DSC 214
Topological Data Analysis
Topic 6: Homology inference, denoising, data sparsification

Instructor: Zhengchao Wan

Today

- Homology inference
- Handling of noise
- Data sparsification

Section 1:
Topology inference from PCD and manifolds

- Input:
  - A set of points $P \subseteq R^d$ sampled on/around X
- Question:
  - How to approximate the persistence module induced by F_X ?

Target filtration (F_X): $X^{r_0} \subseteq X^r \subseteq \cdots X^r \subseteq \cdots$

Intermediate filtration: $P^{r_0} \subseteq P^{r_1} \subseteq \cdots P^r \subseteq \cdots$

$\cong$ By Nerve Lemma

Čech filtration ($\mathscr{C}_X$): $C^{r_0} \subseteq C^{r_1} \subseteq \cdots C^r \subseteq \cdots$

Two sequence interleave

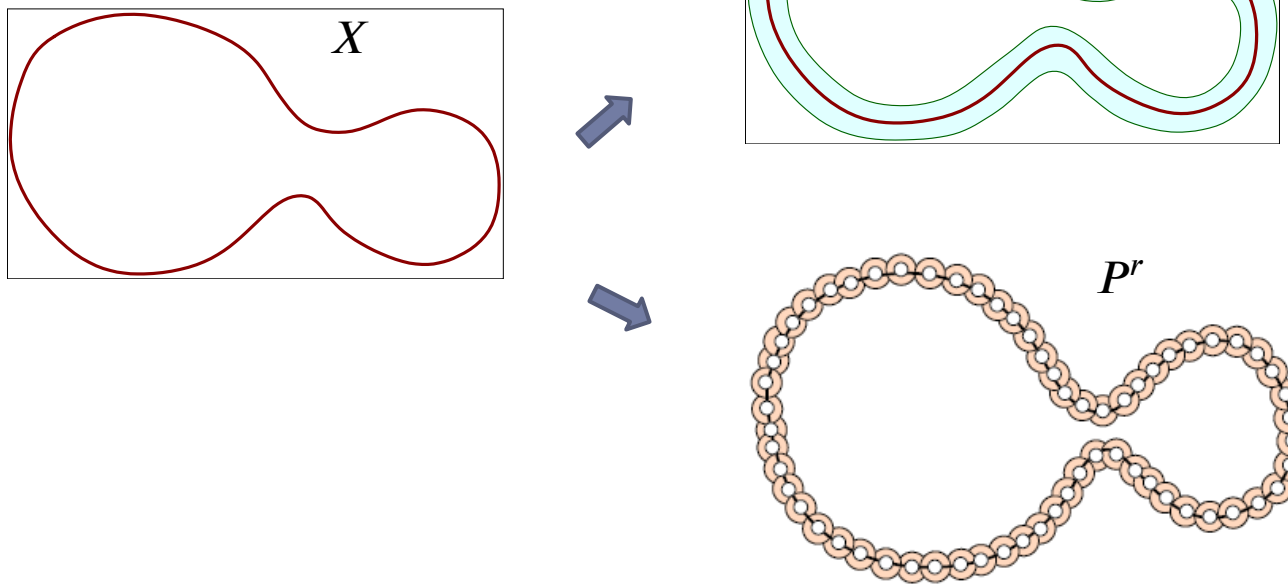
Rips filtration ($\mathscr{R}_X$): $R^{r_0} \subseteq R^{r_1} \subseteq \cdots R^r \subseteq \cdots$

Hausdorff distance between subsets

- If $P \subseteq X$ satisfies that $d_H(P, X) = \inf\{r : X \subseteq P^r\} < \epsilon$

Target filtration (F_X): $X^{r_0} \subseteq X^{r_1} \subseteq \cdots X^r \subseteq \cdots$

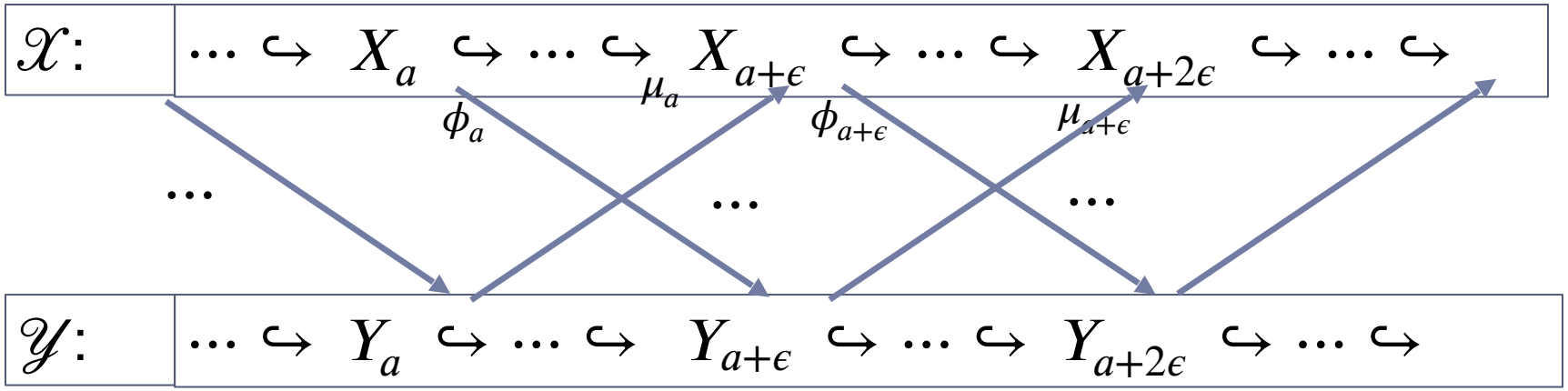
Intermediate filtration: $P^{r_0} \subseteq P^{r_1} \subseteq \cdots P^r \subseteq \cdots$



- Note that
  - $P^r \subset X^{r+\epsilon}$
  - $X^r \subset P^{r+\epsilon}$
- So $d_I(P, F_X) \leq \epsilon$

Recall: Interleaving filtrations

- Given two filtrations $\mathcal{X}$ and $\mathcal{Y}$ ϵ-interleaves if the following diagram commutes.



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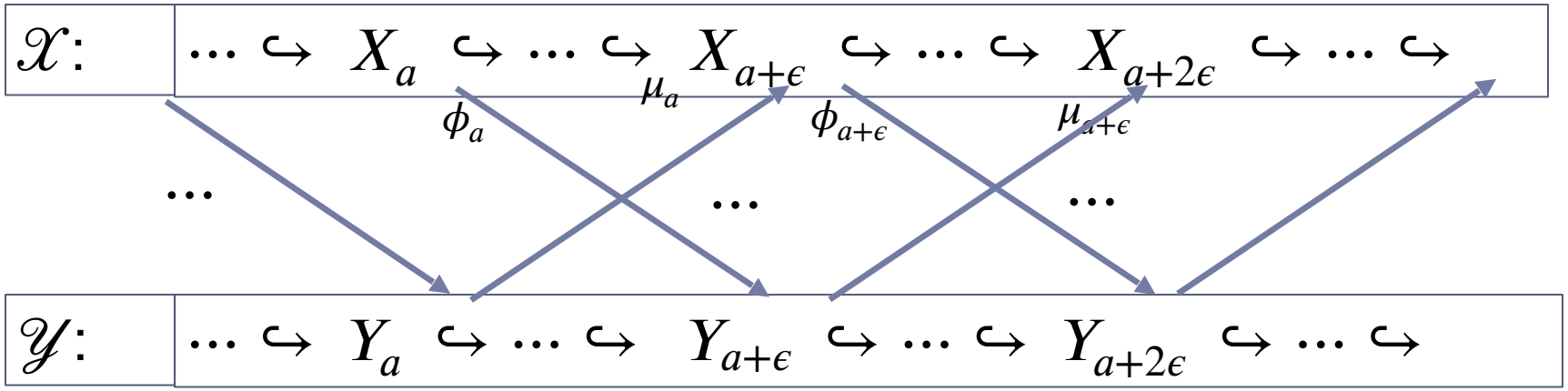


Theorem

Given two ϵ-interleaved filtrations $\mathcal{X}$ and $\mathcal{Y}$, let D_X and D_X be the corresponding persistence diagrams induced by them. We then have:

$$d_B(D_X, D_Y) \leq \epsilon$$

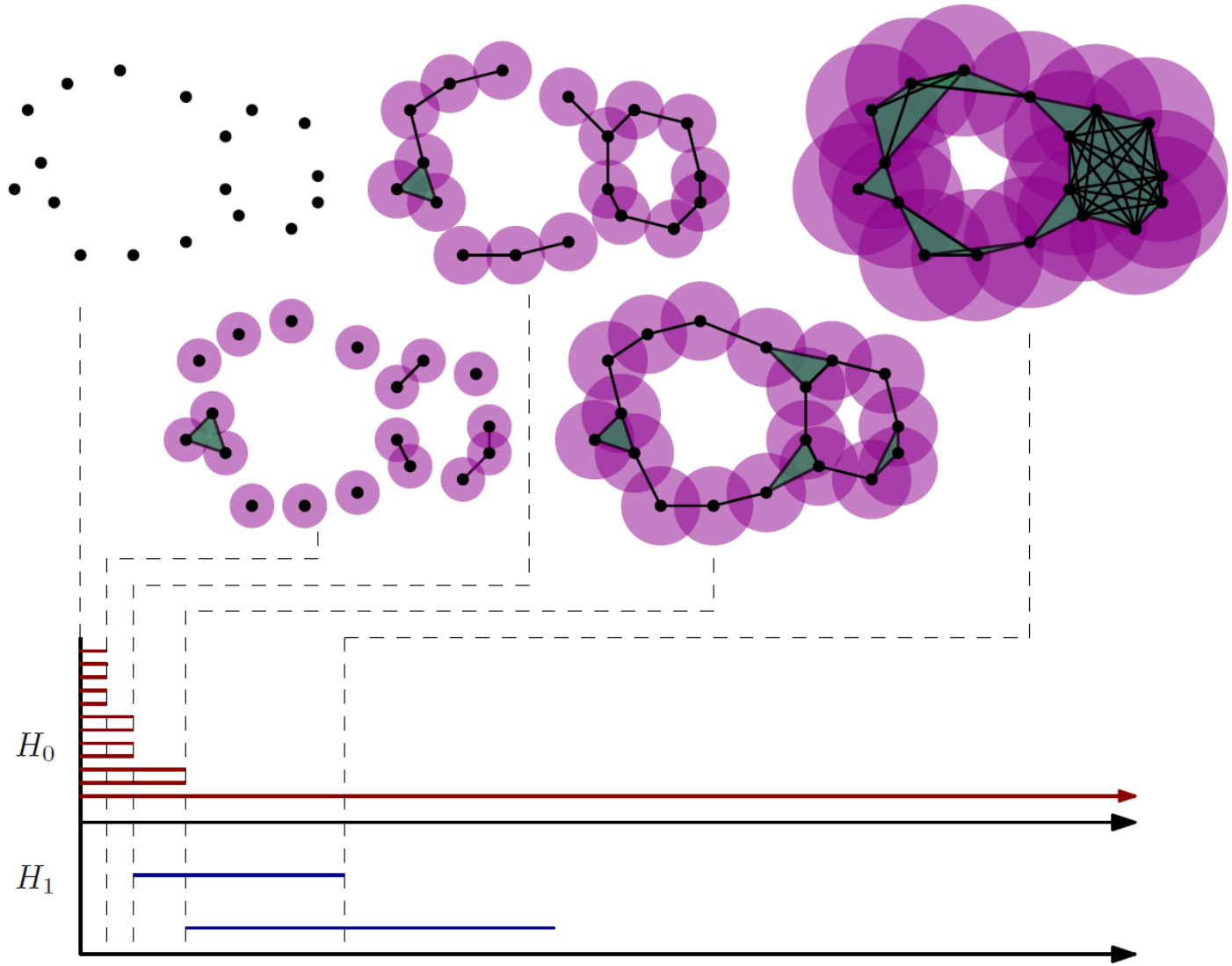
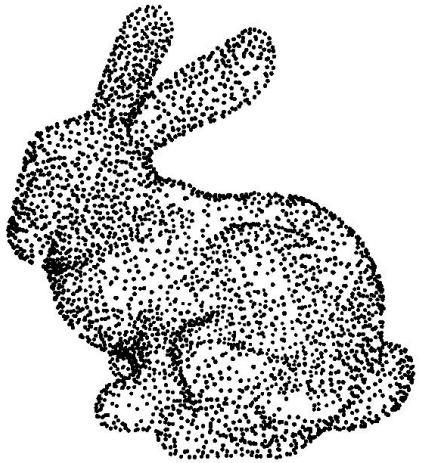


Image courtesy of T. K. Dey



Unorganized PCD

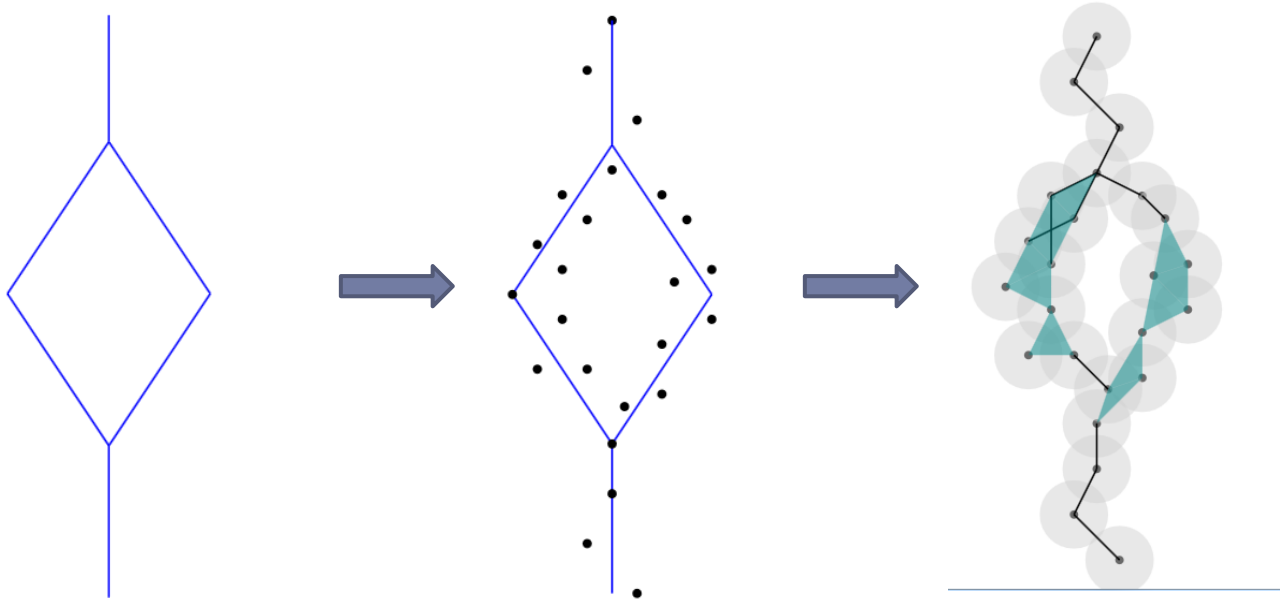
?

