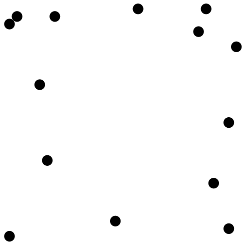
Handling noise and complexity blow-up in topological data analysis.

Mickaël Buchet

The Ohio State University

June 18, 2015

Topological inference



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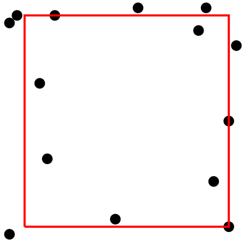

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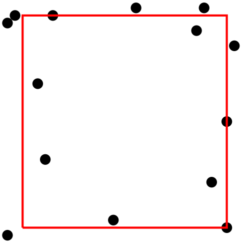

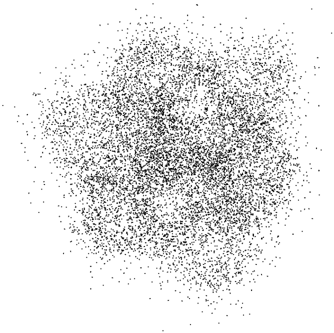

Usual pipeline

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P		F_α		
Point set	$\longrightarrow$	Discrete representation of continuous objects	$\longrightarrow$	Topological information

Challenges

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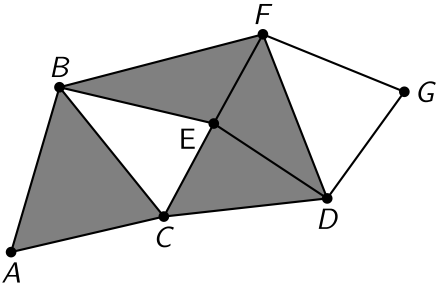
- Size of the data structure
- Complexity of the process
- Robustness to noise

Outline

- Topological information
- Classical data structures
- Sparse data structures
- Handling noise and aberrant values
- Sparsification and parameter free analysis

Homology



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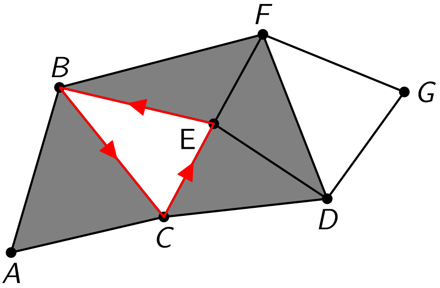

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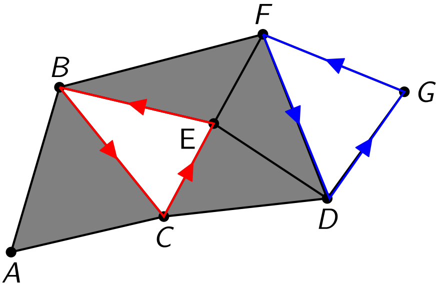

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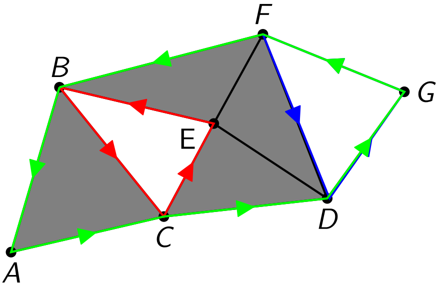
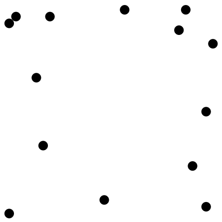


Persistence



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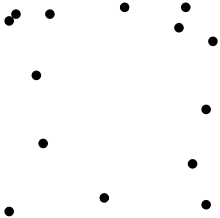

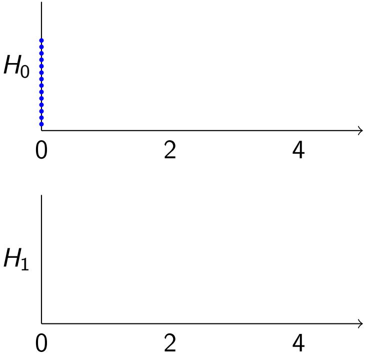

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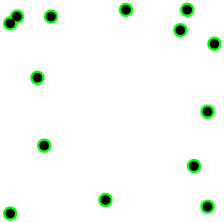

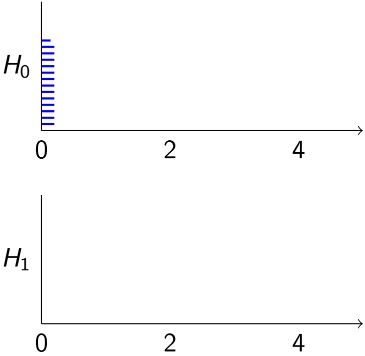

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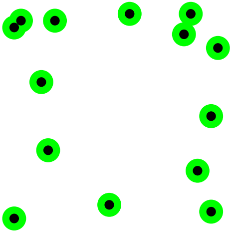

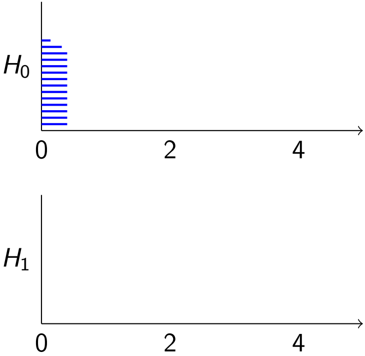

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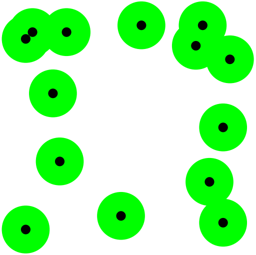

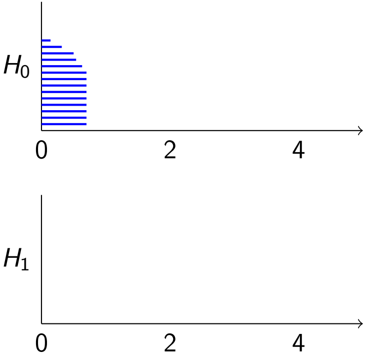

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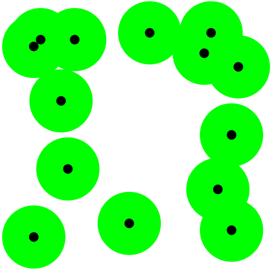

