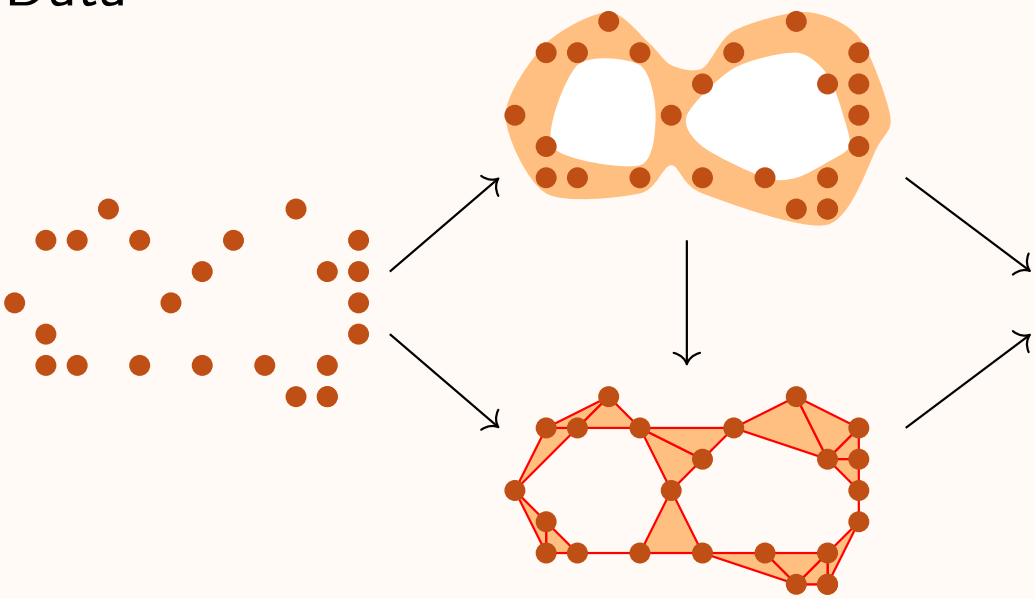
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Plan

- Topological analysis: Reminder on homology theory
- From data cloud to simplicial triangulation
- Topological persistence
- Applications (fluid mechanics, . . .)

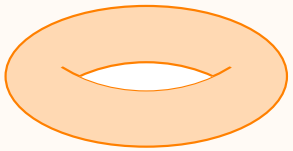
Betti numbers: Measure the topological "complexity"



$\beta_0 = 2,\ \beta_1 = 1,\ \beta_{k\geq 2} = 0$



$\beta_0 = 1,\ \beta_1 = 0,\ \beta_2 = 1$



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- Projective space $\mathbb{P}^n(\mathbb{R})$: $\beta_0 = 1, \quad \beta_1 = \cdots = \beta_{n-1} = 0, \quad \beta_n = 1 - (-1)^n$
- Klein bottle: $(1, 2, 1)$
- $SO(3) : (1, 0, 1), \qquad SO(4) : (1, 0, 0, 2, 0, 0, 1), \qquad SO(5) : (1, 0, 0, 1, 0, 0, 0, 1)$

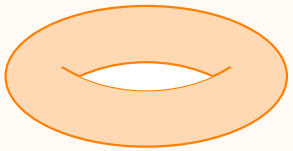
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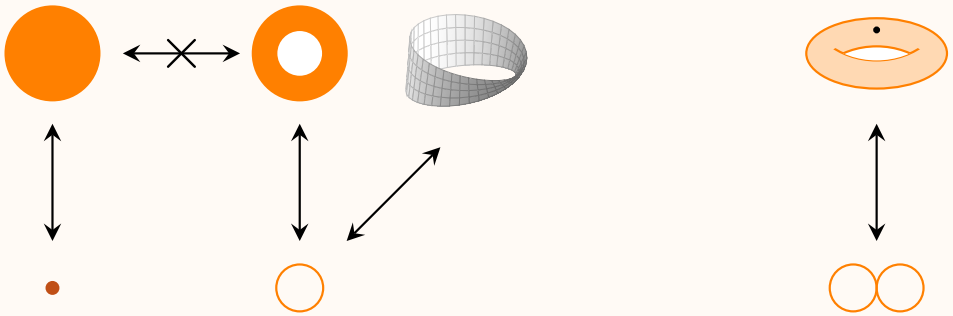
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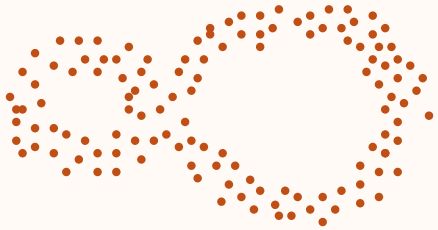
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- Invariant under homomorphism
- Invariant under homotopy (continuous deformation)



Reconstruction of a manifold in $\mathbb{R}^d$

Point cloud $\longrightarrow$ Sub-manifold X of $\mathbb{R}^d$

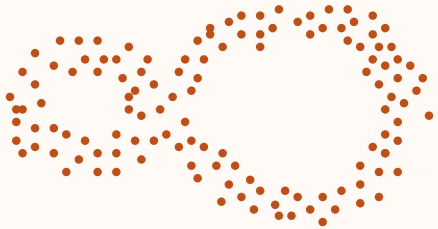


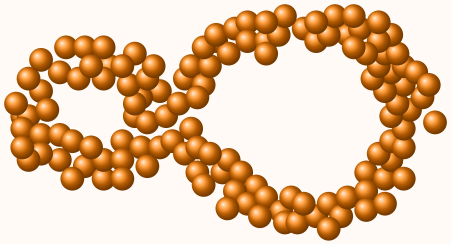
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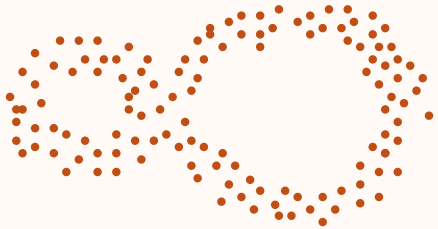


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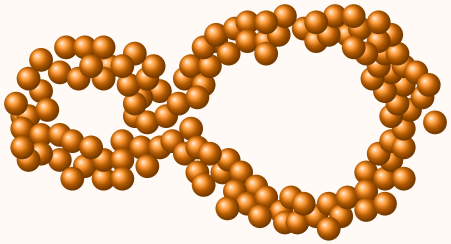
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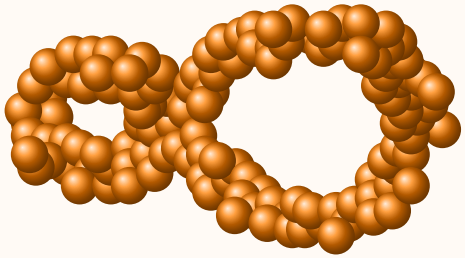
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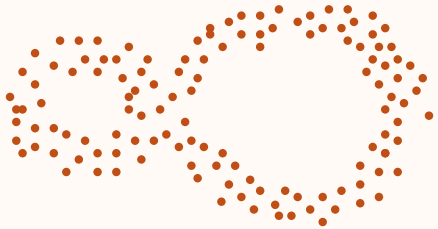




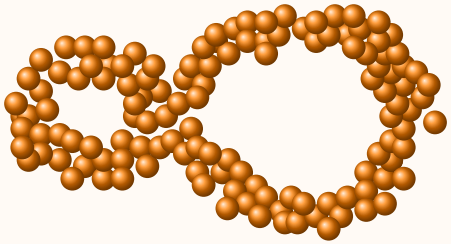
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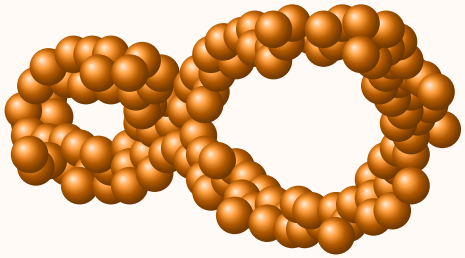
Reconstruction of a manifold in $\mathbb{R}^d$