Topological summary of hidden space

- Input:
  - A set of points $P \subseteq R^d$ sampled on/around X
- Question:
  - How well we approximate the homology of X

- We will be a little more precise on how well we can approximate these topological quantities today.

Pipeline



- PCD —> simplicial complex —> homology estimation
- What follows:
  - Sampling conditions
  - Inference guarantees

Sampling Conditions

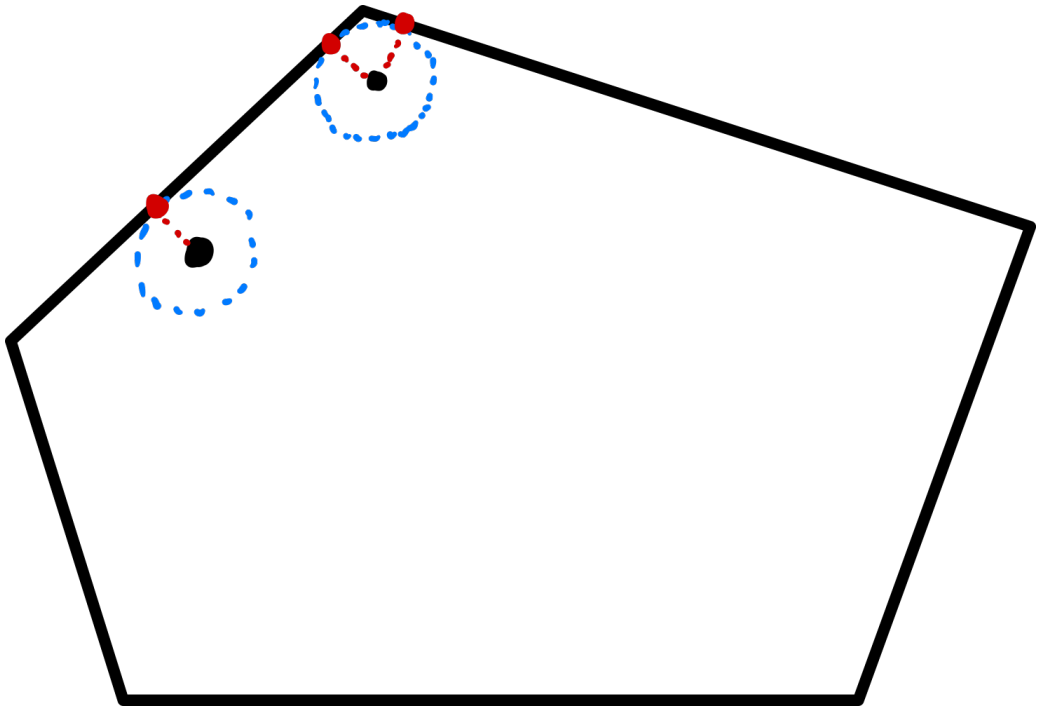
Motivation

- Theoretical guarantees are usually obtained when input points P sampling the hidden domain "well enough".

- Need to quantify the "wellness".
- Two common ones based on:
  - Local feature size (for smooth manifolds)
  - Weak feature size (for general compact subspace of $\mathbb{R}^d$)

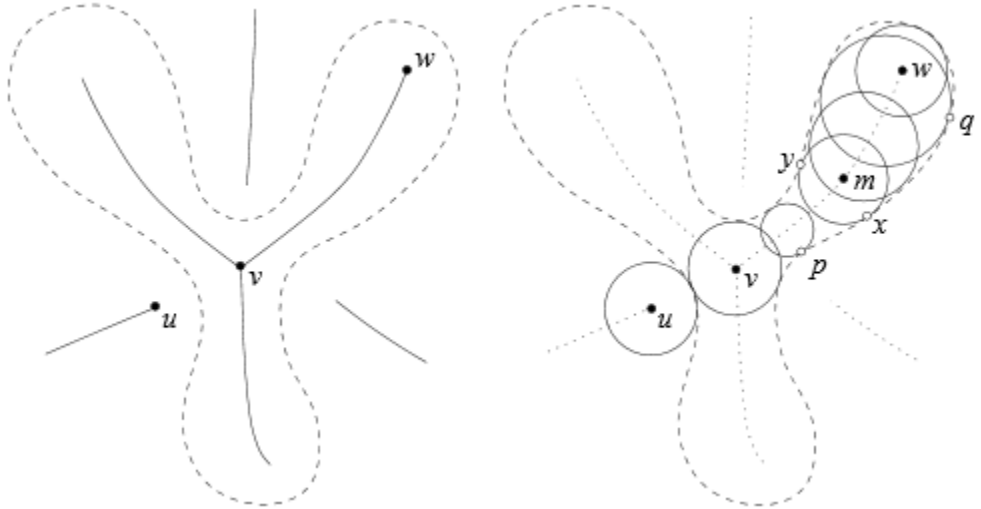
Distance Function

- $X \subset \mathbb{R}^d$: a compact subset of $\mathbb{R}^d$
- Distance function to set $d_X : \mathbb{R}^d \to [0,\infty)$
  - $d_X(x) = \min_{y \in X} d(x, y)$
  - d_X is a 1-Lipschitz function
- X^α: α-offset of X
  - $X^\alpha = \{y \in \mathbb{R}^d \mid d_X(y) \leq \alpha\}$
  - X^α is the sub level set $d_X^{-1}((-\infty, \alpha])$ of d_X
- Given any point $x \in \mathbb{R}^d$
  - $\Gamma(x) := \{\ y \in X \mid d(x,\ y) = d_X(x)\ \}$



Medial Axis

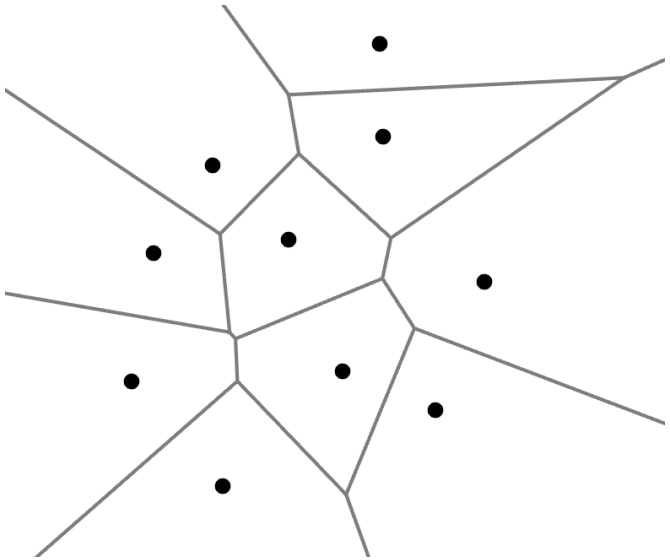
- The *medial axis* Σ of X is the closure of the set of points $x \in \mathbb{R}^d$ such that $\left|\Gamma(x)\right| \geq 2$
  - $\left|\Gamma(x)\right| \geq 2$ means that there is a medial ball $B_r(x)$ touching X at more than 1 point and whose interior is empty of points from X.



Courtesy of [Dey, 2006]

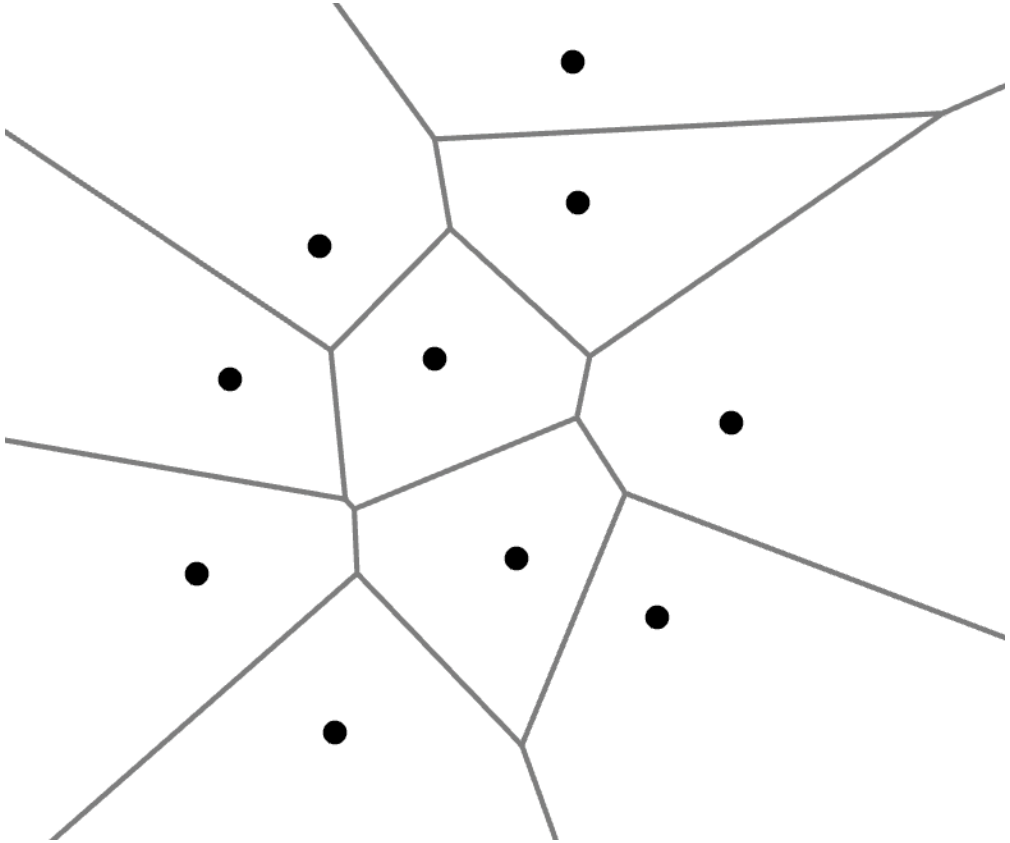
Voronoi Diagram

- Given a finite set $P = \{p_1, \ldots, p_n\} \subset \mathbb{R}^d$, the **Voronoi cell** of p_i is
  - $Vor(p_i) = \{x \in \mathbb{R}^d \,|\, \|x - p_i\| \leq \|x - p_j\|, \forall j \neq i\}$
- The **Voronoi Diagram** of P is the collection of all Voronoi cells.



Medial Axis vs Voronoi Diagram

- When X is a finite set of points. Then, the medial axis agrees with the boundary of Voronoi cells.

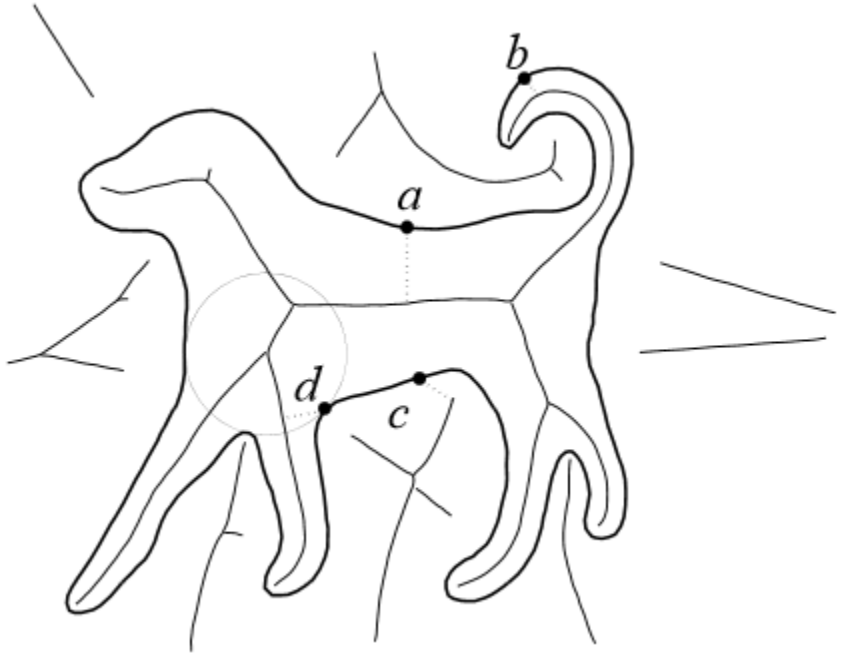


Local Feature Size

- The local feature size $lfs(x)$ at a point $x \in X$ is the distance of x to the medial axis Σ of X
  - That is, $lfs(x) = d(x, \Sigma)$

- This concept is adaptive
  - Large in a place without "features"
- Intuitively:
  - We should sample more densely if local feature size is small.