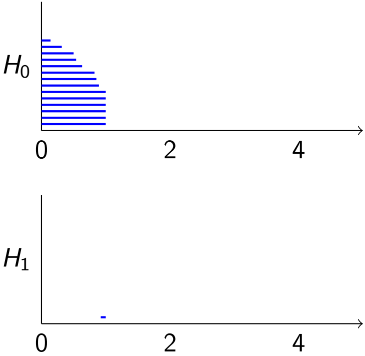

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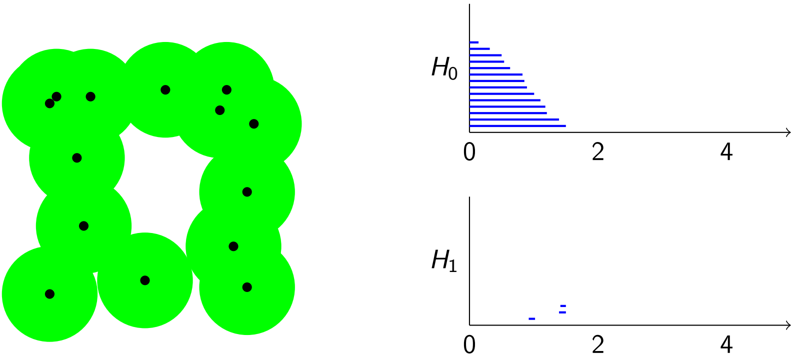

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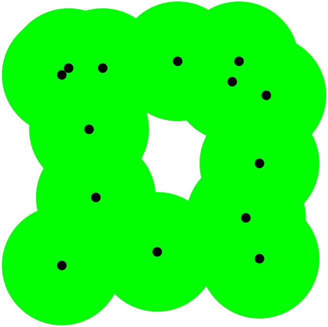

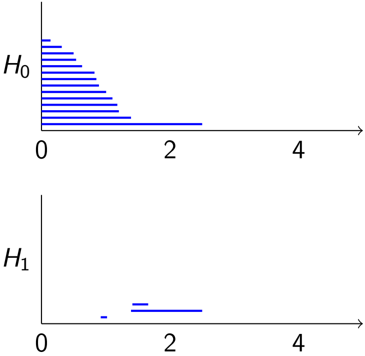

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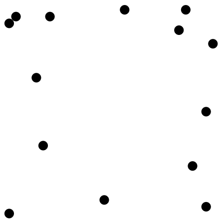
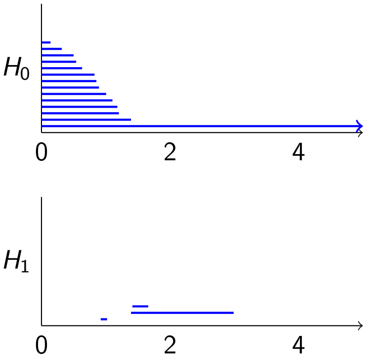
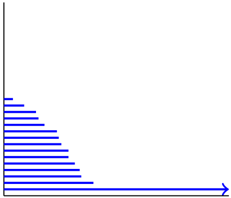
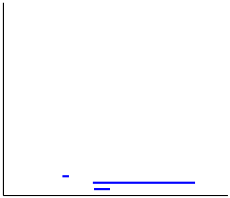




Persistent diagram representation





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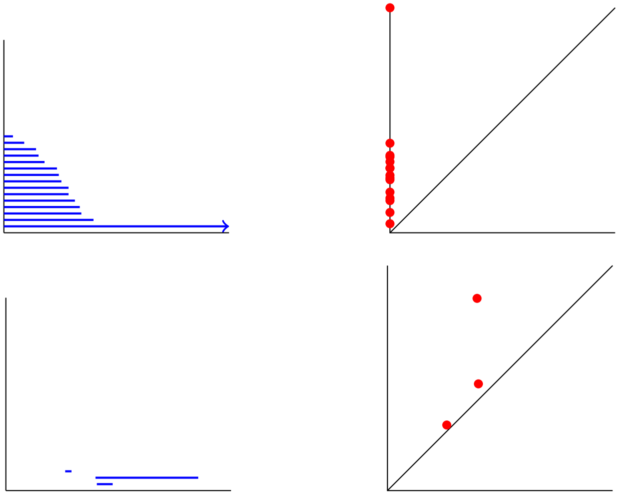

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Čech complex

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$(p_1, \ldots, p_l)$ belongs to the Čech for the parameter α, noted C_α, if :

$$\cap_{i=1}^{n} B(p_i, \alpha) \neq \emptyset$$

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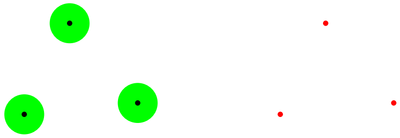

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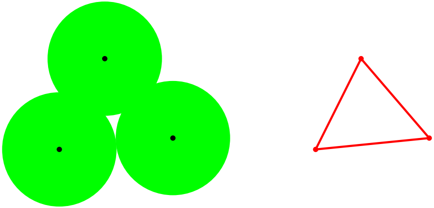

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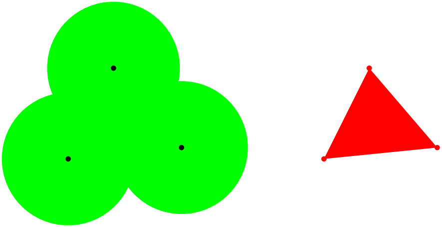

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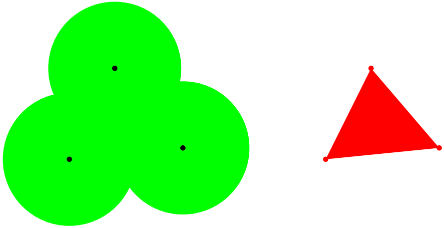

Theorem (Borsuk, 1948)

The Čech complex has the same homology as the union of balls if the space has the good cover property.

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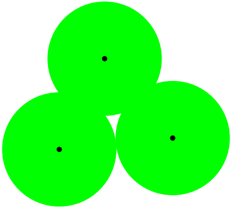

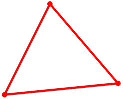

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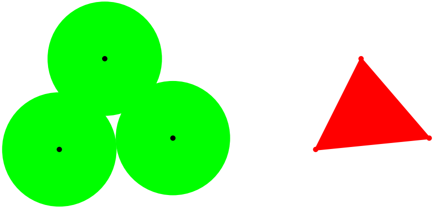
The Rips complex is the maximal complex with the same edges as the Čech complex.