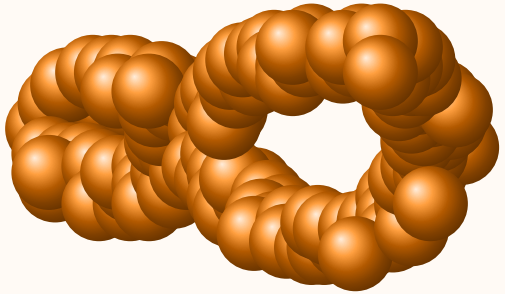
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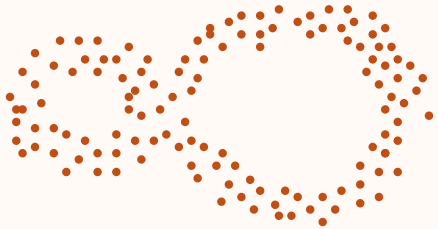




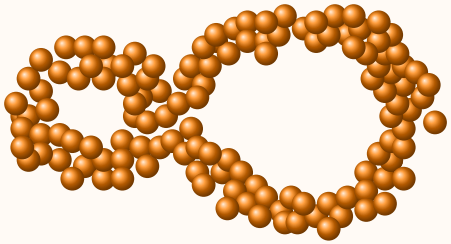
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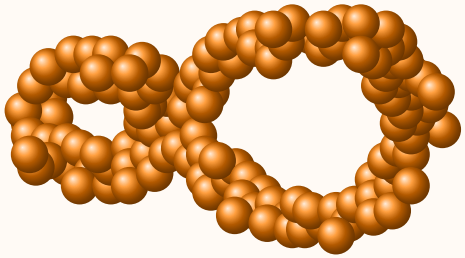
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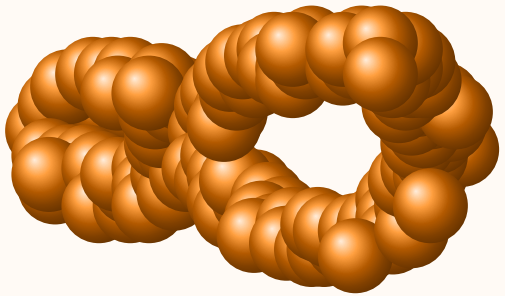
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Point cloud $\longrightarrow$ Sub-manifold M

$\searrow$

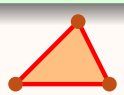
Triangulation: Simplicial complex

Simplicial complex

Geometric k-simplex

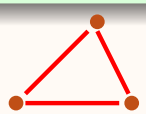
spanned by independent points $v_0, \ldots, v_k \in \mathbb{R}^d$

the convex hull $v_0 \cdots v_k = \left\{ \sum_{i=0}^{k} \lambda_i v_i \in \mathbb{R}^d \quad | \quad \lambda_i \geq 0, \ \sum_{i=0}^{k} \lambda_i = 1 \right\}$

0-simplex:  1-simplex:  2-simplex:  4-simplex: 

Face of a k-simplex $v_0 \cdots v_k$:

any simplex spanned by a subset of $v_0 \cdots v_k$

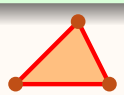
 $\xrightarrow{\textit{Faces}}$  and $\emptyset$

Simplicial complex

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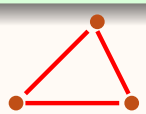
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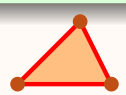
Abstract k-simplex. A set with cardinal $k+1$: $v_0 \cdots v_k$

Simplicial complex

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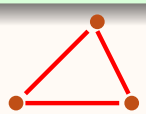
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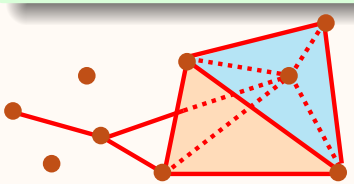
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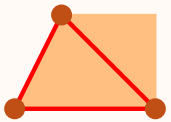
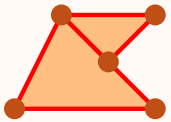
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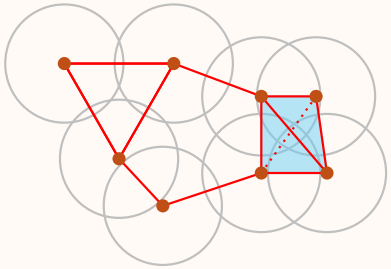
Simplicial complex = Finite collection K of simplices of

- $\sigma \in K$ and τ face of σ $\implies$ $\tau \in K$
- $\sigma \cap \tau \neq \emptyset$ $\implies$ $\sigma \cap \tau$ is a common face of σ and τ



Counter-examples  

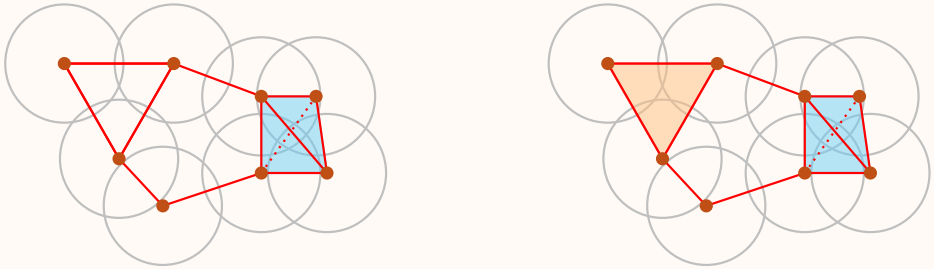
$V = \{v_0, \ldots, v_n\} \subset \mathbb{R}^d$



Cech (abstract) complex

$$Cech(V, r) \quad = \quad \{v_{i_0} \cdots v_{i_k} \quad | \quad \cap_{j=0}^{k} \overline{B}(v_{i_j}, r) \neq \emptyset\}$$

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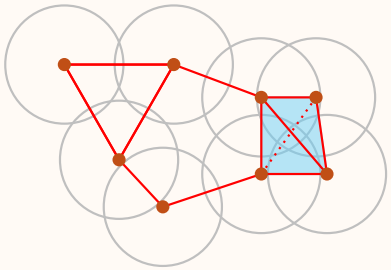
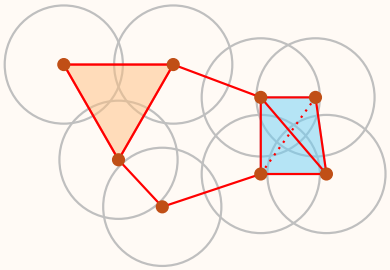
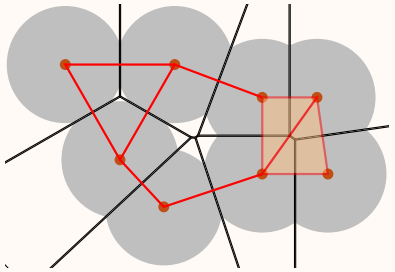
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Vietoris-Rips complex

$$Rips(V, r) \quad = \quad \{v_{i_0} \cdots v_{i_k} \quad | \quad d(v_{i_j}, v_{i_p}) \leq 2r, \quad \forall j, p = 0, \cdots, k\}$$

Easier to compute but more simplicies. Not homotopic equivalent

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Vietoris-Rips complex

$$Alpha(V, r): \quad \overline{B}(v_i, r) \quad \longrightarrow \quad \overline{B}(v_i, r) \cap Voronoi(v_i, r)$$

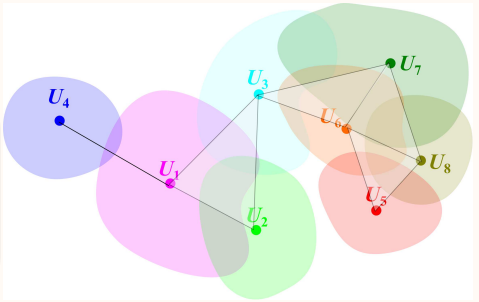
$$Voronoi(v_i, r) = \{x \in \mathbb{R}^d \mid d(v_i, x) \leq d(v_j, x) \ \forall j \neq i\}$$

Less simplices but harder to compute (Voronoi). Homotopic equivalent to Cech.
Natural realization in $\mathbb{R}^d$ if the v_i in general position (no subset $\{v_{i_0}, \cdots, v_{i_{d+1}}\}$ lies on a same hypersphere)

Gonzalez, Garcia-Gonzalez, Chinesta, Cueto: Interpolation on Constitutive manifold of porcine tissues $\subset \mathbb{R}^9$