- The *reach* $\rho(X) = \inf_{x \in X} lfs(x)$



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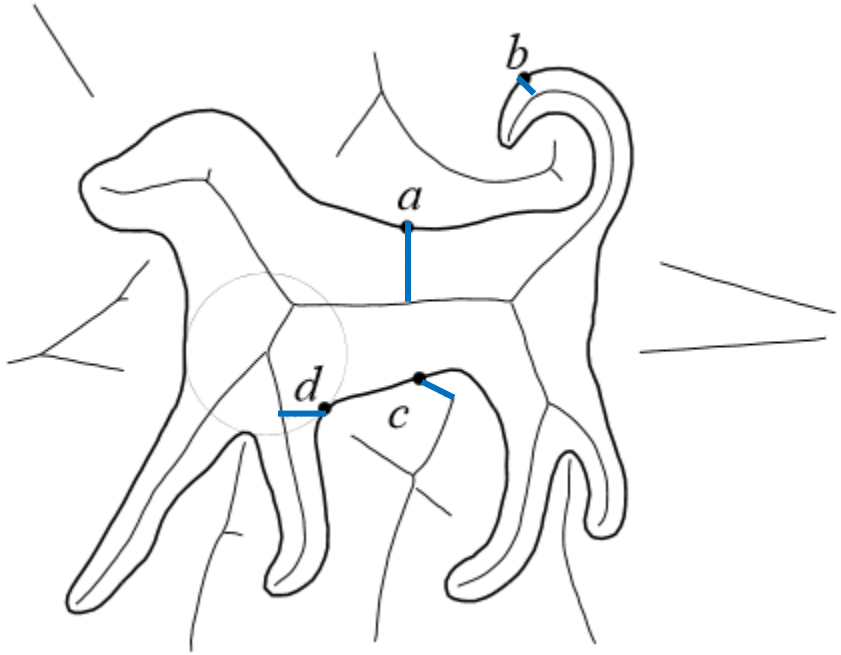


Courtesy of [Dey, 2006]

Smooth Manifold Case

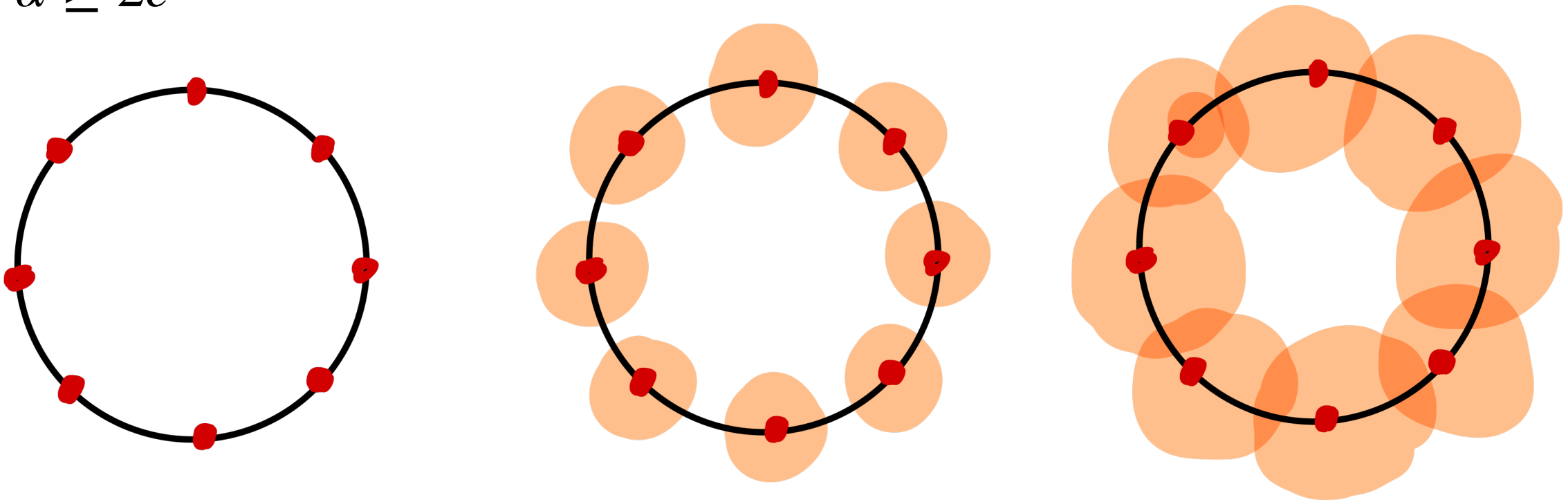
- Let X be a smooth manifold embedded in R^d

Theorem [Niyogi, Smale, Weinberger]

Let $P \subset X$ be such that $d_H(X, P) \leq \epsilon$. If $2\epsilon \leq \alpha \leq \sqrt{\frac{3}{5}}\rho(X)$, there is a deformation retraction from P^α to X .