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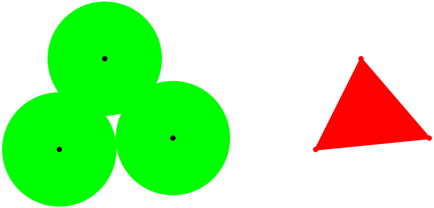
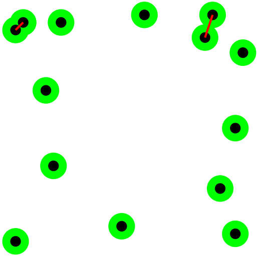


Proposition

$$C_\alpha \subset R_\alpha \subset C_{2\alpha}$$

Illustration



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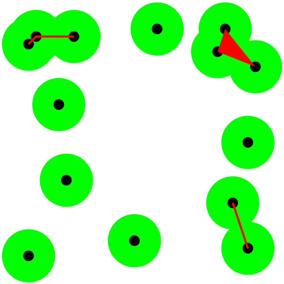

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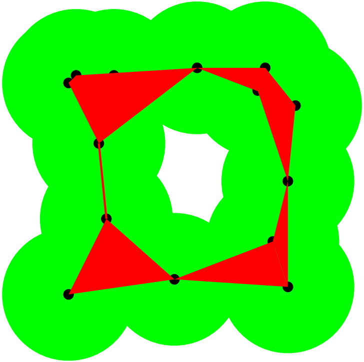

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$$\begin{array}{ccc} R_\delta & \longrightarrow & R_{\delta'} \\ H_*(R_\delta) & \longrightarrow & H_*(R_{\delta'}) \end{array}$$

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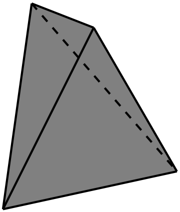
Collapses and contractions (I)

Attali, Lieutier and Salinas 2012, 2013



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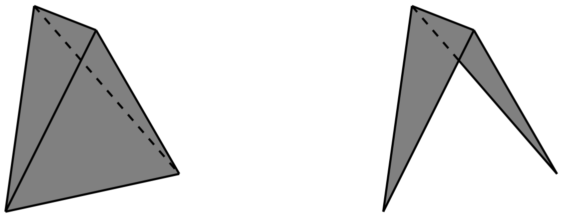

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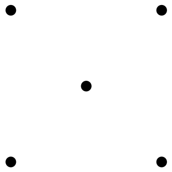
Sparse Rips

Sheehy, 2012



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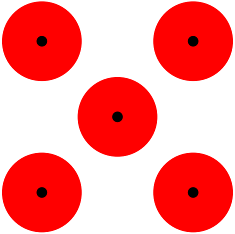

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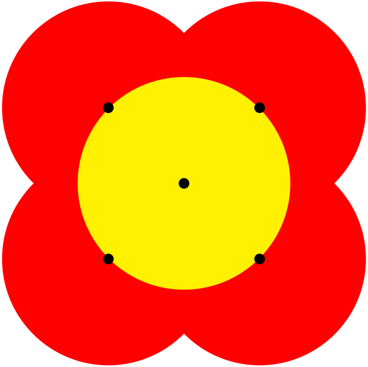

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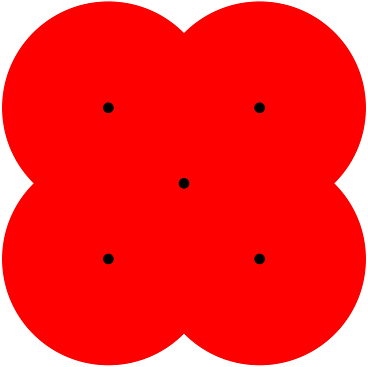
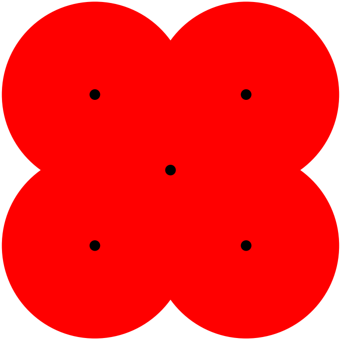


Topological noise

Naively removing points can create topological noise.



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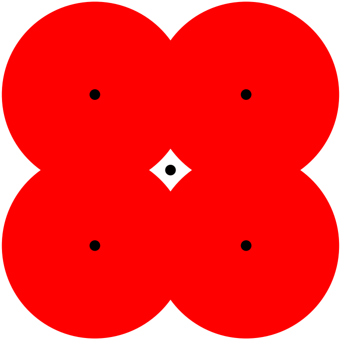

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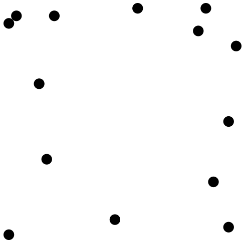

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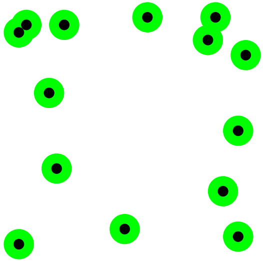

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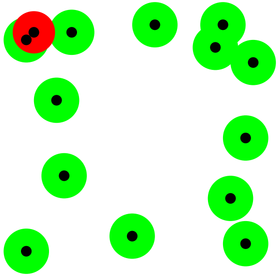

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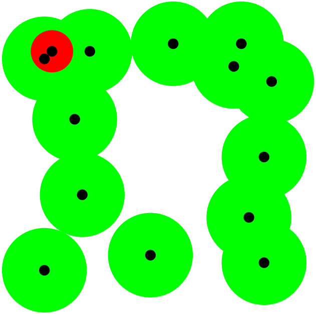

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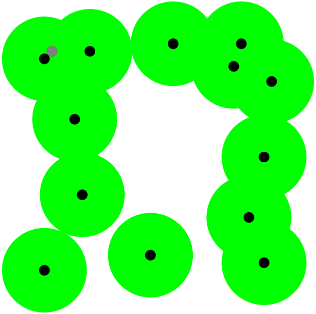

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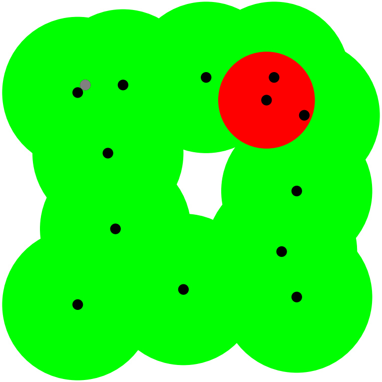

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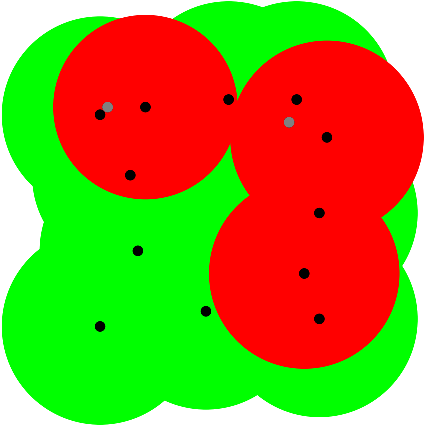

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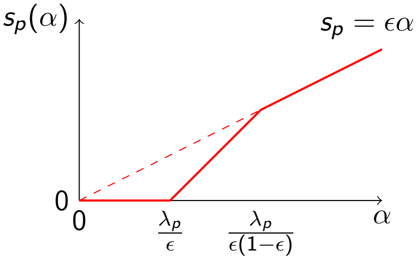
- Fix $\bar{N}_\gamma = \{p \in P | \lambda_p \geq \gamma\}$.
- Perturbed metric : $f_\alpha(p,q) = d_{\mathbb{X}}(p,q) + s_p(\alpha) + s_q(\alpha)$.