In a non-metric space

$U = \{U_0, \cdots, U_n\}$ a set of open/closed subspaces



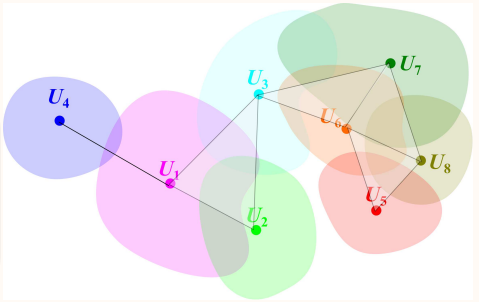
Nerve complex

$$Nerve(U) \quad = \quad \{\{U_{i_0}, \cdots, U_{i_k}\} \subset U \mid \cap_{j=0}^{k} U_{i_j} \neq \emptyset\}$$

Eg: $V = \{v_0, \ldots, v_n\} \subset \mathbb{R}^d$,
$U^r = \{B(v_0, r), \ldots, B(v_n, r)\}$ $\quad Cech(V, r) = Nerve(U^r)$

In a non-metric space

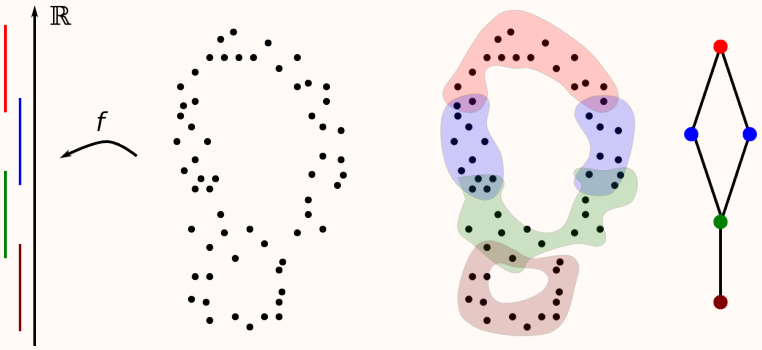
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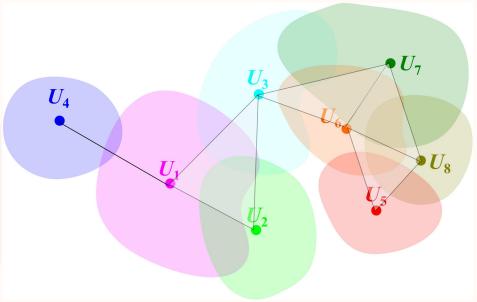


Mapper algorithm with a filter

- A filter $f : V \longrightarrow \mathbb{R}$
- An overlapping covering $\cup_{i=1}^{n} R_i = [\inf f, \sup f]$
- $U_i = f^{-1}(R_i)$
- Refine with a clustering algorithm
- $Nerve(U_i)$

In a non-metric space

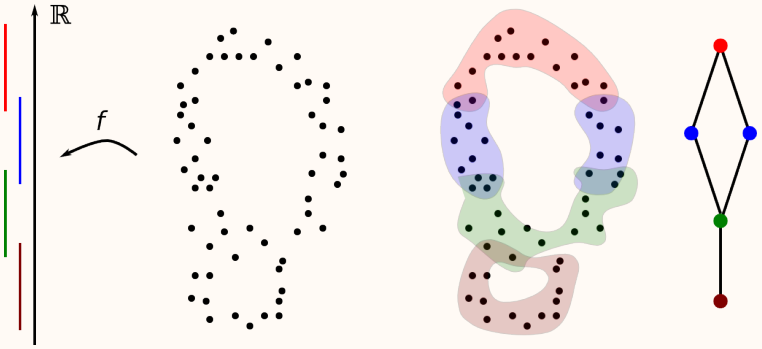
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Nerve complex

$$Nerve(U) \quad = \quad \{\{U_{i_0}, \cdots, U_{i_k}\} \subset U \ \mid \ \cap_{j=0}^{k} U_{i_j} \neq \emptyset\}$$

Eg: $V = \{v_0, \ldots, v_n\} \subset \mathbb{R}^d$,
$U^r = \{B(v_0, r), \ldots, B(v_n, r)\}$ $\quad$ $Cech(V, r) = Nerve(U^r)$

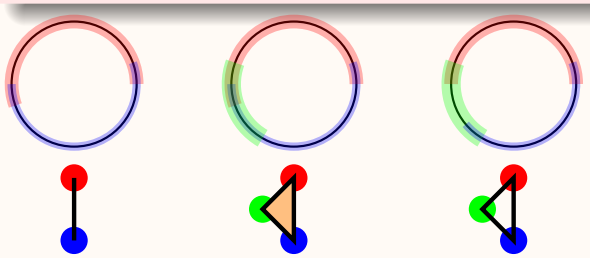


Mapper algorithm with a filter

- A filter $f : V \longrightarrow \mathbb{R}$
- An overlapping covering $\cup_{i=1}^{n} R_i = [\inf f, \sup f]$
- $U_i = f^{-1}(R_i)$
- Refine with a clustering algorithm
- $Nerve(U_i)$

Nerve theorem. $U = \{U_i, \ i = 1, \ldots, n\}$ an open covering of X

If $U_i \cap U_j = \emptyset$ or contractible then X and $Nerve(U)$ are homotopic equivalent



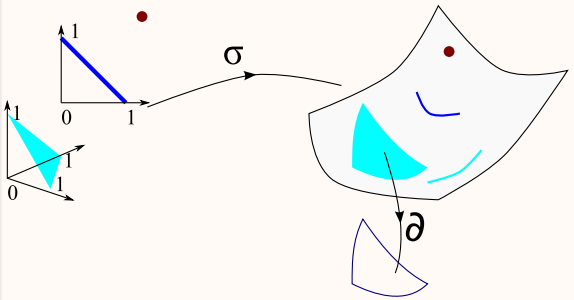
Back on Betti numbers

Singular k-simplex: continuous $\sigma : \Delta_k \longrightarrow M$

k-chain: $\sum_i \alpha^i \sigma_i$ $\quad \alpha^i \in \mathbb{Z}/2\mathbb{Z}$, σ_i k-simplex

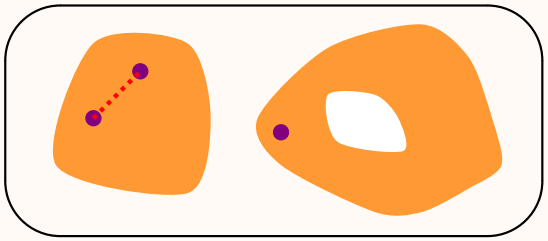
Boundary: $\partial_k \sigma = \sum \sigma_{|face_{k-1}}$

sum of all the restrictions of σ to the $k-1$-faces of Δ_k



k-boundary $=$ element of $\operatorname{Im} \partial_{k+1}$, $\quad k$-cycle $=$ element of $\ker \partial_k$

$\beta_k = \operatorname{rank} H_k$ $\qquad$ où $\qquad H_k = \ker \partial_k / \operatorname{Im} \partial_{k+1}$ $\qquad$ k-th homology group



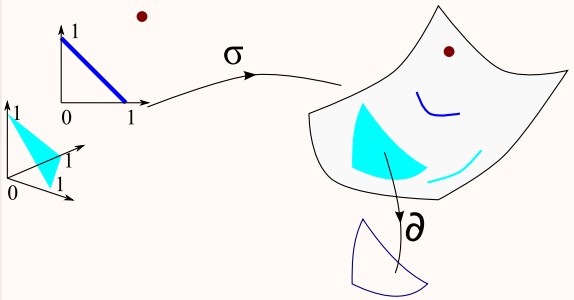
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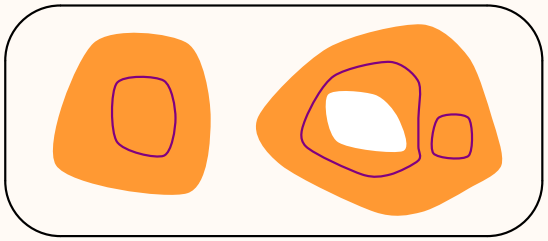
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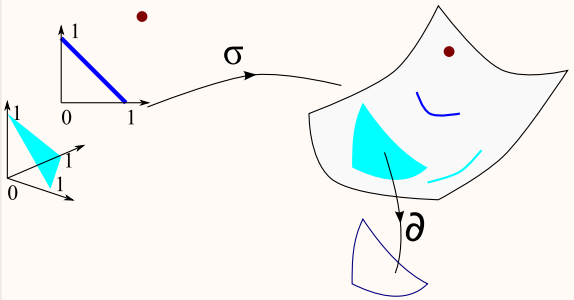
Back on Betti numbers