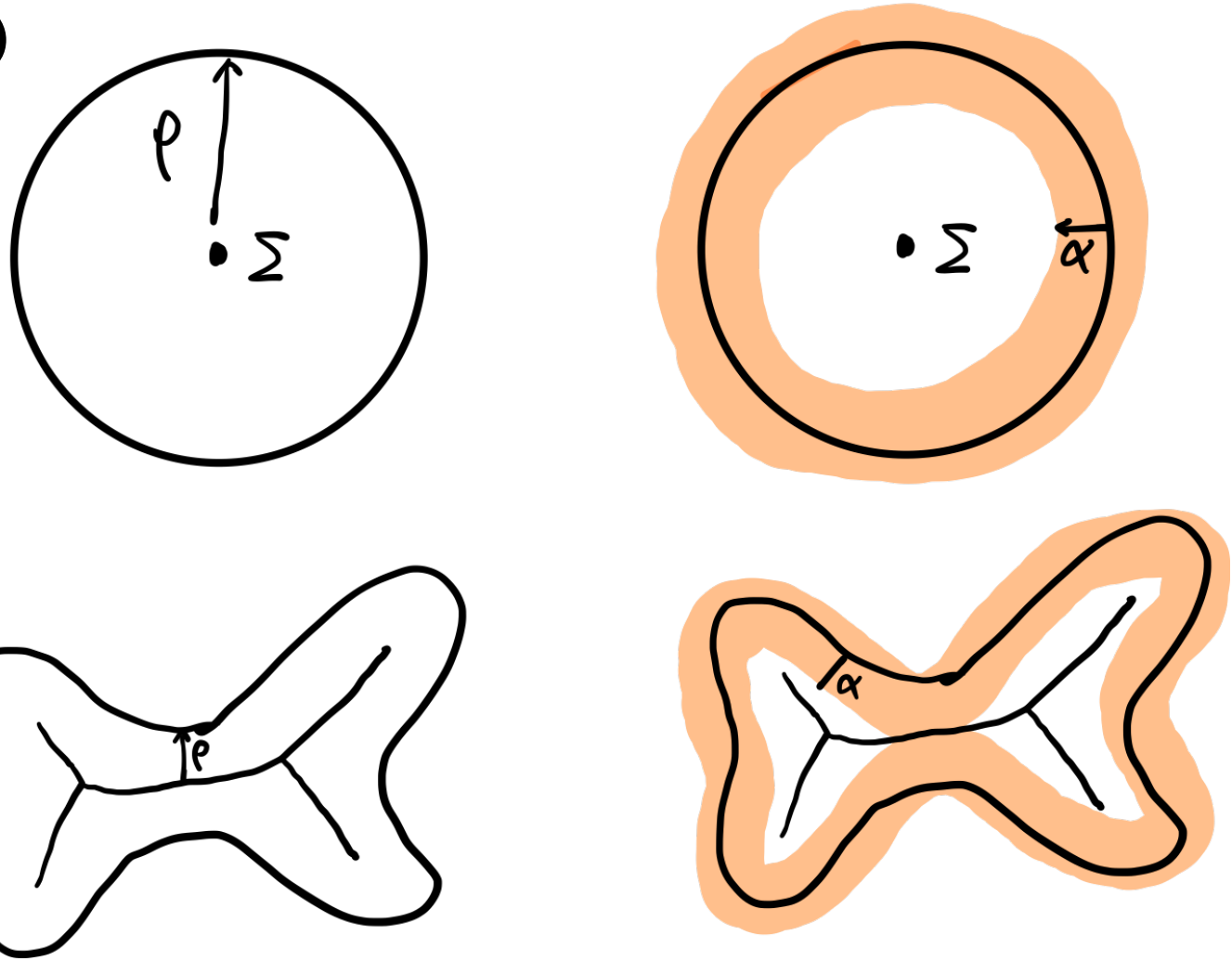
Interpretation

- $\alpha \geq 2\epsilon$

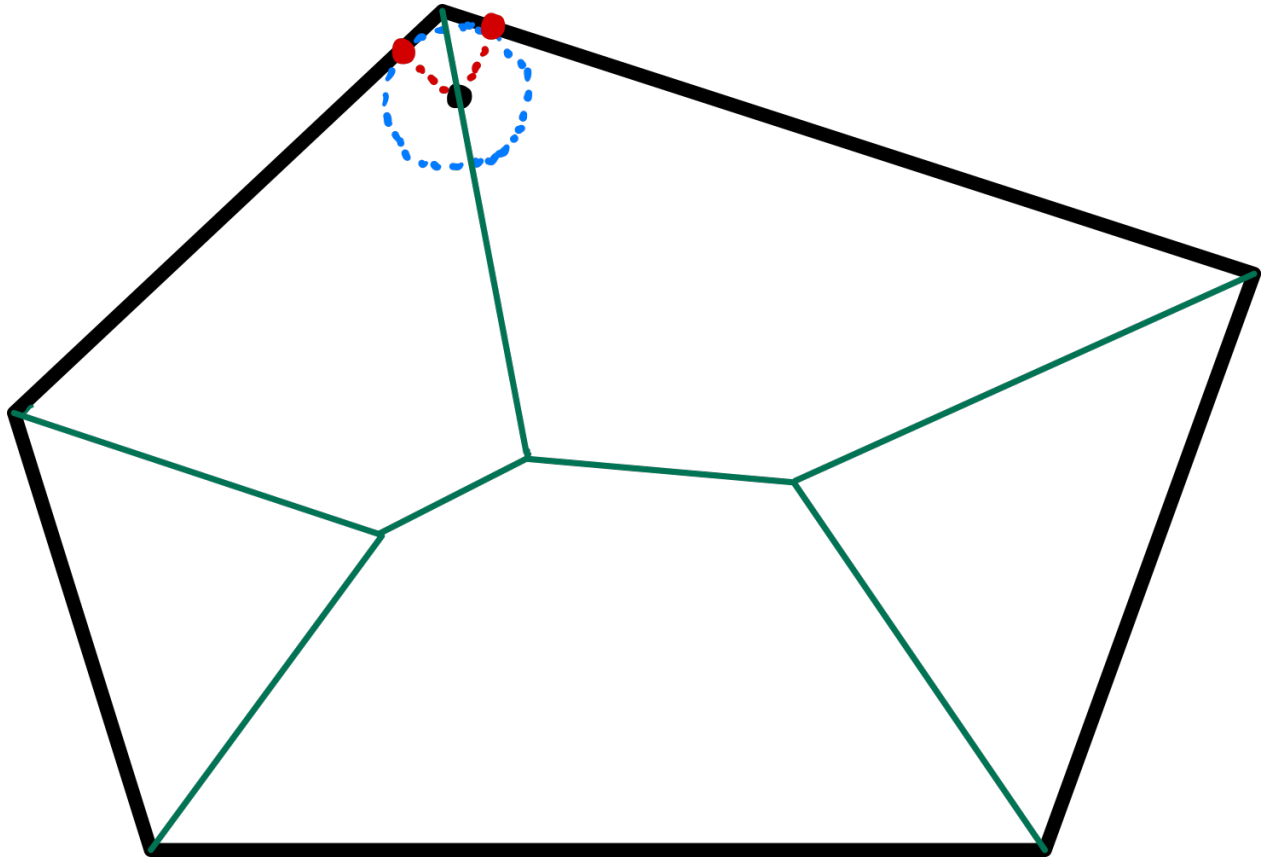


Interpretation

- $\alpha \leq \sqrt{\frac{3}{5}}\rho(X)$

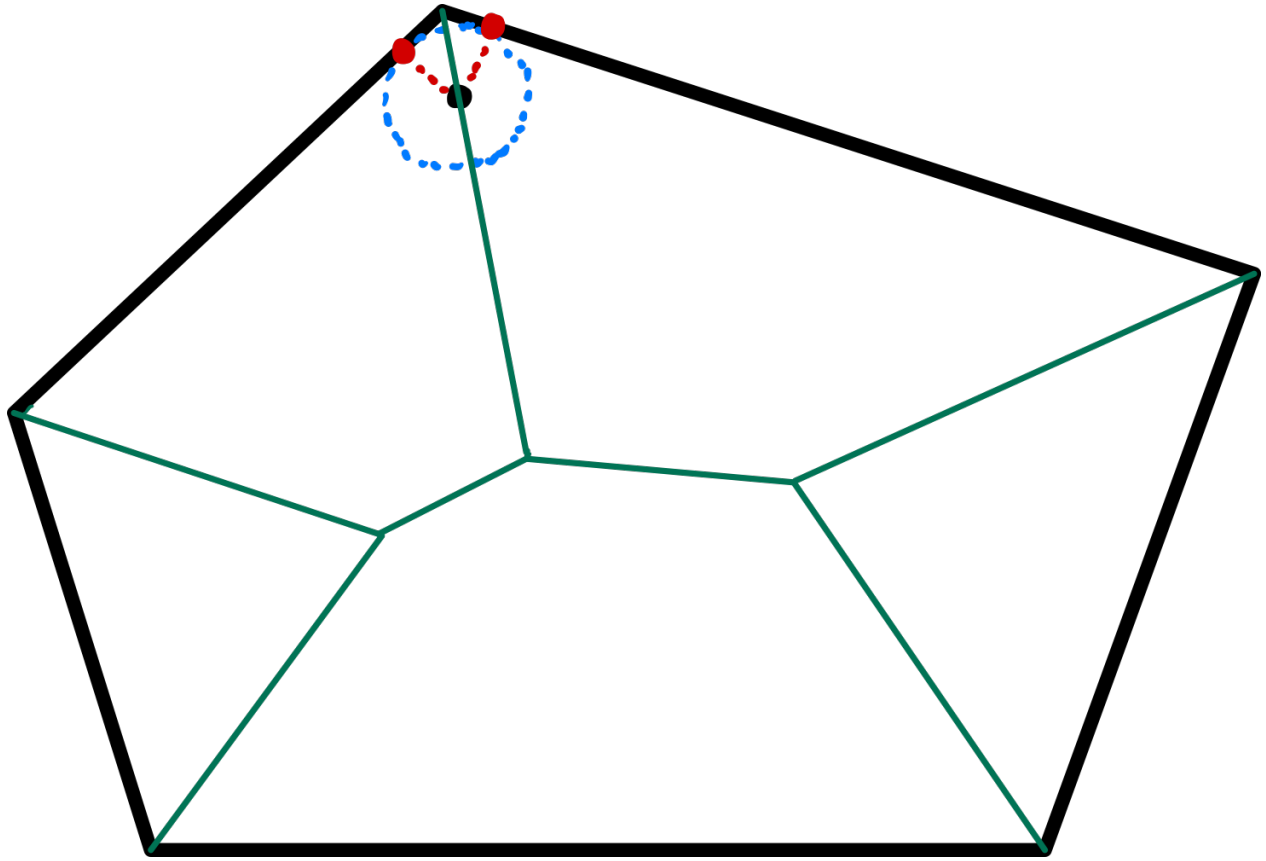


Non-smooth case



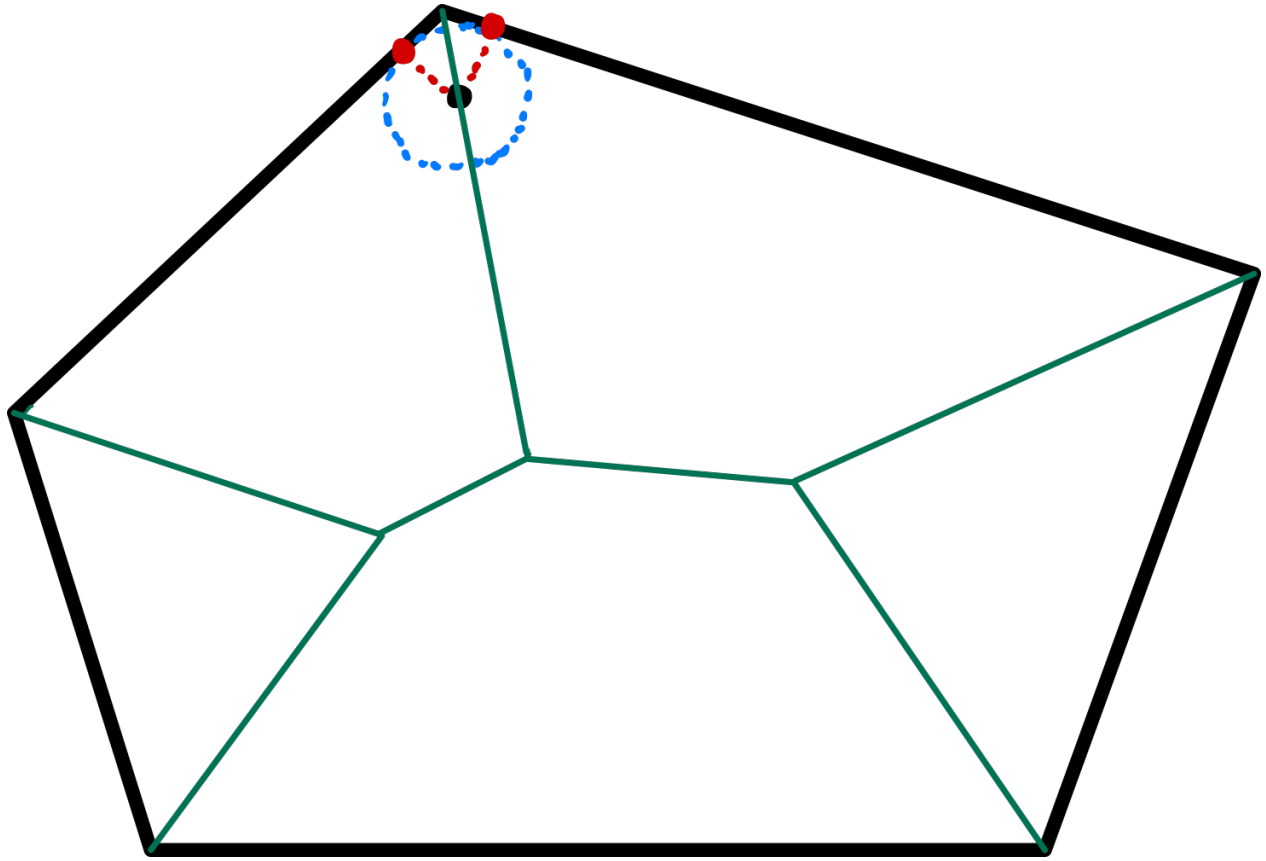
Non-smooth case

- $\rho(X)$ can be 0 for non-smooth shapes



Non-smooth case

- $\rho(X)$ can be 0 for non-smooth shapes
- It is then not suitable for general compact spaces



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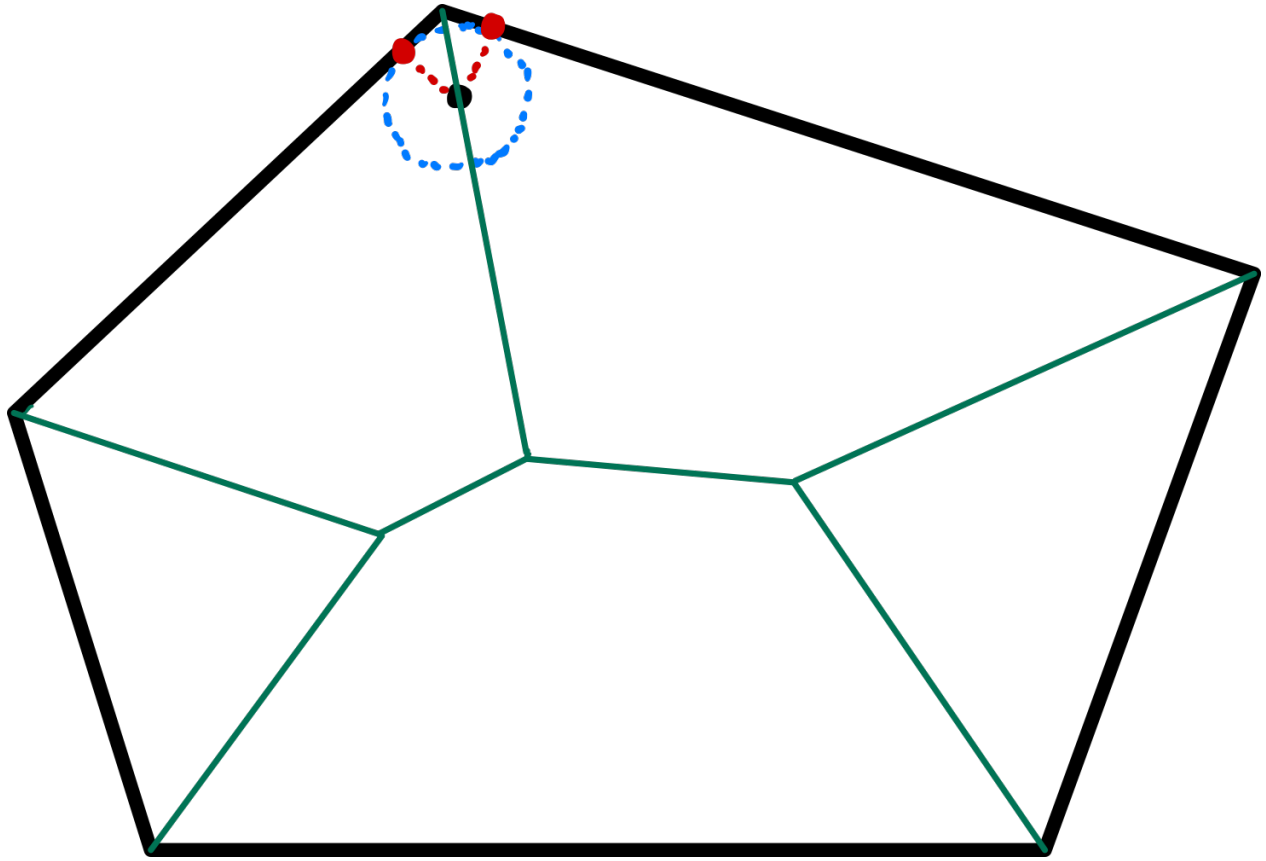

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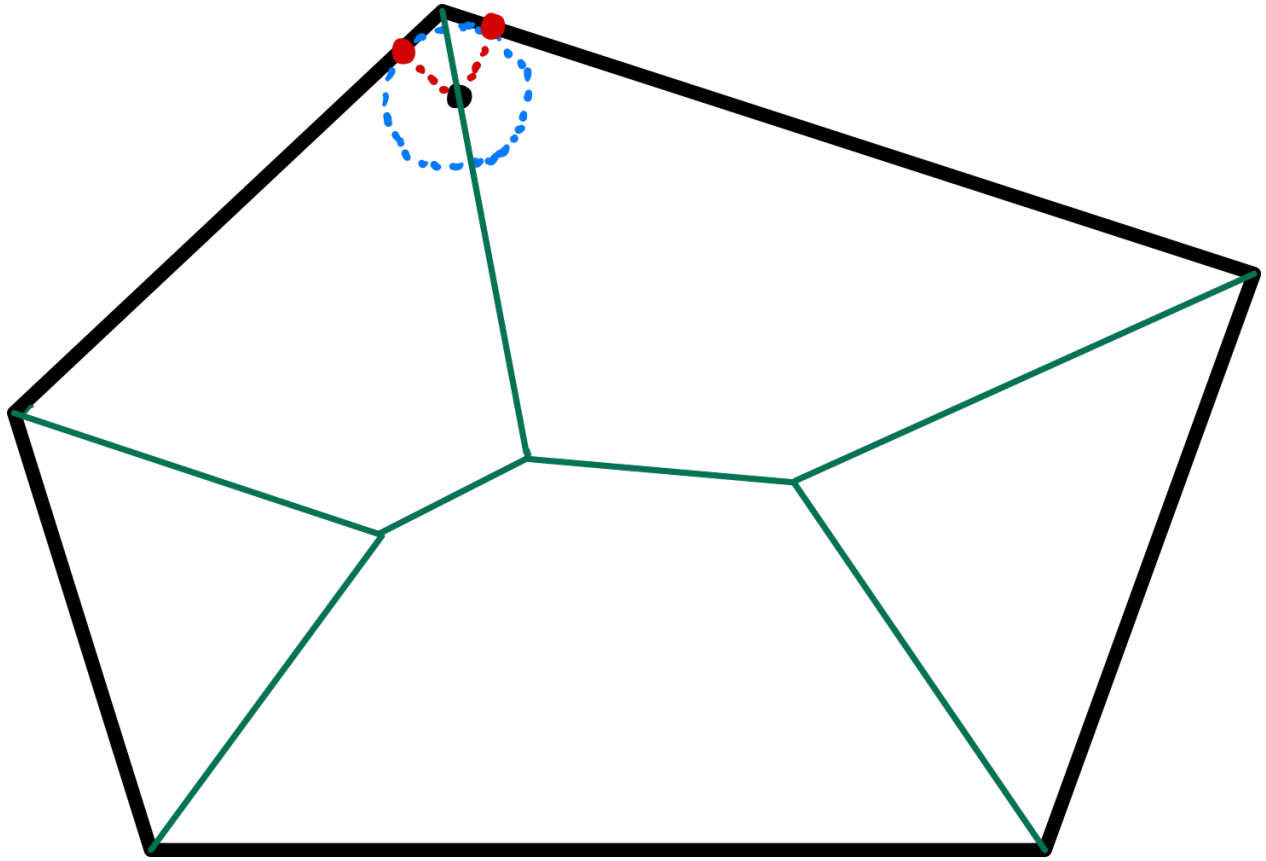
- We are interested in topological changes of $d_X^{-1}((-\infty, \alpha])$
- This reminds us about Morse theory



Recall: Morse theory

Theorem 3 (Homotopy type of sub-level sets). *Let $f : M \to \mathbb{R}$ be a smooth function defined on a manifold M. Given $a < b$, suppose the interval-level set $M_{[a,b]} = f^{-1}([a, b])$ is compact and contains no critical points of f. Then $M_{\leq a}$ is diffeomorphic to $M_{\leq b}$.*

Furthermore, $M_{\leq a}$ is a deformation retract of $M_{\leq b}$, and the inclusion map $i : M_{\leq a} \hookrightarrow M_{\leq b}$ is a homotopy equivalence.