Construction (II)

Definition

The sparse Rips complex is given by:

$$Q_\alpha = \{\sigma \subset \bar{N}_{\epsilon(1-\epsilon)\alpha} | \forall p, q \in \sigma,\ f_\alpha(p, q) < 2\alpha\}$$

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Definition

The sparse Rips filtration is given by:

$$S_\beta = \bigcup_{\alpha \leq \beta} Q_\alpha.$$

Properties of sparse Rips

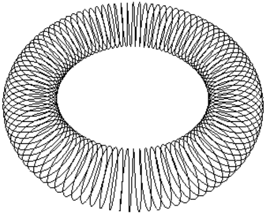
Theorem (Sheehy, 2012)

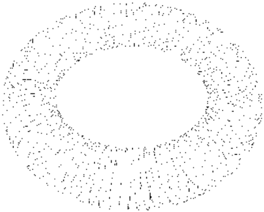
$\{S_\alpha\}$ contains $O(C^l n)$ simplexes where l is the intrinsic dimension of the underlying object.

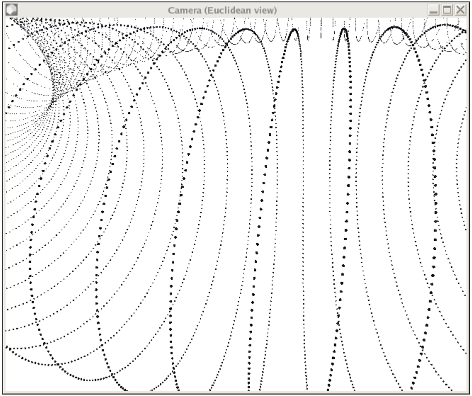
Theorem (Sheehy, 2012)

$\{S_\alpha\}$ is $\frac{1}{1-\epsilon}$-interleaved with the Rips filtration $\{R_\alpha\}$.

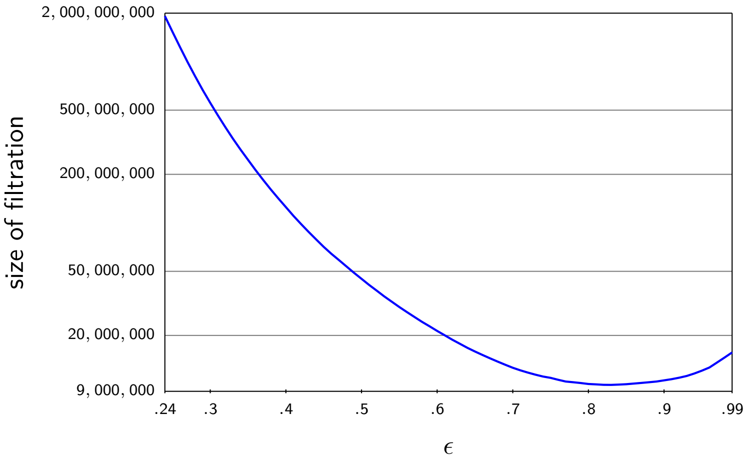
Spiral



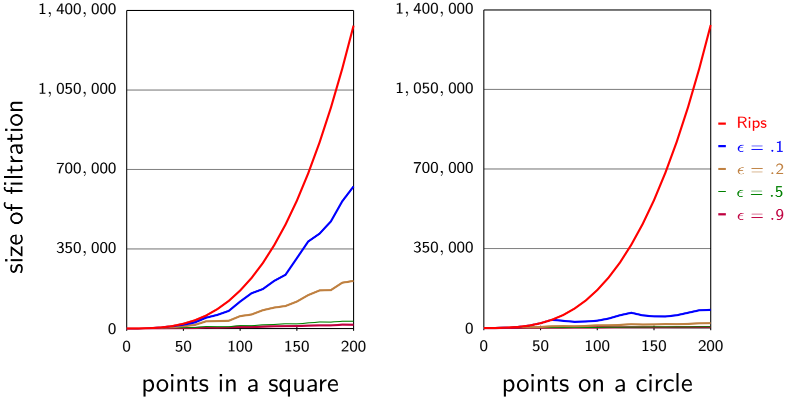




Size of the filtration depending on ϵ

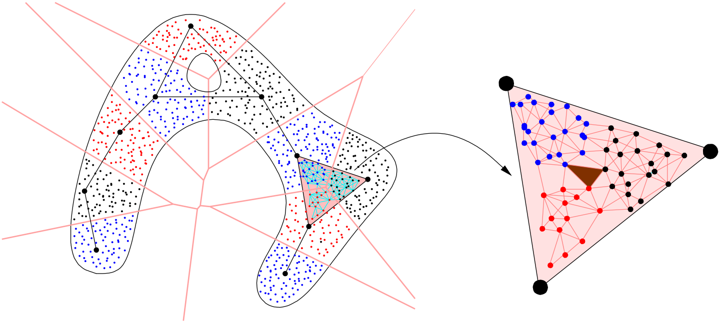


Intrinsic dimension influence



Graph induced complex (I)

Dey, Fan and Wang, 2013



Graph induced complex (II)

- Small construction with good guarantees and complexity for dimension 1.

Graph induced complex (II)

- Small construction with good guarantees and complexity for dimension 1.
- Extensions to higher dimesion needs more complex computations.

Pipeline

Point cloud

Pipeline

$$\text{Point cloud} \xrightarrow{\rotatebox{90}{d_K^{-1}}} \quad \text{Balls}$$

Pipeline

$$\text{Point cloud} \xrightarrow{d_K^{-1}} \text{Balls} \xrightarrow{\text{Nerve}} \text{Čech}$$

Pipeline

$$
\begin{tikzcd}
\text{Point cloud} \arrow[r, "d_K^{-1}"] & \text{Balls} \arrow[r, "\text{Nerve}"] & \text{Čech} \arrow[d, "\text{2-int}"] \\
& & \text{Rips}
\end{tikzcd}
$$

Pipeline

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\text{Point cloud} \arrow[r, "d_K^{-1}"] & \text{Balls} \arrow[r, "\text{Nerve}"] & \text{Čech} \arrow[d, "\text{2-int}"] \\
& \text{Sparse Rips} & \text{Rips} \arrow[l, "\frac{1}{1-\epsilon}\text{-int}"']
\end{tikzcd}$$

Pipeline

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\text{Point cloud} \arrow[r, "d_K^{-1}"] & \text{Balls} \arrow[r, "\text{Nerve}"] & \text{Čech} \arrow[d, "2\text{-int}"] \\
\text{Information} & \text{Sparse Rips} \arrow[l, "\text{Algorithm}"'] & \text{Rips} \arrow[l, "\frac{1}{1-\epsilon}\text{-int}"']
\end{tikzcd}$$

Pipeline

$$
\begin{tikzcd}
\text{Point cloud} \arrow[r, "d_K^{-1}"] \arrow[d, red] & \text{Balls} \arrow[r, "\text{Nerve}"] & \text{Čech} \arrow[d, "2\text{-int}"] \\
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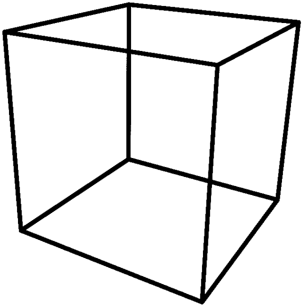
Outline