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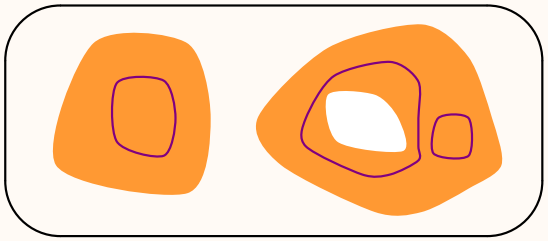
Boundary: $\partial_k \sigma = \sum \sigma_{|face_{k-1}}$

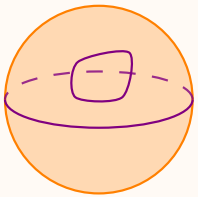
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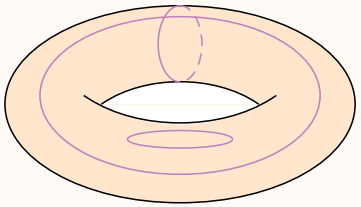


k-boundary $=$ element of $\operatorname{Im} \partial_{k+1}$, $\quad k$-cycle $=$ element of $\ker \partial_k$

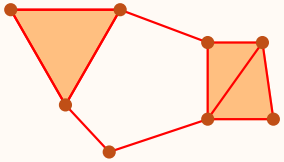
$\beta_k = \operatorname{rank} H_k$ $\quad$ où $\quad H_k = \ker \partial_k / \operatorname{Im} \partial_{k+1}$ $\quad$ k-th homology group







Homology of a simplicial complex K



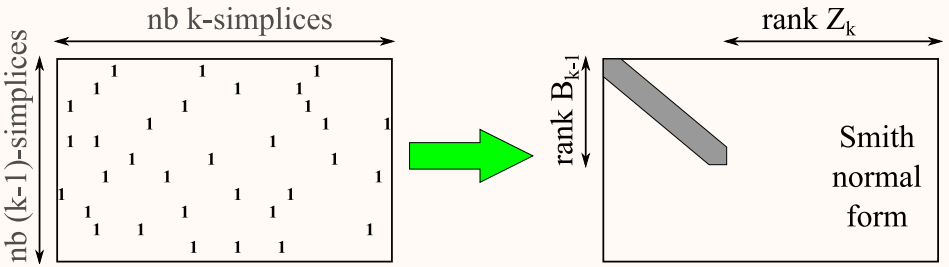
k-chain: $\sum_i \alpha^i \sigma_i$, $\quad \alpha^i \in \mathbb{Z}/2\mathbb{Z}$, $\quad \sigma_i$ k-simplex

Boundary: $\partial_k v_0 \cdots v_k = \sum_{i=0}^{k} v_0 \cdots \widehat{v_i} \cdots v_k$



k-boundary $=$ element of $\operatorname{Im} \partial_{k+1}$, $\quad k$-cycle $=$ element of $\ker \partial_k$

$\beta_k = \operatorname{rank} H_k \qquad$ où $\qquad H_k = \ker \partial_k / \operatorname{Im} \partial_{k+1}$

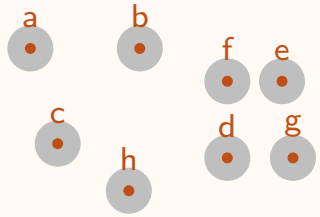


$\beta_k = \operatorname{rank} Z_k - \operatorname{rank} B_k$

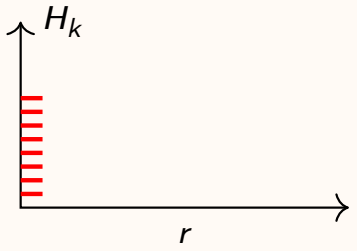
$Z_k = \ker \partial_k$,
$B_k = \operatorname{Im} \partial_{k+1}$

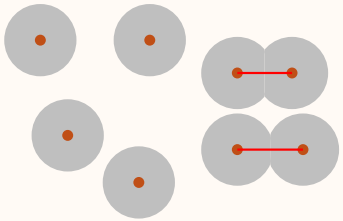
Smith normal form ($\simeq$SVD) of ∂_k

Evolution with r in $Cech(P, r)$, $Rips(P, r)$, $Alpha(P, r)$?