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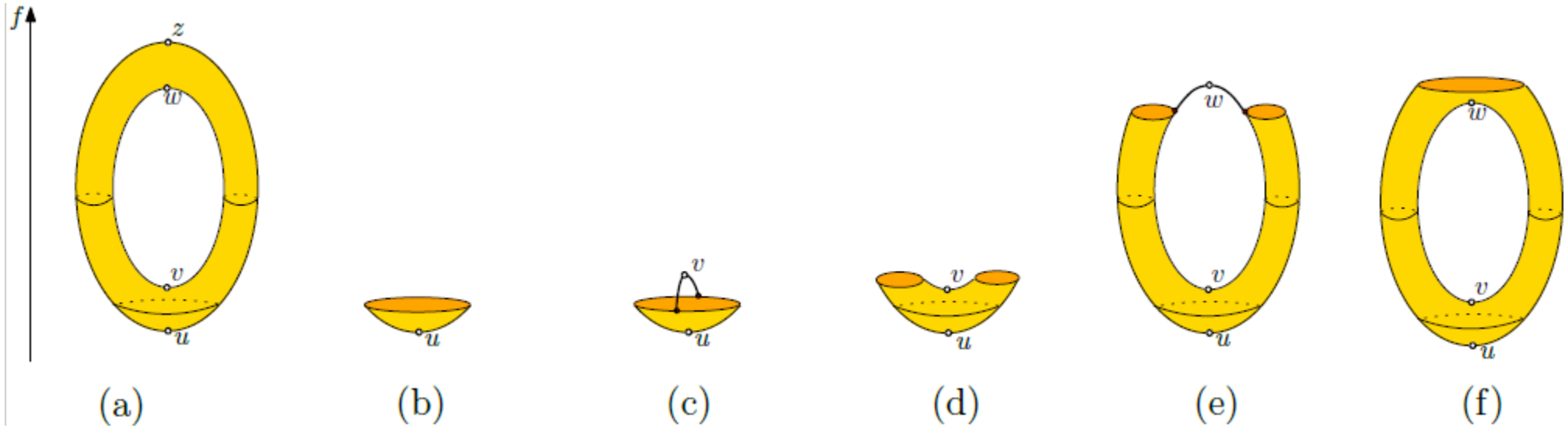

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Theorem 4. *Given a Morse function $f : M \to \mathbb{R}$ defined on a smooth manifold M, let p be an index-k critical point of f with $\alpha = f(p)$. Assume $f^{-1}([\alpha - \varepsilon, \alpha + \varepsilon])$ is compact for a sufficiently small $\varepsilon > 0$ such that there is no other critical points of f contained in this interval-level set other than p. Then the sublevel set $M_{\leq \alpha+\varepsilon}$ has the same homotopy type as $M_{\leq \alpha-\varepsilon}$ with a k-cell attached to its boundary* $\mathrm{Bd}\, M_{\leq \alpha-\varepsilon}$.

Animation

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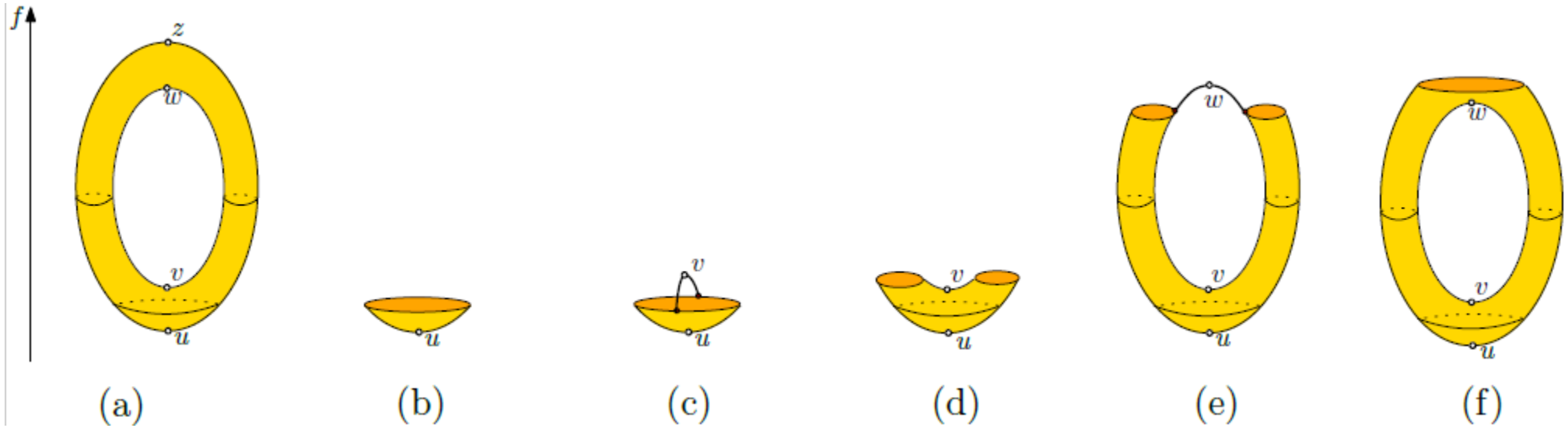
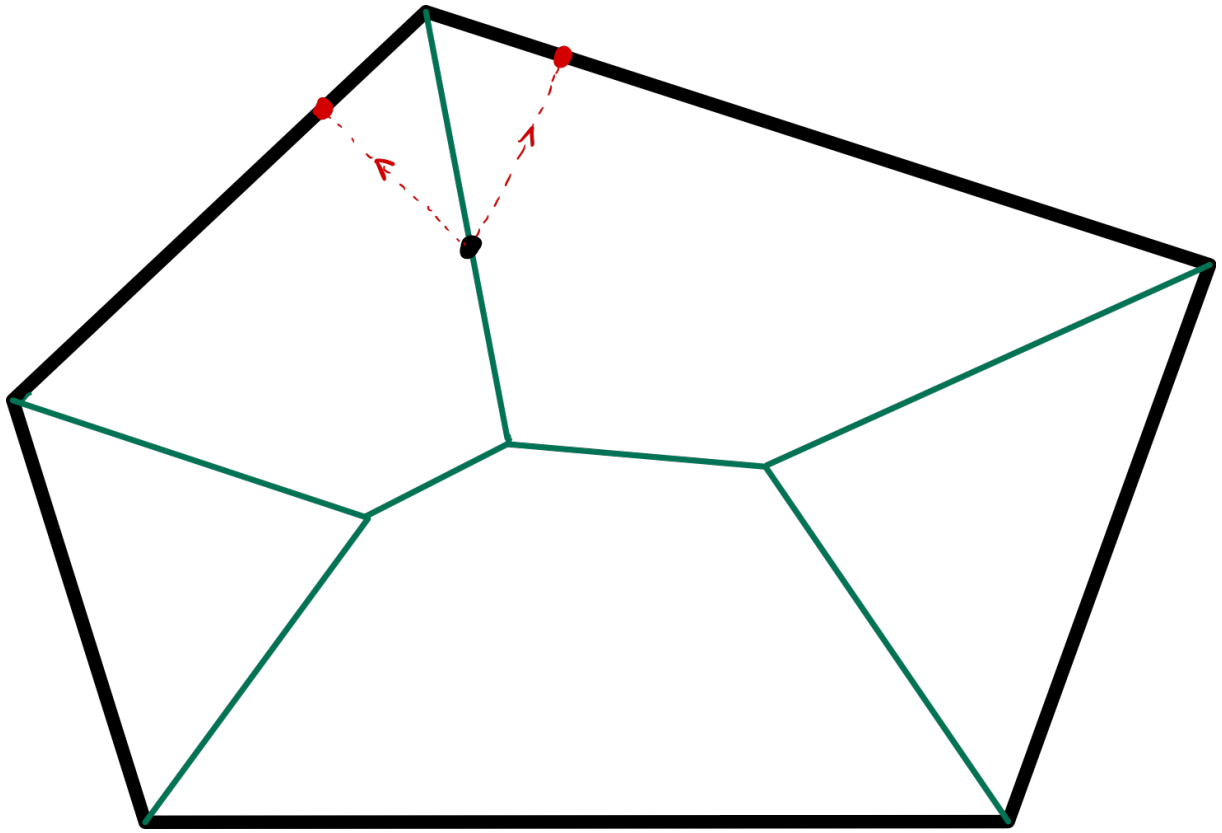


Animation

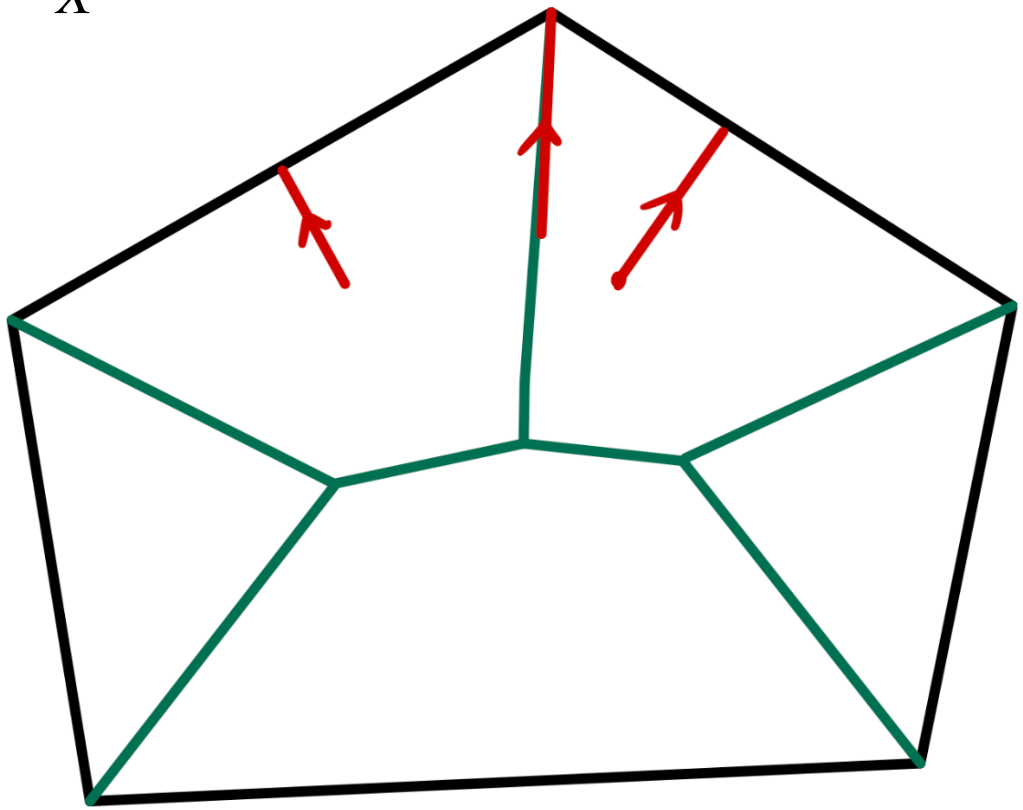
Morse theory for distance function?

- Distance function d_X not differentiable on $\Sigma \cup X$



Gradient of Distance Function

- Can we take the average of different directions for points in Σ to define gradient of d_X?

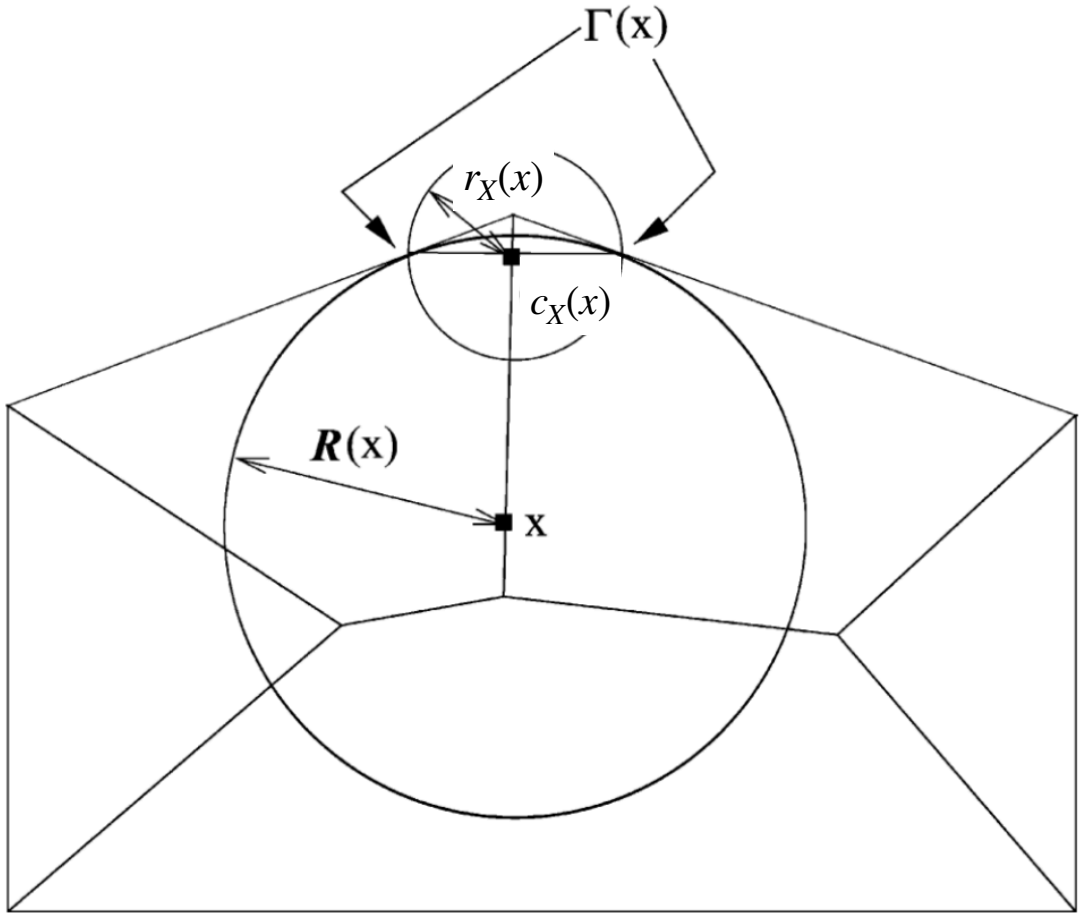


Gradient of Distance Function

- Distance function not differentiable on the $\Sigma \cup X$
- Still can define a generalized concept of gradient
  - *[Grove'93] [Lieutier, 2004]*
- For $x \in \mathbb{R}^d \backslash X$,
  - Let $c_X(x)$ and $r_X(x)$ be the center and radius of the smallest enclosing ball of point(s) in $\Gamma(x)$
  - The *generalized gradient* of distance function