- Topological information
- Classical data structures
- Sparse data structures
- Handling noise and aberrant values
- Sparsification and parameter free analysis

Outliers (I)



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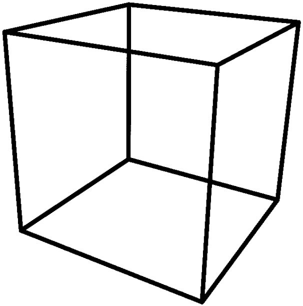
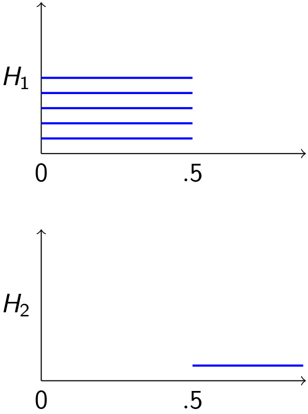
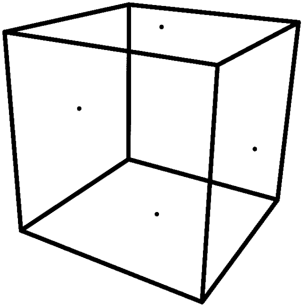
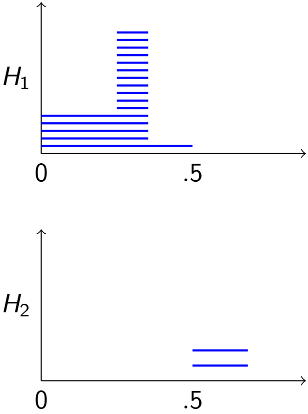




Outliers (II)





Distance to a measure

Definition (Chazal, Cohen-Steiner, Mérigot, 2011)

Let μ be a measure and $m \in]0, 1[$, then

$$d_{\mu,m}(x) = \frac{1}{\sqrt{m}} \inf_{\nu \in \mathrm{Sub}_m(\mu)} W_2(m\delta_x, \nu)$$

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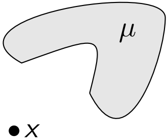

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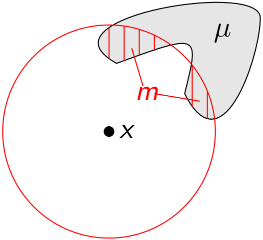


Case of an empirical measure

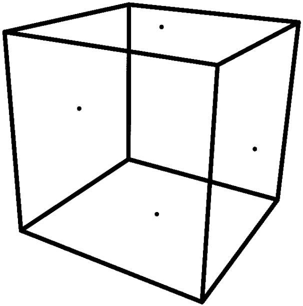
Proposition

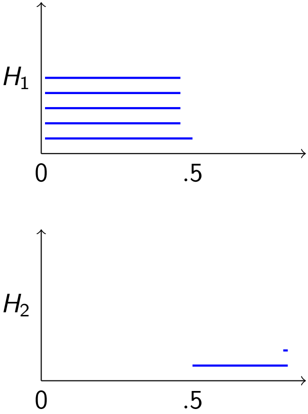
Let μ be the empirical on P and $k = m|P|$ is an integer then:

$$d_{\mu,m}(x) = \sqrt{\frac{1}{k}\sum_{i=1}^{k} d_{\mathbb{X}}(x, p_i(x))^2}$$

where $p_i(x)$ is the i^{th}-neighbour of x in P.

Results





Barycentric decomposition

Proposition

In Euclidean spaces, the distance to an empirical measure is a power distance.

Barycentric decomposition

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$$d_{\mu,m}(x)^2 = \frac{1}{k}\sum_{i=1}^{k} ||x - p_i(x)||^2$$

Barycentric decomposition

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\begin{aligned}
d_{\mu,m}(x)^2 &= \frac{1}{k}\sum_{i=1}^{k} ||x - p_i(x)||^2 \\
&= ||x - bar(x)||^2 + \frac{1}{k}\sum_{i=1}^{k} ||p_i(x) - bar(x)||^2
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where $bar(x) = \sum_{i=1}^{k} p_i(x)$

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&= ||x - bar(x)||^2 + w_{bar(x)}^2 \\
&= \min_{b\in B} \left(||x-b||^2 + w_b^2\right)
\end{aligned}
$$

where $bar(x) = \sum_{i=1}^{k} p_i(x)$ and B is the set of all barycentres of k points.

Power distances

Definition

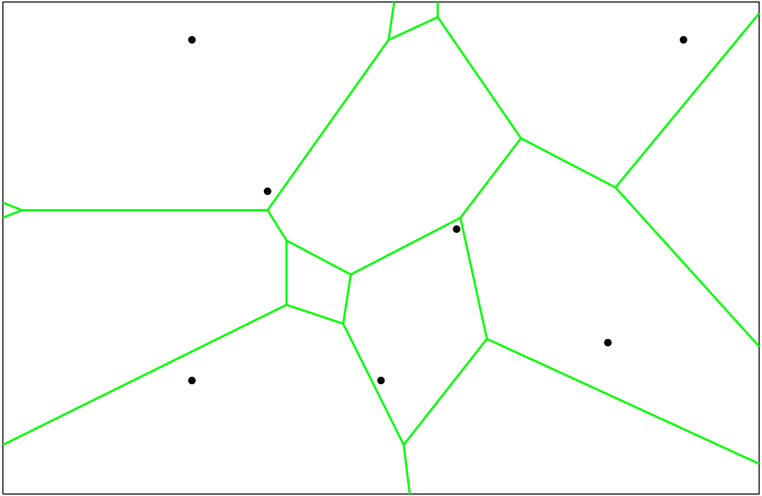
Let P be a point set and $w : P \to \mathbb{R}$ a weight function. The power distance associated with (P, w) is defined by:

$$f(x) = \sqrt{\min_{p \in P} ||x - p||^2 + w(p)^2}$$

Sub-level sets of a power distance f are unions of balls.

$$f^{-1}(]-\infty, \alpha]) = \bigcup_{p \in P} \bar{B}(p, \sqrt{\alpha^2 - w(p)^2})$$

k^{th}-order Voronoi diagram



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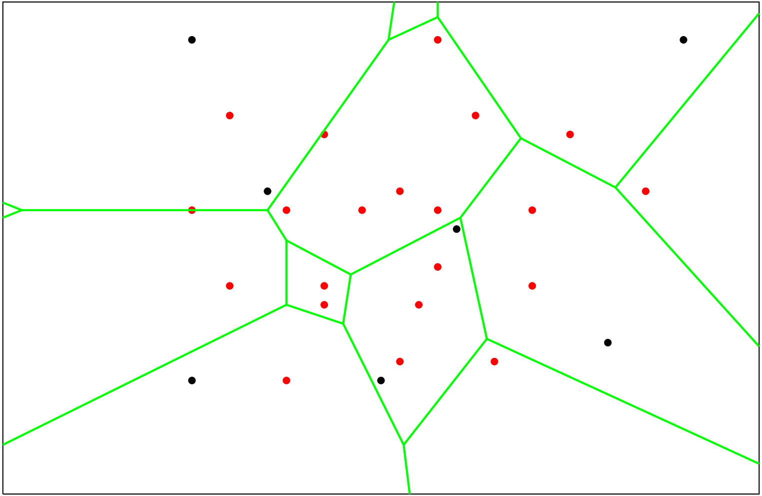