$K^{r1} = \{a, b, c, d, e, f, g, h\}$

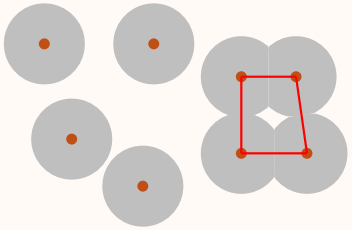




$K^{r2} = \{a, b, c, d, e, f, g, h$

$ef, dg\}$

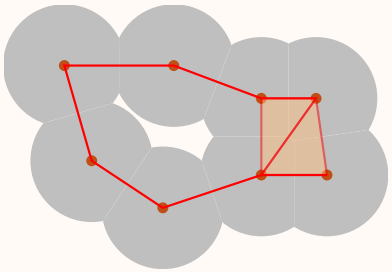




$K^{r3} = \{a, b, c, d, e, f, g, h$

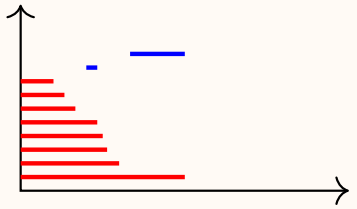
$ef, dg, fd, eg\}$



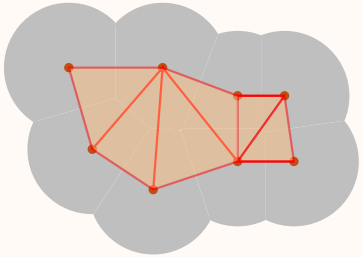


$K^{r4} = K^{r3} \cup \{def, deg,$

$ch, bf, ac, ab, hd\}$



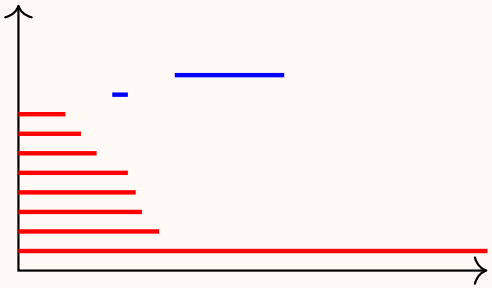
Persistence barcode and diagram

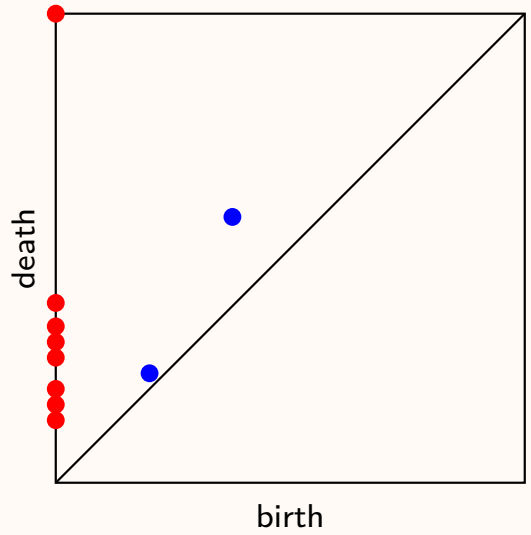


$K^{\infty} = K^{r_4} \cup \{abc, deg,$

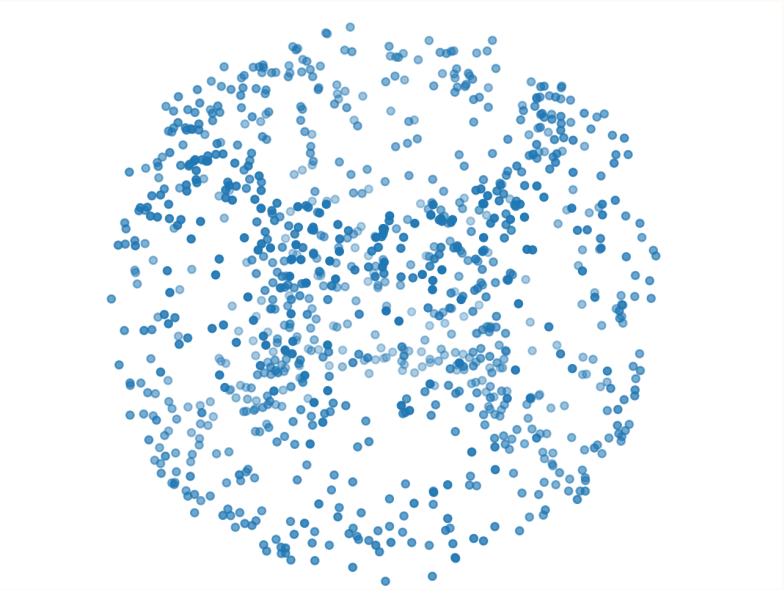
$ch, bf, ac, ab, hd\}$

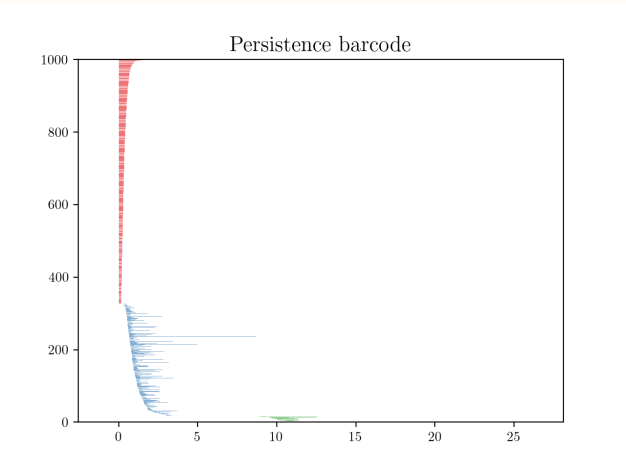


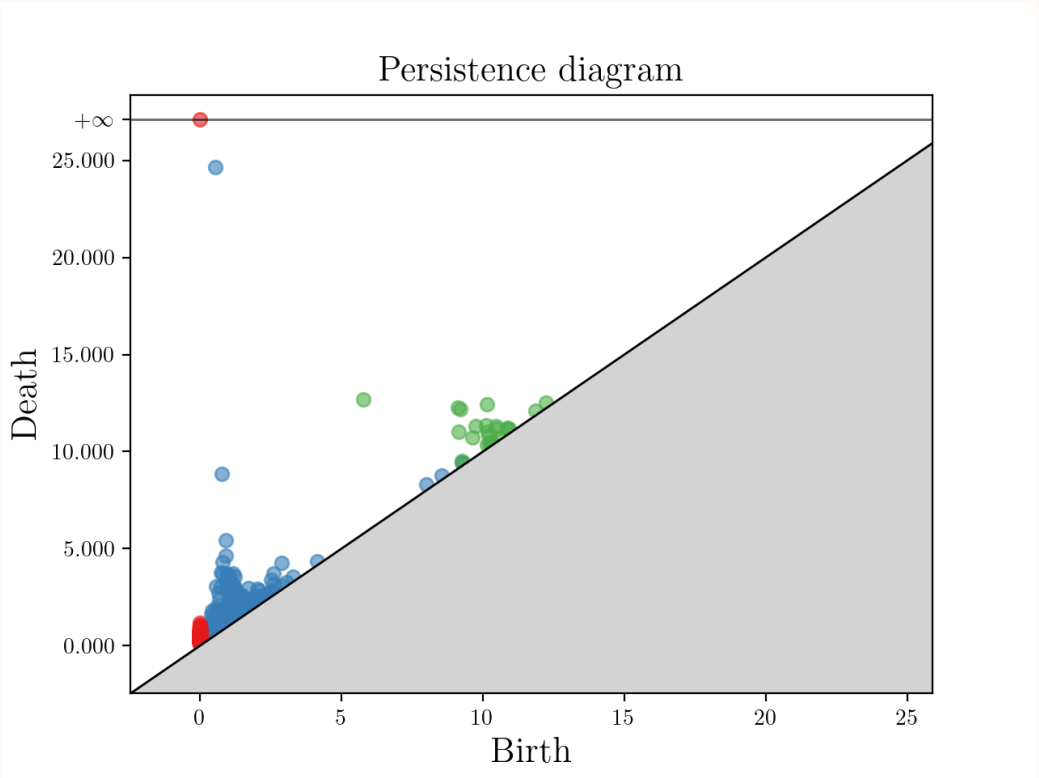




Analysis of a noisy 3D point data







Compression/noise reduction: remove a point if it does not change *too much* the diagram

Gudhi [Maria et al, 2007]

In a distance sense

Filtration of a complexe K

- family $(K^r)_{r \in R}$ of subcomplexes of K, $R \subset \mathbb{R}$ st
- $r_1 \leq r_2 \implies K^{r_1} \subseteq K^{r_2}$, and $\cup_{r \in R} K^r = K$

Persistence barcode/diagram: compact encoding of the evolution of the topology with r

Only a finite number of r is needed in practice

Filtration of a complexe K

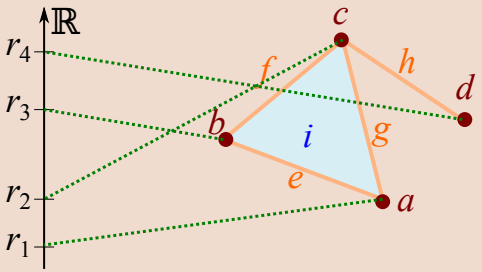
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Persistence barcode/diagram: compact encoding of the evolution of the topology with r

Only a finite number of r is needed in practice

Sublevel set filtration from a mapper

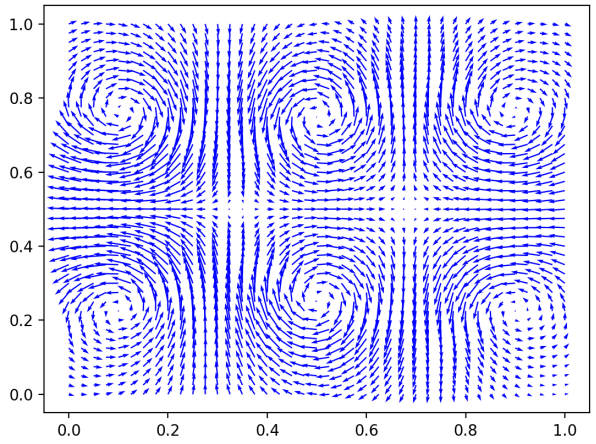
- Mapper f: $v \in \mathit{Vertex}(K) \longmapsto \mathbb{R}$
- Extension: f: $K \longrightarrow \mathbb{R}$ with $fv_0 \cdots v_k = \max_{i=0,\ldots,k} f(v_i)$
- Sublevel sets: $K^r = f^{-1}(]-\infty, r])$

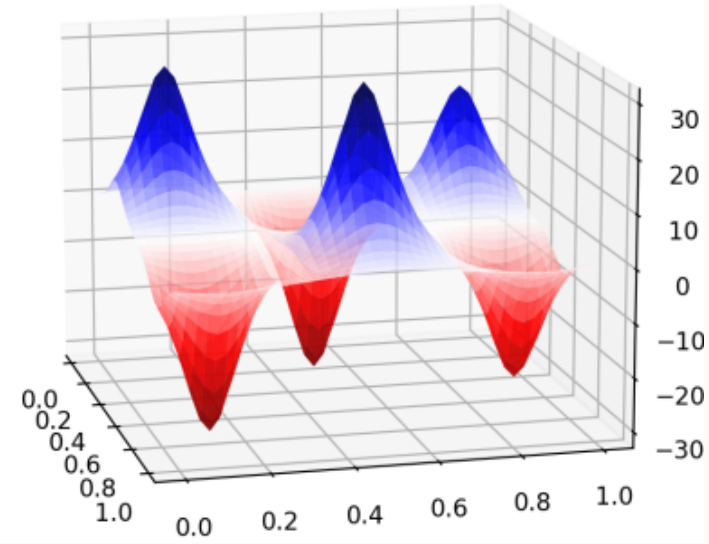


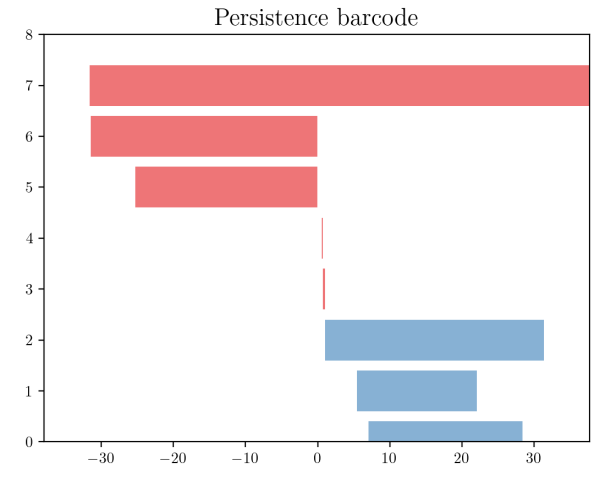
$K^{r_1} = \{a\}, \quad K^{r_2} = \{a, c, ac\}, \quad K^{r_3} = \{a, c, ac, b, ba, bc, abc\}$