$$\nabla_X(x) = \frac{x - c_X(x)}{d_X(x)}$$

- Flow lines induced by the generalized gradient



Courtesy of Lieutier 2004

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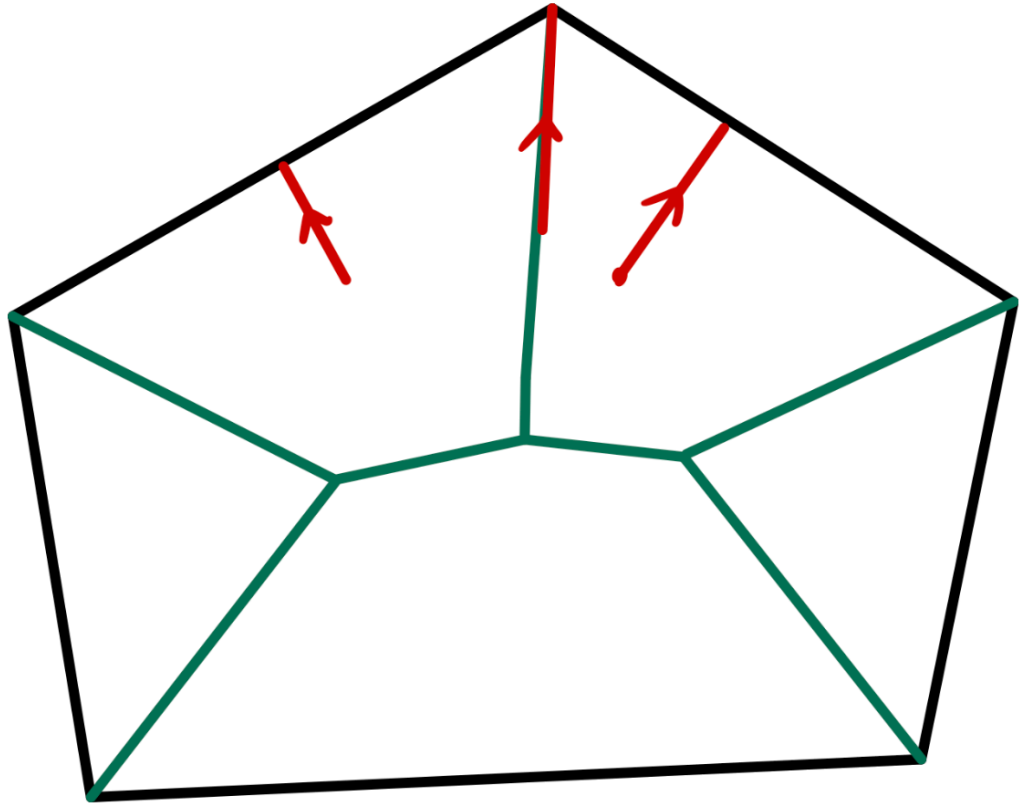
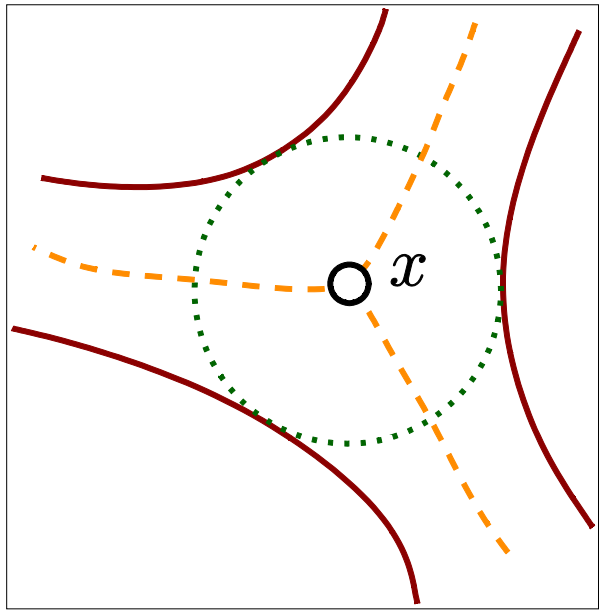
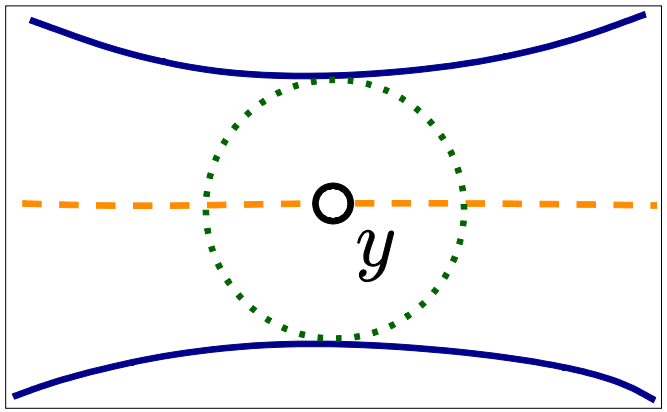


Critical Points

- A critical point of the distance function is a point whose generalized gradient $\nabla_X(x)$ vanishes, i.e., $c_X(x)$ coincides with x

- A critical point is in its medial axis Σ





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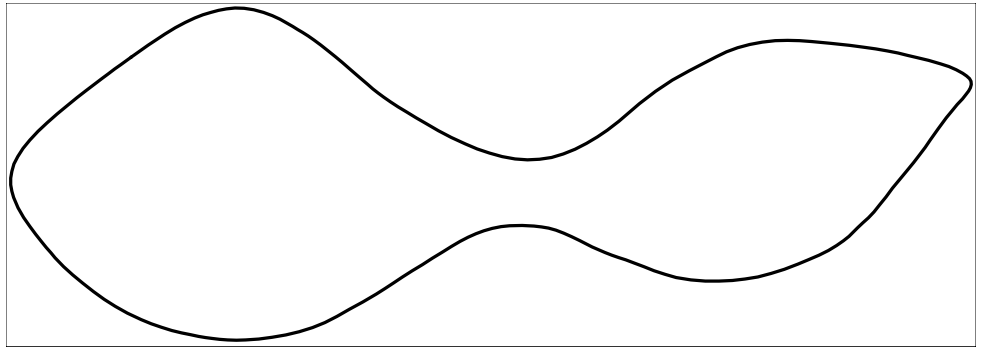

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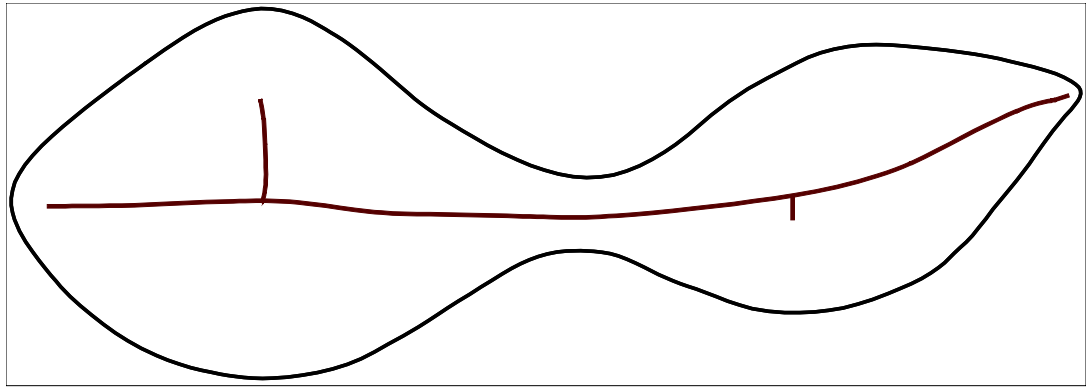

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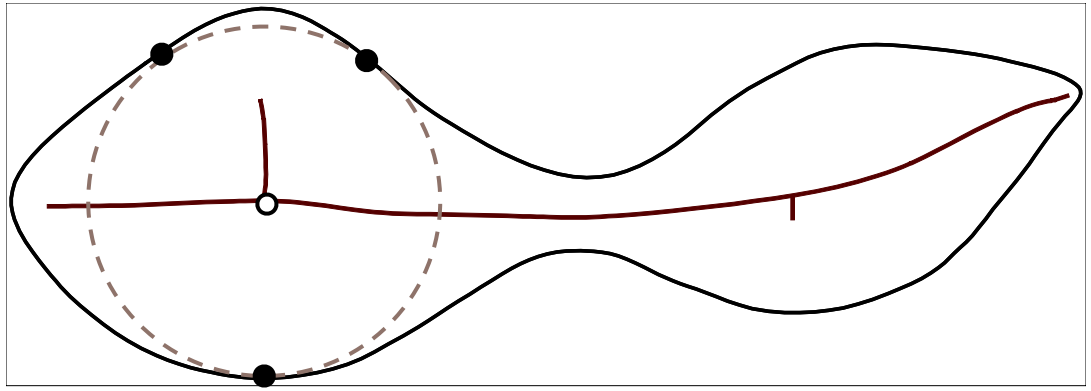

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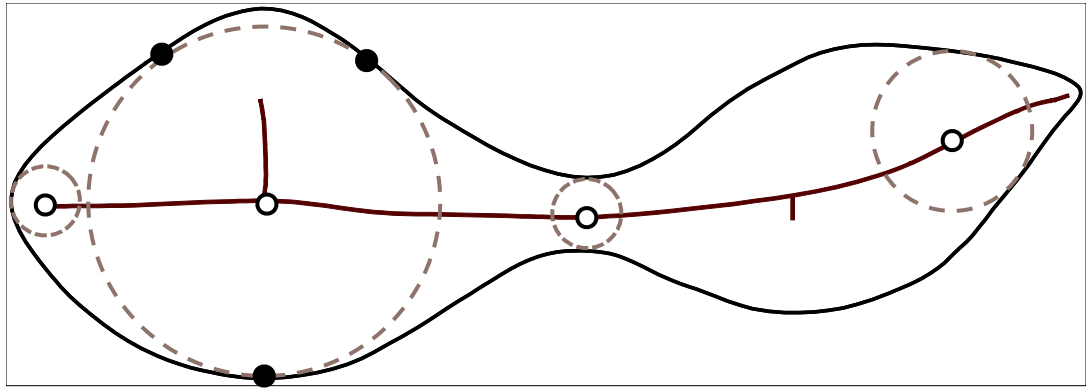
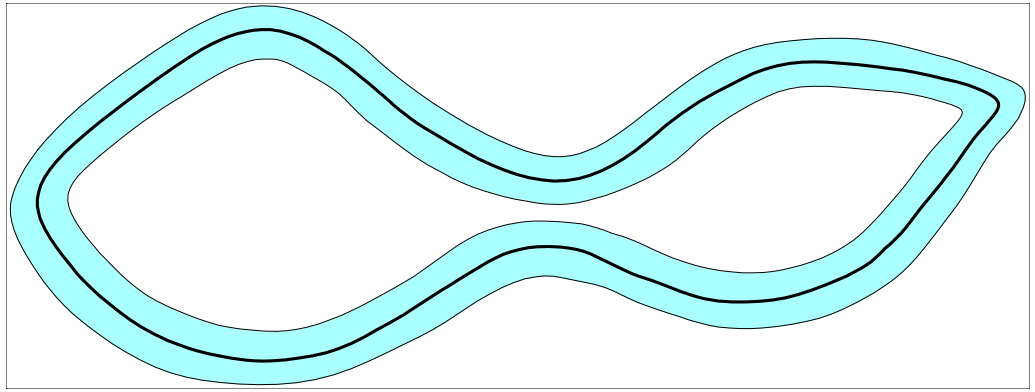
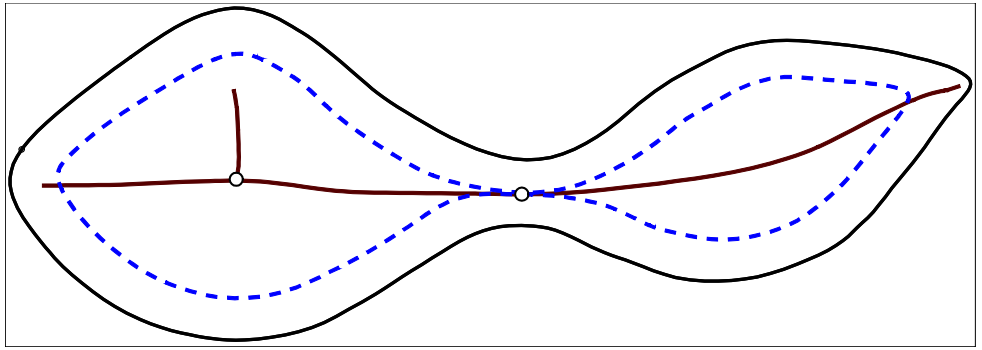


When does offset changes its topology?