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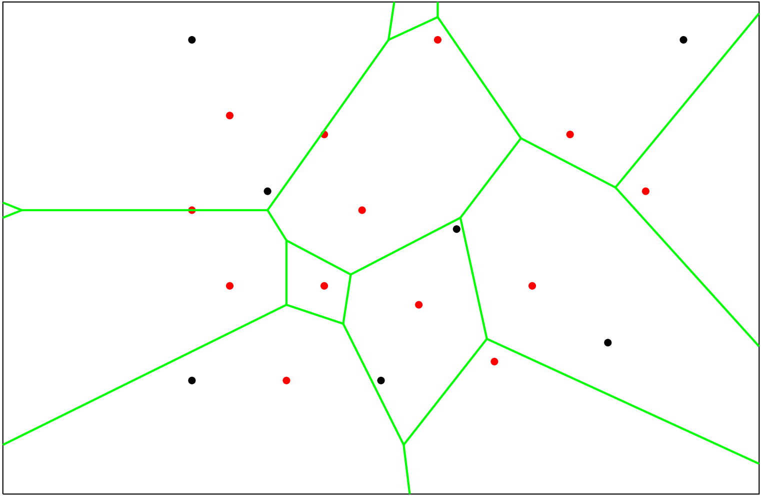

Size of k^{th}-order Voronoi diagram

Sub-level sets of $d_{\mu,m}$ are unions of balls.

$$d_{\mu,m}^{-1}(]-\infty,\alpha]) = \bigcup_{b\in B} \bar{B}(b, \sqrt{\alpha^2 - w_b^2})$$

Theorem (Clarkson, Shor, 1989)

The number of non-empty cells in Voronoi diagrams from order 1 to k is

$$O\left(n^{\lfloor \frac{d+1}{2} \rfloor} k^{\lceil \frac{d+1}{2} \rceil}\right).$$

Using the weighted metric

We used a weighted Rips filtration to compute the persistence diagram:

$$R_\alpha = \left\{ \sigma \subset P | \forall p, q \in P,\ d_{\mathbb{X}}(p,q) \leq \sqrt{\alpha^2 - w_p^2} + \sqrt{\alpha^2 - w_q^2} \right\}$$

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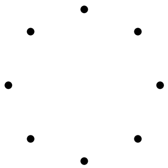

Adaptation to the weighted Rips

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Theorem (Buchet et al., 2015)

R_α and T_α are κ-interleaved where $\kappa = 1 + \frac{\sqrt{1+t^2}\epsilon}{1-\epsilon}$, id est :

$$\begin{tikzcd}
R_\alpha \arrow[r, hook] & R_{\kappa\alpha} \\
T_\alpha \arrow[u, hook] \arrow[ur, hook] \arrow[r, hook] & T_{\kappa\alpha} \arrow[u, hook]
\end{tikzcd}
\qquad\qquad
\begin{tikzcd}
R_\alpha \arrow[r, hook] \arrow[dr, "\pi_{\frac{\alpha}{1-\epsilon}}"] & R_{\kappa\alpha} \\
T_\alpha \arrow[u, hook] \arrow[r, hook] & T_{\kappa\alpha} \arrow[u, hook]
\end{tikzcd}$$

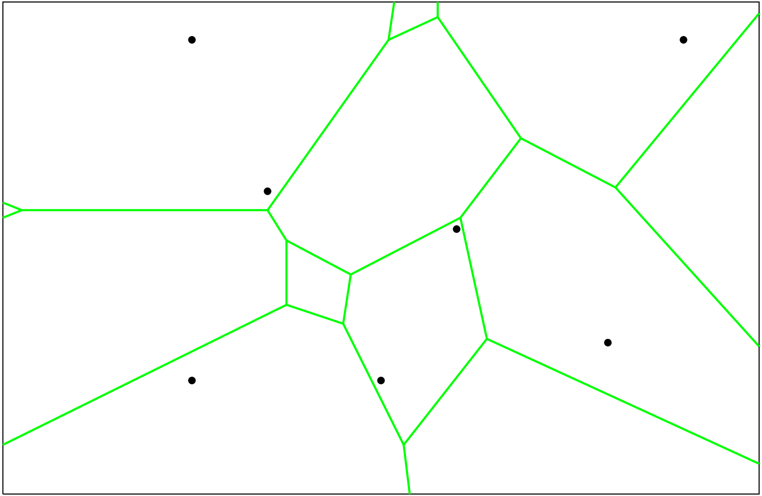
Witnessed k-distance

Approximation by sampling barycentres.

Definition (Guibas, Mérigot, Morozov, 2011)

$$d^W_{\mu,m}(x) = \min_{p \in P} \sqrt{||x - bar(p)||^2 + w^2_{bar(p)}}$$

Building the witnessed k-distance



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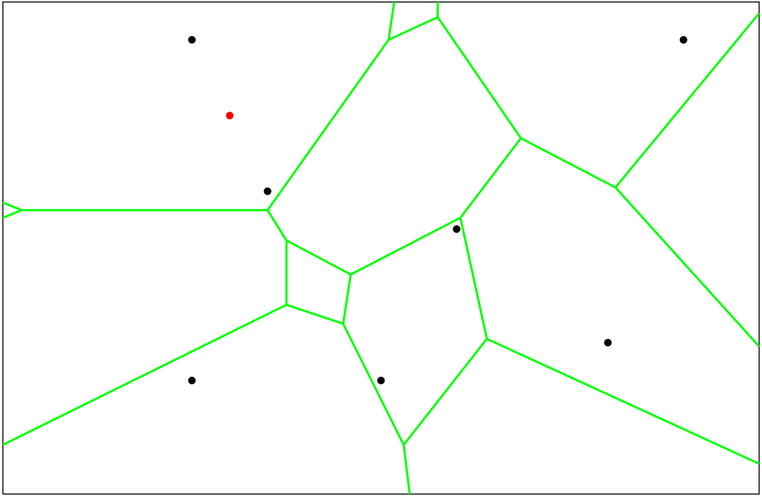