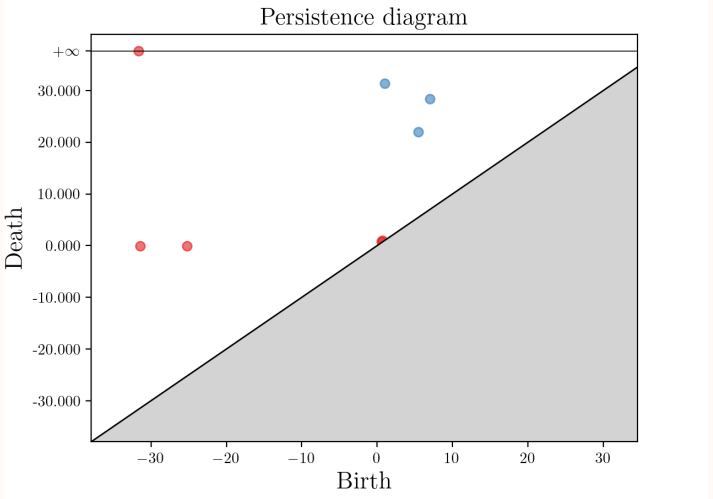
$K^{r_4} = K^{r_3} \cup \{d, cd\} = K$

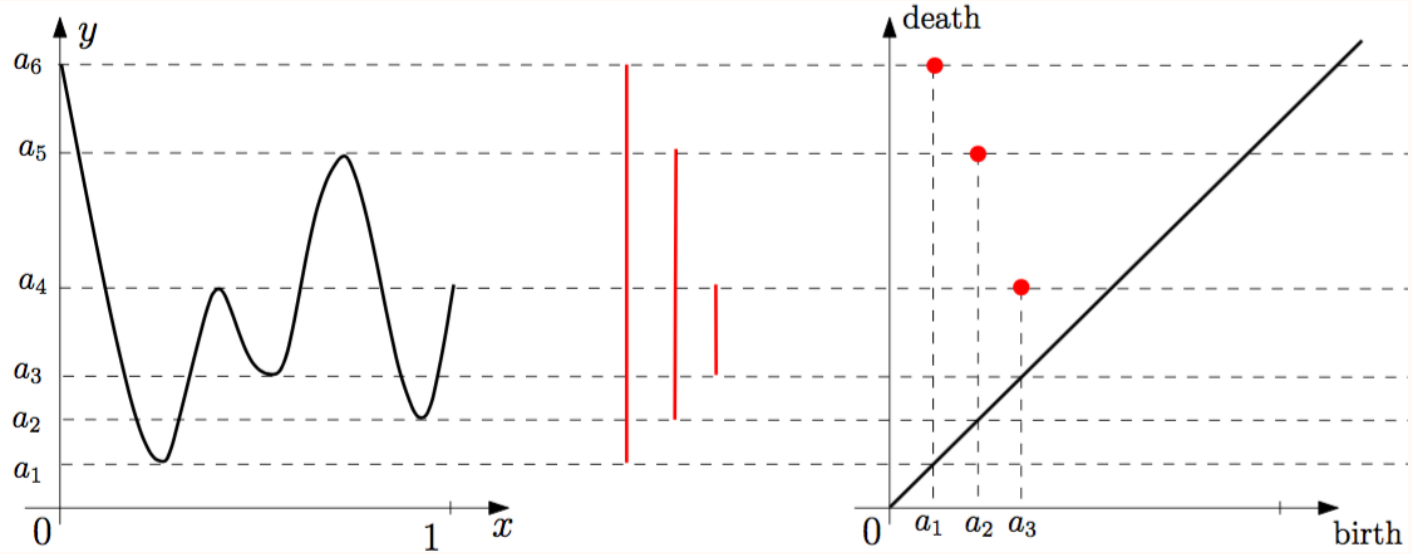
6-vertex flow. Filtration f =vorticity

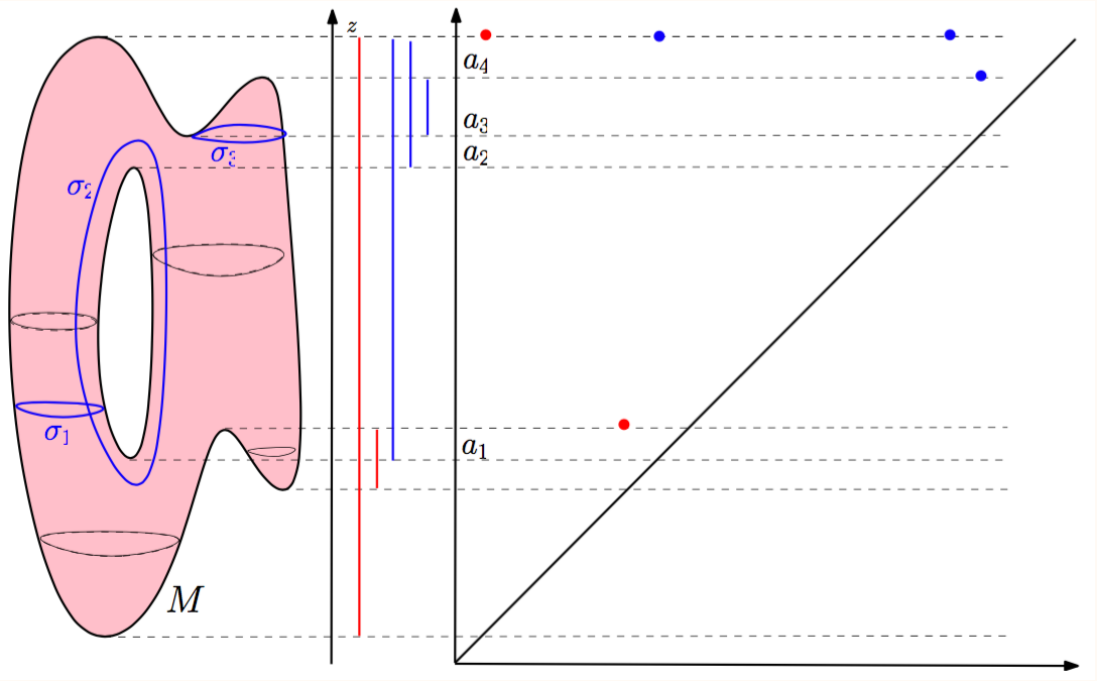




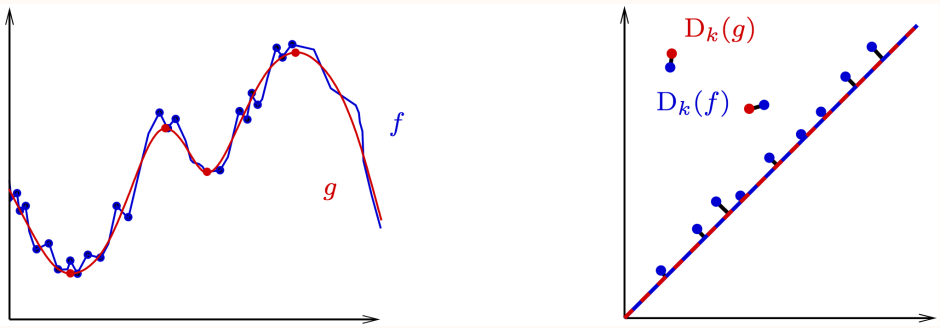





y
a_6
a_5
a_4
a_3
a_2
a_1
0
1
x
death
0
a_1
a_2
a_3
birth


z
a_4
a_3
a_2
a_1
σ_3
σ_2
σ_1
M

Metric on the space of Diagrams

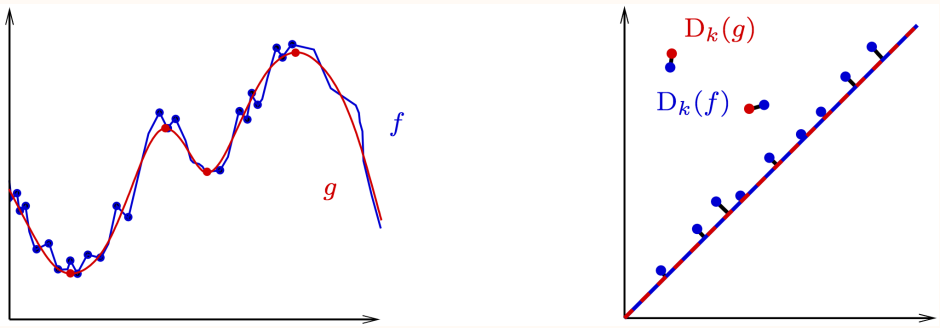


Wasserstein distance

$$W_p(D, D') = \inf_{\beta \in B} \left(\sum_{x \in D} \|x - \beta(x)\|_p^p \right)^{1/p} \qquad B = \{\textit{bijection } D_1 \cup \Delta \longrightarrow D_2 \cup \Delta\}$$