- When they sweep past critical points!





Critical point theory for distance function

- Theorem [Offset Homotopy] [*Grove'93*]

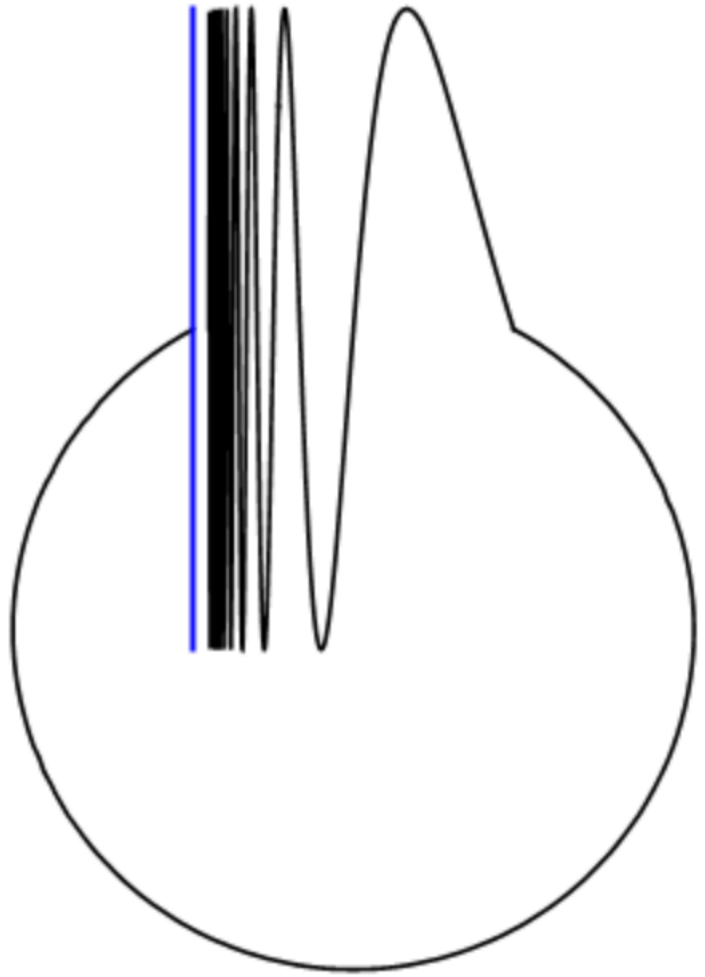
  If $0 < \alpha < \alpha'$ are such that there is no critical value of d_X in the closed interval $[\alpha,\ \alpha']$, then $X^{\alpha'}$ deformation retracts onto X^{α}. In particular, $H(X^{\alpha}) \cong H(X^{\alpha'})$.

- Remarks:
  - For the case of compact set X, note that it is possible that X^{α}, for sufficiently small $\alpha > 0$, may not be homotopy equivalent to $X^0 = X$.
  - Intuitively, by above theorem, we can approximate $H(X^{\alpha})$ for any small positive α from a thickened version (offset) of X^{α}.

Critical point theory for distance function

- Theorem [Offset Homotopy] [*Grove'93*]

  If $0 < \alpha < \alpha'$ are such that there is no critical v … l
  $[\alpha,\ \alpha']$, then $X^{\alpha'}$ deformation retracts onto X … $(X^{\alpha'})$.



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Weak Feature Size

- Given a compact $X \subset \mathbb{R}^d$, let $C \subset \mathbb{R}^d$ denote
  - the set of critical points of the distance function d_X
  - Note $C \subset \Sigma$

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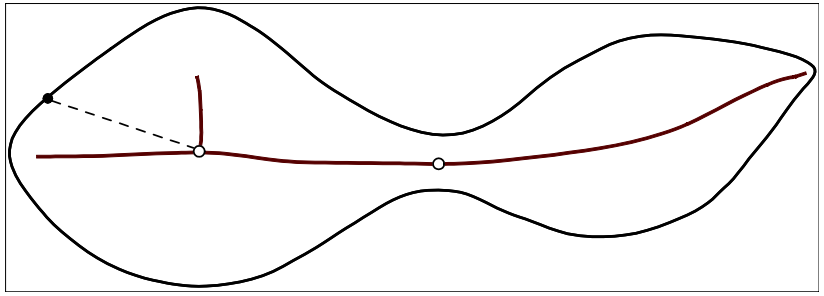

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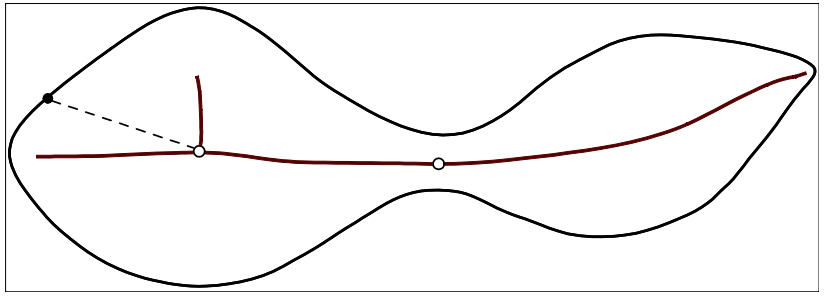

- Given a compact $X \subset R^d$, the *weak feature size* is
  - $wfs(X) = \inf_{x \in X} d(x, C)$
- Equivalently,
  - $wfs(X)$ is the infimum of the positive critical value of d_X

- $\rho(X) \leq wfs(X)$

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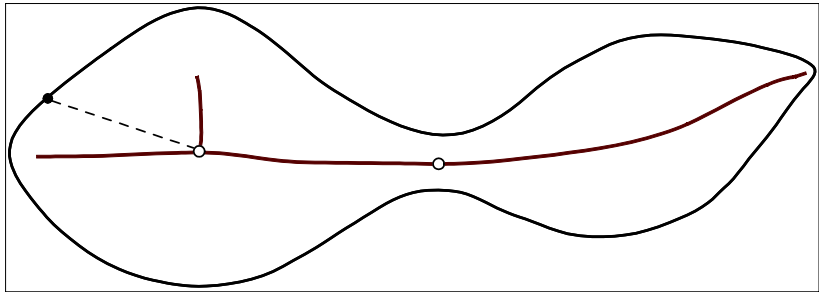

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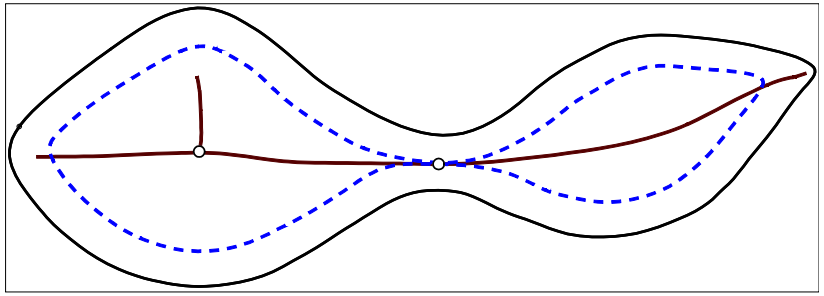
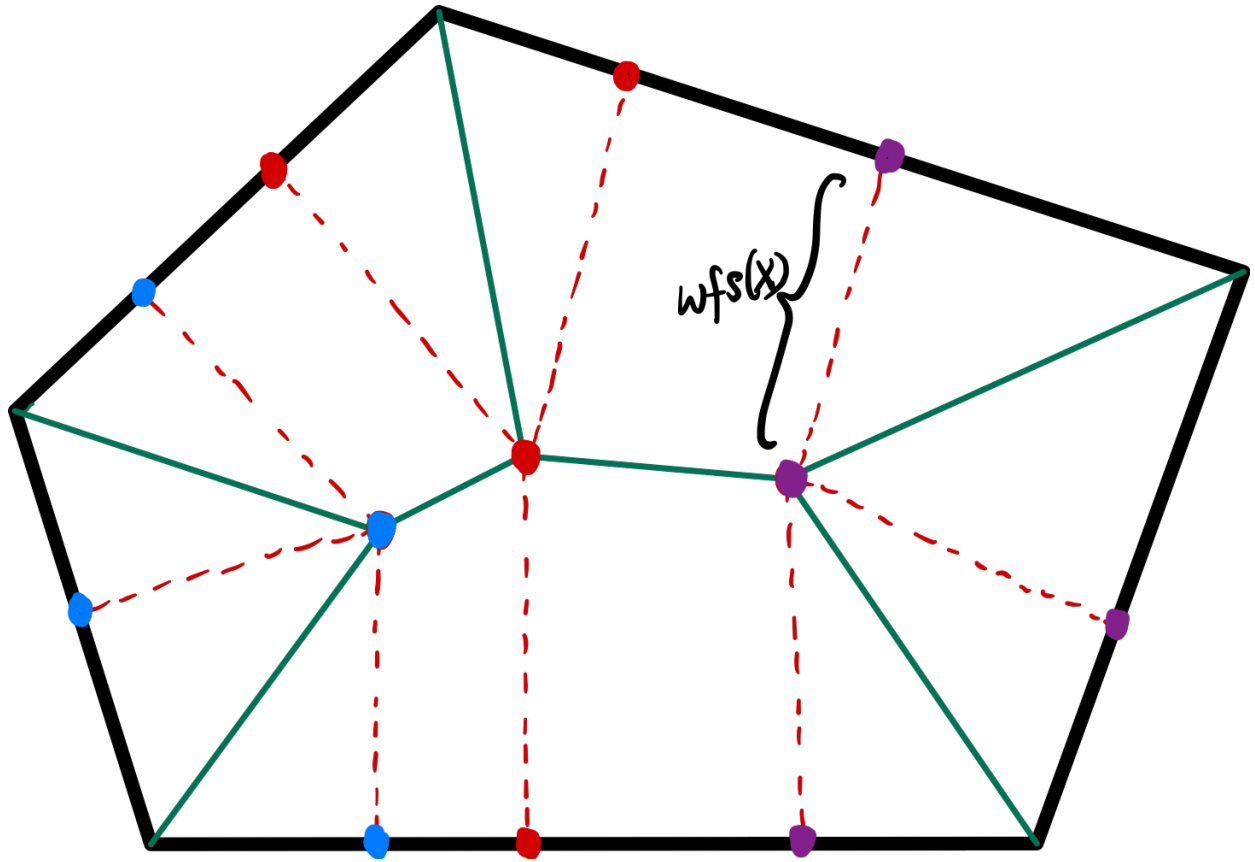


- $\rho(X) \leq wfs(X)$

Example



Typical Sampling Conditions

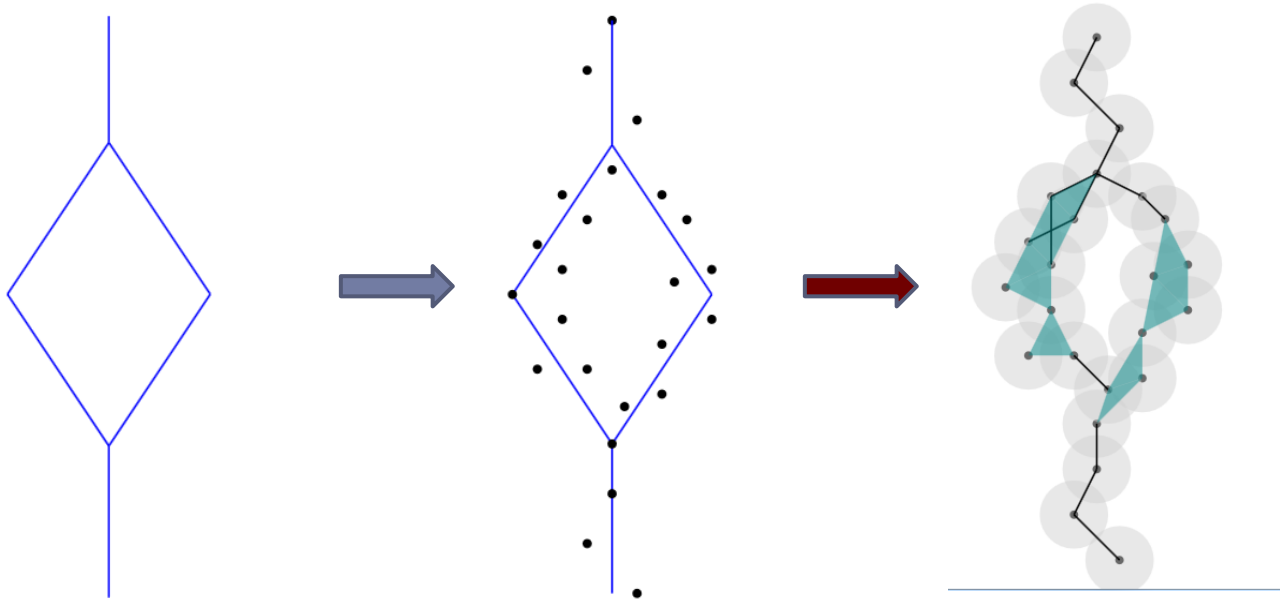
- Hausdorff distance $d_H(A,\ B)$ between two sets A and B
  - smallest value α such that $A \subseteq B^{\alpha}$ and $B \subseteq A^{\alpha}$
- No noise version:
  - A set of points P is an ϵ-sample of X

    if $P \subset X$ and $d_H\,(P,\ X) \leq \epsilon$
- With noise version:
  - A set of points P is an ϵ-sample of X if $d_H\,(P,\ X) \leq \epsilon$

- The Hausdorff distance should be **smaller** than the reach (for manifold) or the weak feature size for general compact subsets