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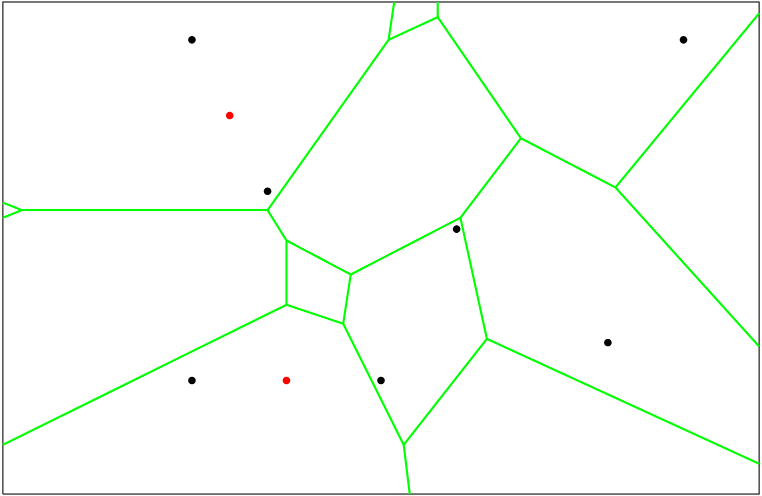

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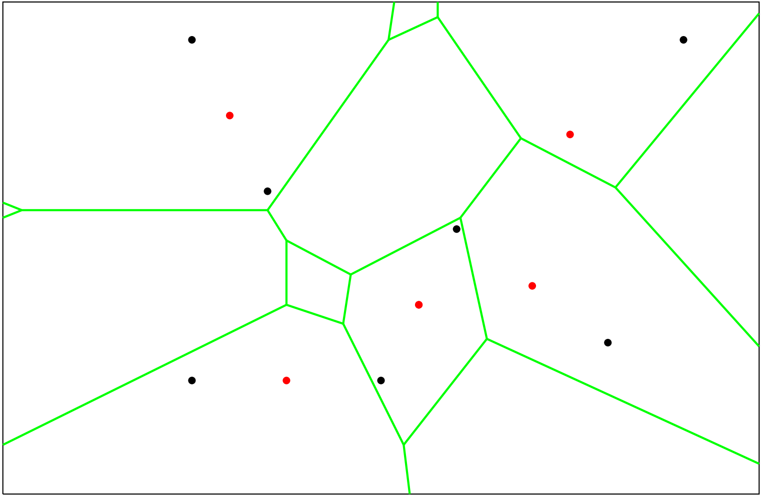

Guarantees of the witnessed k-distance

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Theorem (GMM, 2011; Buchet et al., 2015)

$$d_{\mu,m} \leq d^W_{\mu,m} \leq \sqrt{6} d_{\mu,m}$$

Approximation supported by the points

Using a power distance supported by input points.

Definition (Buchet et al., 2015)

$$d^P_{\mu,m}(x) = \min_{p \in P} \sqrt{d_{\mathbb{X}}(x,p)^2 + d_{\mu,m}(p)^2}$$

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$$d_{\mu,m}^{P}(x) = \min_{p \in P} \sqrt{d_{\mathbb{X}}(x,p)^2 + d_{\mu,m}(p)^2}$$

Theorem (Buchet et al., 2015)

In Euclidean space:

$$\frac{1}{\sqrt{2}} d_{\mu,m} \leq d_{\mu,m}^{P} \leq \sqrt{3} d_{\mu,m}$$

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Theorem (Buchet et al., 2015)

In Euclidean space:

$$\frac{1}{\sqrt{2}} d_{\mu,m} \leq d^P_{\mu,m} \leq \sqrt{3} d_{\mu,m}$$

In any metric space:

$$\frac{1}{\sqrt{2}} d_{\mu,m} \leq d^P_{\mu,m} \leq \sqrt{5} d_{\mu,m}$$

All these bounds are tight.

Pipeline

Point cloud

Pipeline

Point cloud $\xrightarrow{{d^{P}_{\mu,m}}^{-1}}$ Balls

Pipeline

$$\text{Point cloud} \xrightarrow{{d^P_{\mu,m}}^{-1}} \text{Balls} \xrightarrow{\text{Nerve}} \text{w. Čech}$$

Pipeline

$$
\begin{tikzcd}
\text{Point cloud} \arrow[r, "{d_{\mu,m}^{P}}^{-1}"] & \text{Balls} \arrow[r, "\text{Nerve}"] & \text{w. Čech} \arrow[d, "\text{2-int}"] \\
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\end{tikzcd}
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Parameter free analysis

Is it possible to obtain a good analysis in an (almost) parameter-free mehod?

Parameter free analysis

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Yes, if we have a good sampling.

Good samplings for the distance to a measure

We assume that we have a point cloud P describing an underlying compact set K in a metric space $\mathbb{X}$. Given a mass parameter m, what is a "good" sampling to use the distance to a measure?

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The (ϵ, r) sampling.

1. $\forall x \in K,\ d_{\mu,m}(x) \leq \epsilon.$

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The (ϵ, r) sampling.

1. $\forall x \in K,\ d_{\mu,m}(x) \leq \epsilon.$
2. $\forall y \in \mathbb{X},\ d_K(y) \leq r \implies d_K(y) \leq d_{\mu,m}(y) + \epsilon.$

Good samplings for the distance to a measure

We assume that we have a point cloud P describing an underlying compact set K in a metric space $\mathbb{X}$. Given a mass parameter m, what is a "good" sampling to use the distance to a measure?

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Good samplings for the distance to a measure

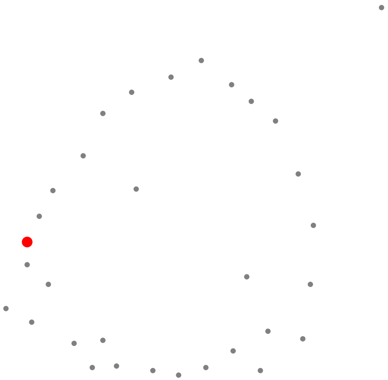
We assume that we have a point cloud P describing an underlying compact set K in a metric space $\mathbb{X}$. Given a mass parameter m, what is a "good" sampling to use the distance to a measure?

The (ϵ, r, c) uniform sampling.

1. $\forall x \in K,\ d_{\mu,m}(x) \leq \epsilon.$
2. $\forall y \in \mathbb{X},\ d_K(y) \leq d_{\mu,m}(y) + \epsilon.$
3. $\forall p \in P,\ d_{\mu,m}(p) \geq \frac{\epsilon}{c}.$

Decimation

Decimation



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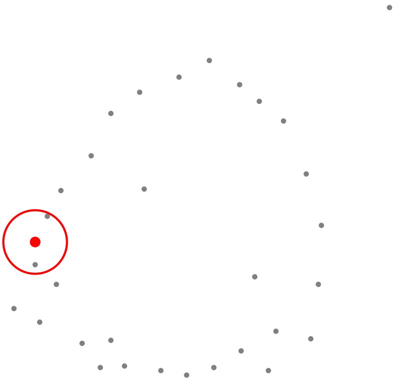

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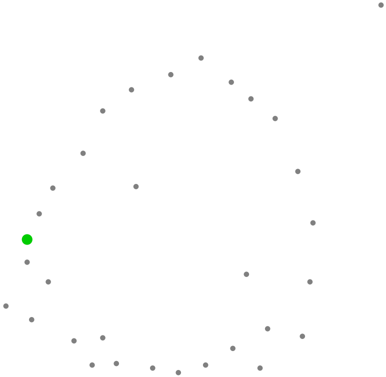