Bottlneck distance: $W_\infty(D, D') = \inf_{\beta \in B} \sup_{x \in D} \|x - \beta(x)\|_p$

Metric on the space of Diagrams



Wasserstein distance

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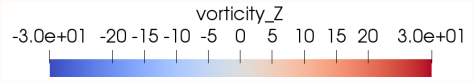
Bottlneck distance: $W_\infty(D, D') = \inf_{\beta \in B} \sup_{x \in D} \|x - \beta(x)\|_p$

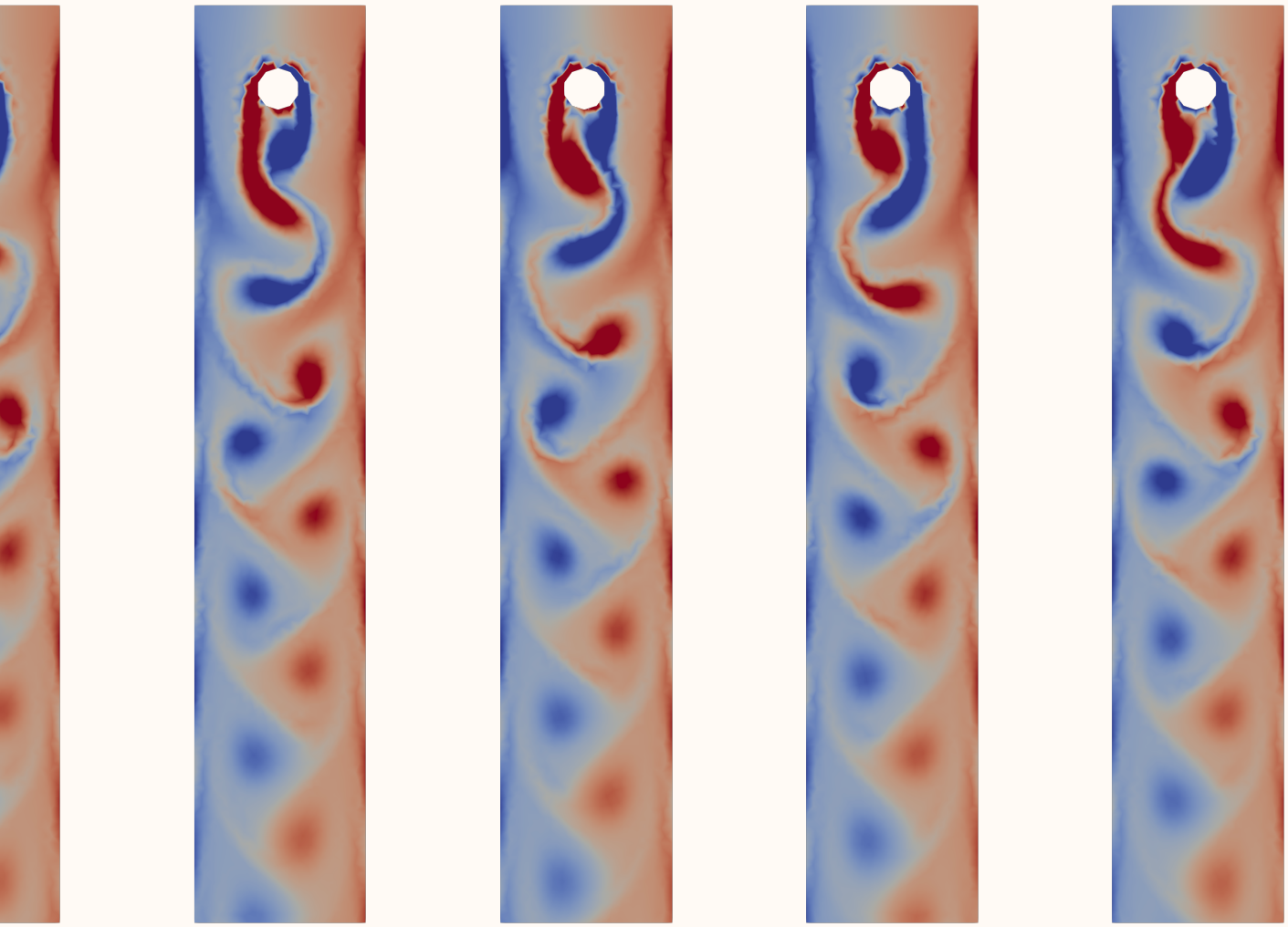
Stability. Tame functions $f, g : X \longrightarrow \mathbb{R}$

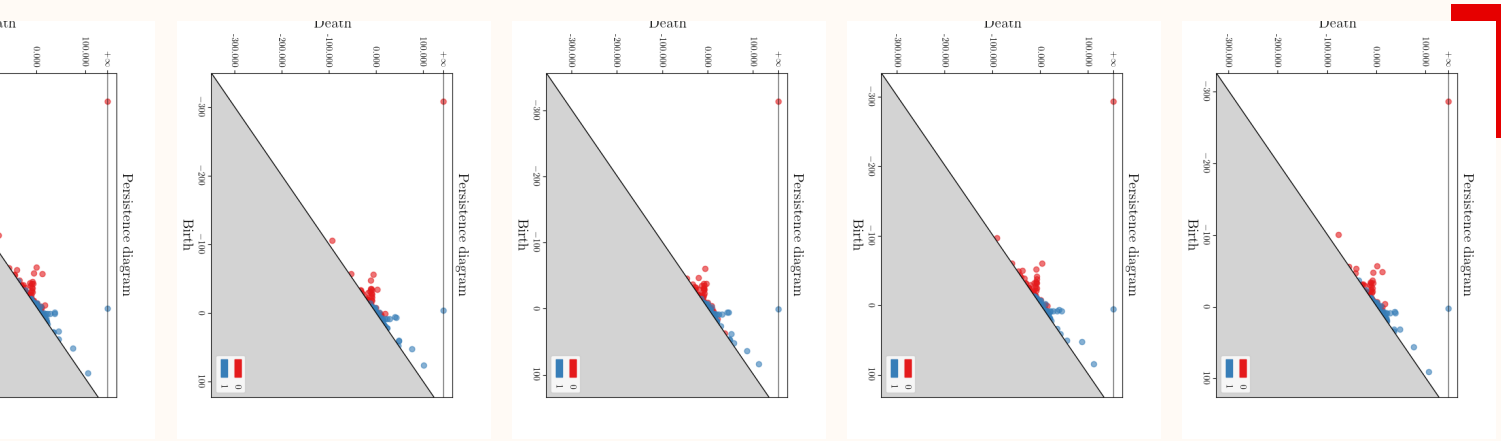
$$W_\infty(\ D(f)\ ,\ D(g)\ ) \leq \|f - g\|_\infty$$

Bottlneck distance [Cohen-Steiner, Edelsbrunner, Harer, 2007]. Wasserstein distance [Skraba, Turner, 2021]

$\omega \in [-286, 300]$. Color limited to:





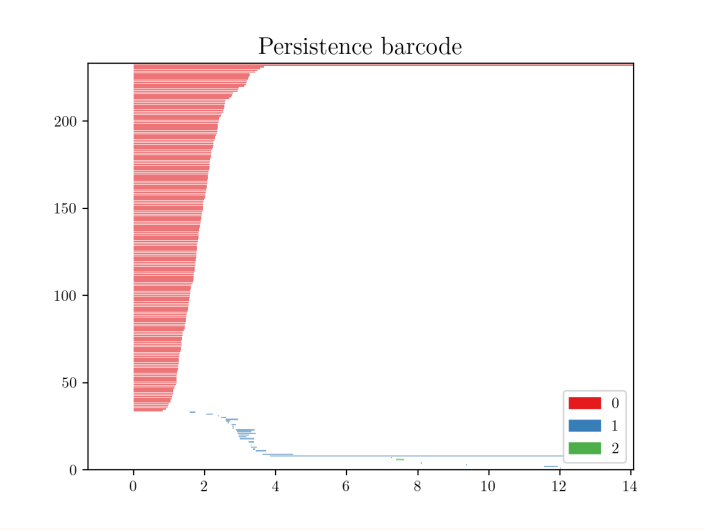


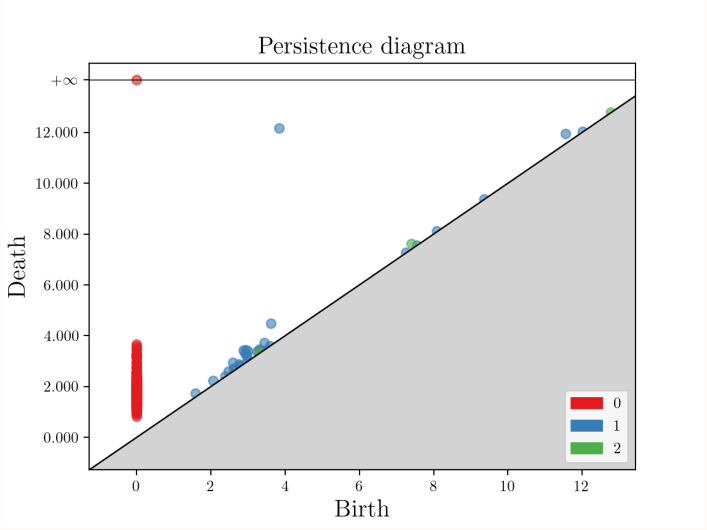
Topological persistence analysis on diagrams

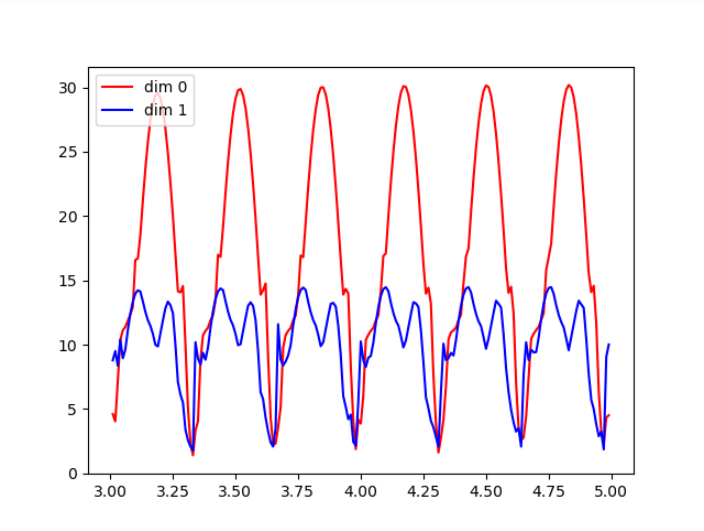
$V = \{Diag_{dim=0}(t_i),\ t_i \geq 3s\}$

Flow well-established from $t_0 = 3s$

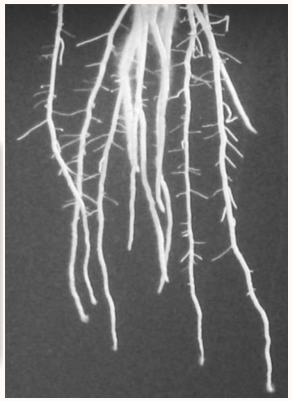
Rips complex with W_∞







Comparison/Classification



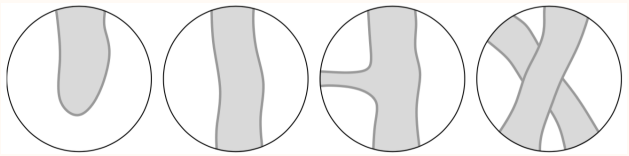
Root architecture

Image intensity: $f : P \subset \mathbb{R}^2 \longrightarrow [0,1]$
Foreground $F = f^{-1}([\epsilon, 1])$
Background $B = f^{-1}([0, \epsilon[)$

Local analysis at $x \in F$.
Filtration: discretisation of $F^r = F \cap B(x, r)$
Consider homology group relative to the boundary $F \cap \mathbb{S}^1(x, r)$

- tip: $\beta_1 = 1$ (on a long r-interval)
- branch: $\beta_1 = 2$
- fork: $\beta_1 = 3$
- crossing: $\beta_1 = 4$

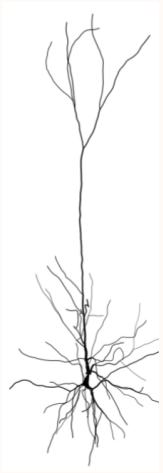
$\mathbb{S}^1$=circle



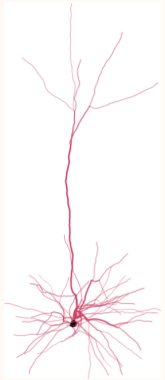
[Edelsbrunner, Harer. 2010]

Rough surface characterization. [Frahi, Argerich, Yun, Falco, Barasinski, Chinesta, 2020]

Neuronal synthesis



$\longrightarrow$ Persistence diagram $\longrightarrow$



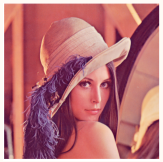
$\longrightarrow$



- Same morpho-electrical properties
- Statistical study

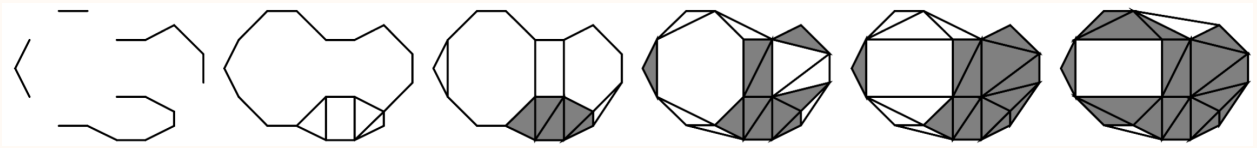
[Kanari et al., 2020]

Image segmentation



	$p = 0$	$p = 2$	$p = 4$
$\alpha = 2$	23 Regions	22 Regions	13 Regions
$\alpha = 4$	47 Regions	34 Regions	21 Regions
$\alpha = 6$	43 Regions	28 Regions	22 Regions

- $V = \{\text{edge}\}$
- $K^\alpha = Alpha(V, \alpha)$:



- Fix a scale α and a persistence param p.
  - p-persistent region: hole at α_0 which are unfilled at $\alpha_0 + p$
  - p-transient region: hole at α_0 which are filled at $\alpha_0 + p$
- Merge neighbor similar (eg. mean color) p-transient regions if it does not change the p-persistent Betti number

[Letscher, Fritts, 2007]

- Compression/noise reduction: remove a p if $W_p(\ D(V), D(V - \{p\})\ ) < \infty$

- Barycenter/interpolation $\longleftarrow$ distance. Non-unicity
  Pers. diagr $D \simeq$ Radon measure $\sum_{x \in D} \delta_x \Longrightarrow$ unique barycentre

  {Radon meas.}+optimal transp. is convex

  [Understanding topo. and geom. of space of pers. diagr. opt. part. transp. 2020]

- Pers. diagr $\longrightarrow$ Probability measure
  Expectation, moments

Do not compute β_k for each r

Filtration of K $\longrightarrow$ total order on K

$\{a\}$, $\{a, b\}$, $\{a, b, c\}$, $\{a, b, c, ac\}$, $\{a, b, c, ac, d\}$, $\{a, b, c, ac, d, cd\}$,
$\{a, b, c, ac, d, cd, ad\}$, $\{a, b, c, ac, d, cd, acd\}$, $\{a, b, c, ac, d, cd, acd, ab\}$

	a	*b*	*c*	*ac*	*d*	*cd*	*ad*	*acd*	*ab*
a				1			1		1
b									1
c				1		1			
ac								1	
d						1	1		
cd								1	
ad								1	
acd									
ab									

size: card K $\times$ card K

rank $Z_k^r = \text{card}\{\sigma \ k-\text{simplex of } K^r \mid column(\sigma) = 0\}$ After reduction

rank $B_k^r = \text{card}\{\sigma \ (k+1)-\text{simplex of } K^r \mid column(\sigma) \neq 0\}$ After reduction

$\beta_k^r = Z_k^r - B_k^r$

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a				1			1		1
b									1
c				1		1	1		
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