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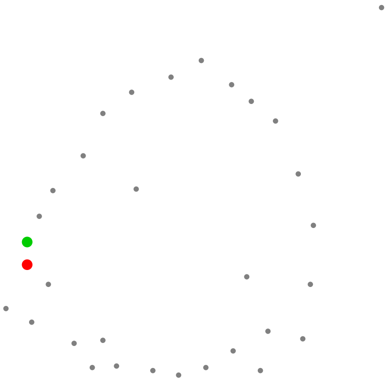

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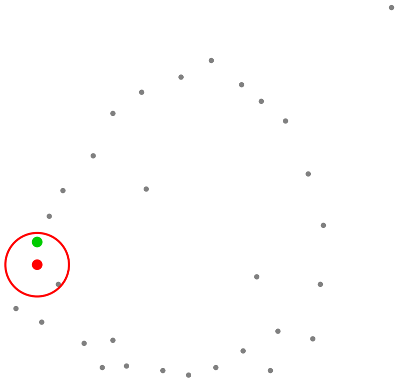
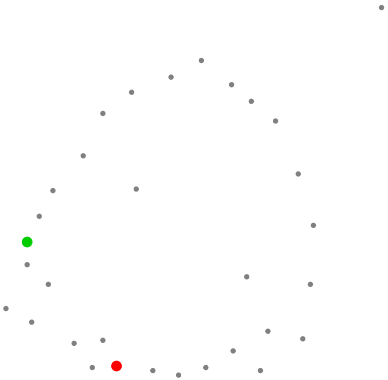
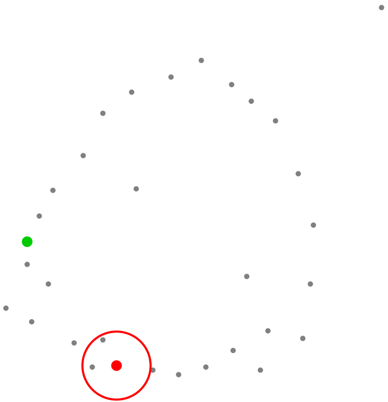


Decimation



Decimation



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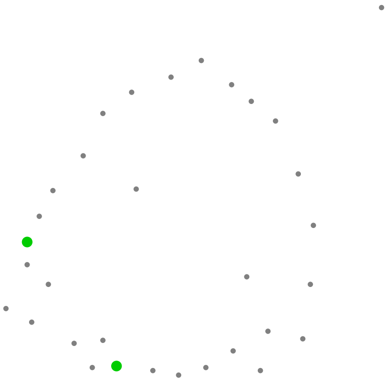

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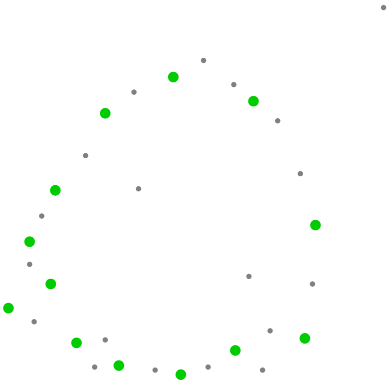

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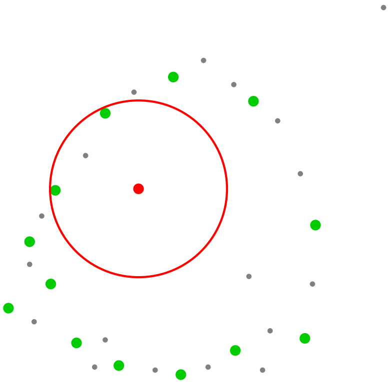
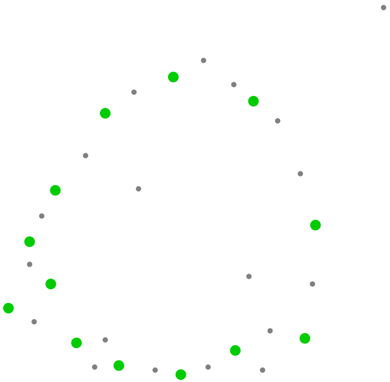


Decimation



Algorithm

1. $Q_0 = \emptyset$
2. Sort P according to increasing distance to the empirical measure.
3. For i from 1 to $n = |P|$, if $B(p_i, 2d_{\mu,m}(p_i)) \cap Q_{i-1} = \emptyset$:
    - then $Q_i = Q_{i-1} \cup p_i$
    - else $Q_i = Q_{i-1}$.

Guarantees

Theorem

If P is an (ϵ, ∞) sampling of K then:

$$d_H(Q_n, K) \leq 7\epsilon.$$

Theorem

If P is an (ϵ, ∞) uniform sampling of $K \subset \mathbb{R}^d$, with $\epsilon < \frac{1}{28}\mathrm{wfs}(K)$. Then for all α, $\alpha' \in [7\epsilon, \mathrm{wfs}(K) - 7\epsilon]$ such that $\alpha' - \alpha > 14\epsilon$ and for all $\lambda \in (0, \mathrm{wfs}(K))$, we have

$$H_*(X^\lambda) \cong H_*(C_\alpha(Q_n) \hookrightarrow C_{\alpha'}(Q_n)).$$

Adaptive setting

We assume that a feature size function f exists on K which is 1-Lipschitz. The sampling conditions become, for an (ϵ, ∞, c) uniform sampling.

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3. $\forall p \in P,\ d_{\mu,m}(p) \geq \frac{\epsilon}{c} f(\bar{p})$.

Adaptive guarantees

Theorem

Given an input point P which is an (ϵ, ∞) adaptive sample of a compact K with $\epsilon \leq \frac{1}{2}$, our algorithm returns a 7ϵ Hausdorff adaptive sampling of K.

Id est:

$$\forall x \in K,\ \exists q \in Q_n,\ d_{\mathbb{X}}(x,q) \leq 7\epsilon f(x)$$

$$\forall q \in Q_n,\ \exists x \in K,\ d_{\mathbb{X}}(x,q) \leq 7\epsilon f(\bar{q})$$

Theorem

Given a set L and the feature function $f = d_L$, we consider an (ϵ, ∞, c)-uniform adaptive sample P of K. If $c \leq 2$, $\epsilon \leq \frac{1}{396}$ and $G_{\frac{1}{3}} \cap M_{\frac{\pi}{4}} = \emptyset$ then for any sufficiently small $\beta > 0$, $H_*(d_K^{-1}([0,\beta])) \cong H_*(B_{.032} \hookrightarrow B_{15.6})$.

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- Aberrant noise can be handled using the distance to a measure.
- The distance to a measure is compatible with classical data structures.
- Classical data structures have sparse approximations usable in practice.
- Noisy data set can be sparsified with guarantees given only one parameter.

References

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