Homology Inference from PCD

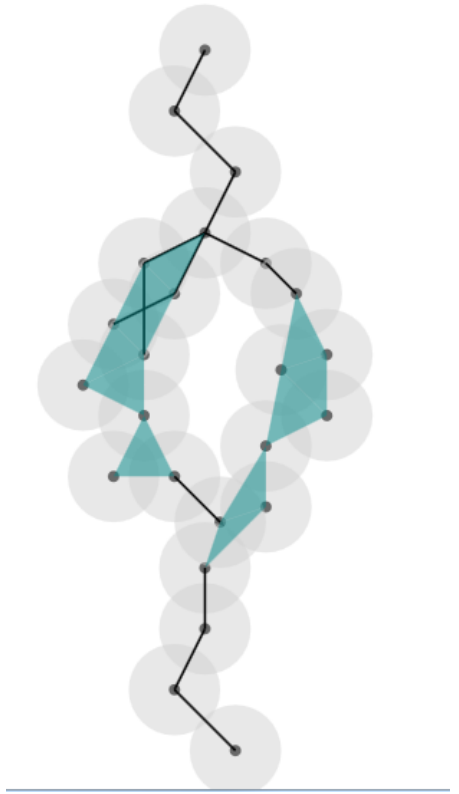
Problem Setup



- A hidden compact X (or a manifold M)
- An ϵ-sample P of X
- Recover homology of X from some complex built on P
  - will focus on Čech complex and Rips complex

Union of Balls

- $X^{\alpha} = \bigcup_{x \in X} B(x,\ \alpha)$
- $P^{\alpha} = \bigcup_{p \in \mathrm{P}} B\left(p,\ \alpha\right)$



- Intuitively, P^{α} approximates offset X^{α}
- The Čech complex $C^{\alpha}(P)$ is the Nerve of P^{α}
- By Nerve Lemma, $C^{\alpha}(P)$ is homotopy equivalent to P^{α}

Smooth Manifold Case

- Let X be a smooth manifold embedded in R^d

Theorem [Niyogi, Smale, Weinberger]

Let $P \subset X$ be such that $d_H(X,\ P) \leq \epsilon$. If $2\epsilon \leq \alpha \leq \sqrt{\frac{3}{5}}\rho(X)$, there is a deformation retraction from P^α to X .

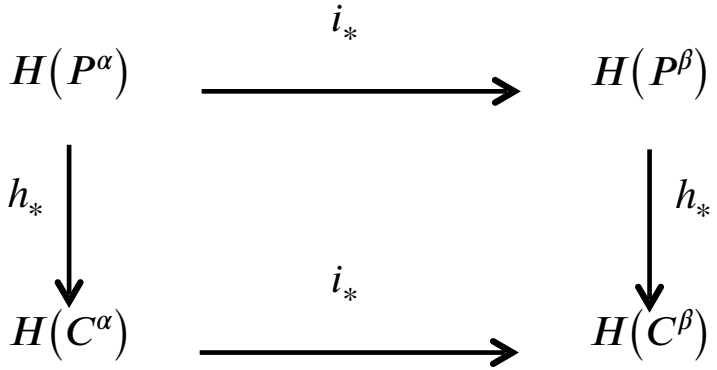
Corollary A

Under the conditions above, we have

$H_*(X) \cong H_*(P^\alpha)$

Convert to Cech Complexes

- Lemma A *[Chazal and Oudot, 2008]*:
- The following diagram commutes:



Corollary B

Let $P \subset X$ be s.t. $d_H(X, P) \leq \epsilon$. If

$$2\epsilon \leq \alpha \leq \beta \leq \sqrt{\frac{3}{5}}\rho(X), H_*(X) \cong H_*(C^\alpha) \cong H_*(C^\beta)$$

where the second isomorphism is induced by inclusion.

- How about using Rips complex instead of Čech complex?
- Recall that

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

inducing

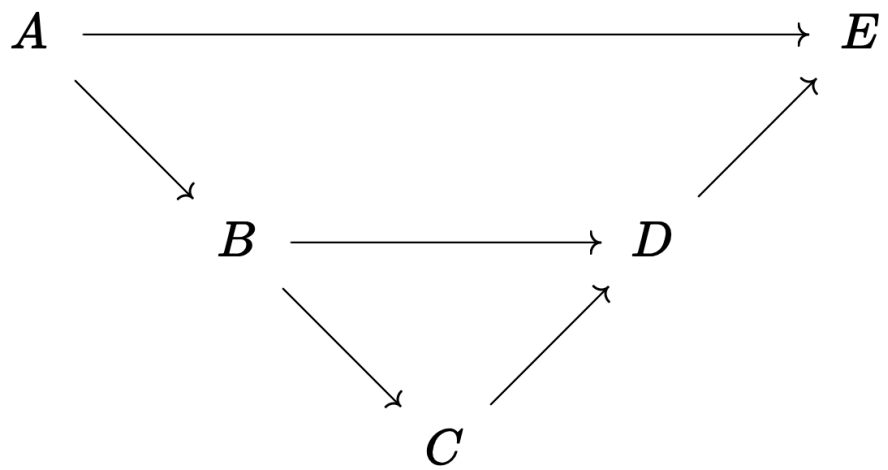
$$H(C^r) \rightarrow H(R^r) \rightarrow H(C^{2r})$$

- Idea *[Chazal and Oudot 2008]*:
  - Forming interleaving sequence of homomorphism to connect them with the homology of the input manifold X and its offsets X^{α}

From Rips Complex

- Lemma B:

  Given a sequence $A \to B \to C \to D \to E$ of linear maps between finite dimensional vector spaces, if $rank(A \to E) = \dim C$ then $rank(B \to D) = \dim C$.



From Rips Complex

- Lemma B:

  Given a sequence $A \to B \to C \to D \to E$ of linear maps between finite dimensional vector spaces, if $rank(A \to E) = \dim C$ then $rank(B \to D) = \dim C$.

- Rips and Čech complexes:

$$C^{\alpha}(P) \subseteq R^{\alpha}(P) \subseteq C^{2\alpha}(P) \subseteq R^{2\alpha}(P) \subseteq C^{4\alpha}(P)$$
$$\Rightarrow H_*(C^{\alpha}) \to H_*(R^{\alpha}) \to H_*(C^{2\alpha}) \to H_*(R^{2\alpha}) \to H_*(C^{4\alpha})$$

- Applying Lemma B, if $H_*(C^{\alpha}) \cong H_*(C^{2\alpha}) \cong H_*(C^{4\alpha}) \cong H_*(X)$ then

$$rank(H_*(R^{\alpha}) \to H_*(R^{2\alpha})) = \dim H_*(C^{2\alpha}) = \dim H_*(X)$$

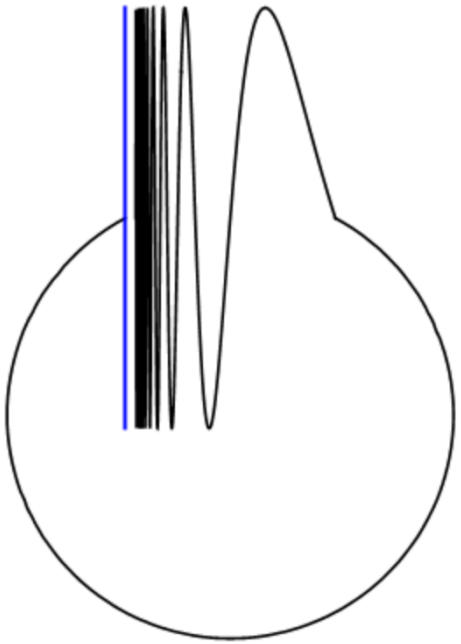
From Rips Complex

From Rips Complex

- Theorem [Homology Inference]
- Let $X \subset \mathbb{R}^d$ be a manifold and let $P \subset X$ be such that $d_H(X,\ P) \leq \epsilon$. If $2\epsilon \leq \alpha \leq \frac{1}{4}\sqrt{\frac{3}{5}}\rho(X)$, we have $rank(H_*(R^\alpha) \to H_*(R^{2\alpha})) = \dim H_*(X)$, in other words, the persistent Betti number of the VR filtration recovers the Betti number of X

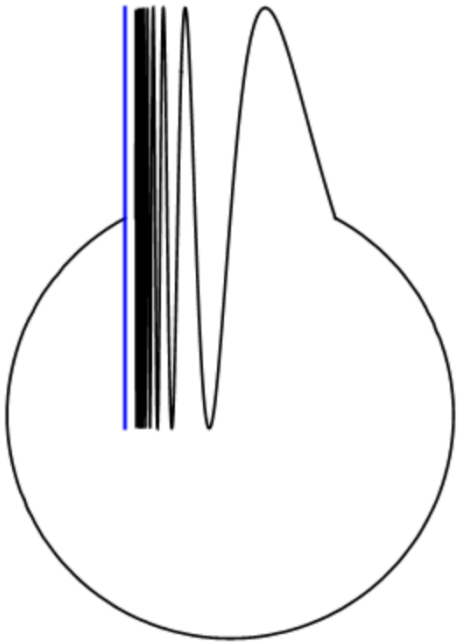
The Case of Compact Set

- $H_*(X^\lambda)$ may not be isomorphic to $H_*(X)$ even for sufficiently small $\lambda > 0$
- We no longer have isomorphism between $H_*(X)$ and $H_*(P^\alpha)$



The Case of Compact Set

- $H_*(X^\lambda)$ may not be isomorphic to $H_*(X)$ even for sufficiently small $\lambda > 0$
- We no longer have isomorphism between $H_*(X)$ and $H_*(P^\alpha)$
- We then only try to infer $H_*(X^\lambda)$ for small $\lambda > 0$ using pairs of spaces



The Case of Compact Set

Corollary A

Let $P \subset X$ be such that $d_H(X,\ P) \leq \epsilon$. If $2\epsilon \leq \alpha \leq \sqrt{\frac{3}{5}}\rho(X)$, we have $H_*(X) \cong H_*(P^\alpha)$

The Case of Compact Set

- In contrast to Corollary A, now we have the following (using critical point theory and Lemma B).

- Lemma C *[Chazal and Oudot 2008]*:
  Let $P \subset \mathbb{R}^d$ be a finite set such that $d_H(X,\ P) < \epsilon$ for some $\epsilon < \frac{1}{4} wfs(X)$. Then for all $\alpha,\ \beta \in \left[\epsilon,\ wfs(X) - \epsilon\right]$ such that $\beta - \alpha \geq 2\epsilon$, and for all $\lambda \in \left(0,\ wfs(X)\right)$, we have $H\left(X^{\lambda}\right) \cong image\left(i_*\right)$, where $i_*: H\left(P^{\alpha}\right) \to H\left(P^{\beta}\right)$ is the homomorphism between homology groups induced by the canonical inclusion $i: P^{\alpha} \to P^{\beta}$.

The Case of Compact Set

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- $X^\lambda \simeq X^{\lambda'}$ for $\lambda, \lambda' \in (0, wfs(X))$
- $X^{\alpha-\epsilon} \subseteq P^\alpha \subseteq X^{\alpha+\epsilon} \subseteq P^\beta \subseteq X^{\beta+\epsilon}$
- Using Nerve theorem, this can be transformed into a result regarding Cech filtrations

The Case of Compact Set

The Case of Compact Set

- Theorem [Homology Inference] *[Chazal and Oudot 2008]*:

  Let $P \subset \mathbb{R}^d$ be a finite set such that $d_H(X, P) < \epsilon$ for some $\epsilon < \frac{1}{9} wfs(X)$. Then for all $\alpha \in \left[2\epsilon, \frac{1}{4}\left(wfs(X) - \epsilon\right)\right]$ all $\lambda \in \left(0, wfs(X)\right)$, we have $H\left(X^{\lambda}\right) \cong image\left(j_*\right)$, where j_* is the homomorphism between homology groups induced by canonical inclusion $j: R^{\alpha} \to R^{4\alpha}$.

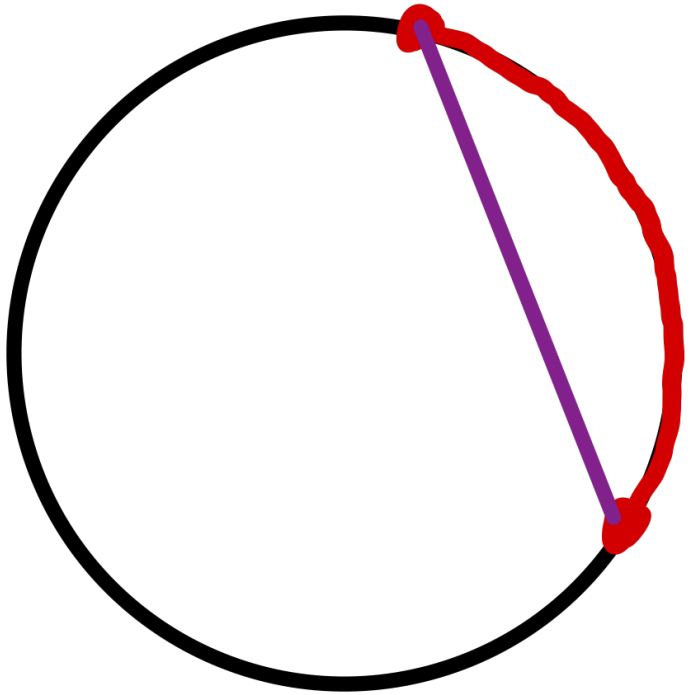
Summary of Homology Inference

- NSW theorem or the critical point theory of d_X gives us information on topological change in the filtration $\{X^r\}$
- The Hausdorff distance gives rise to interleaving between $\{X^r\}$ and $\{P^r\}$
- Nerve Theorem relates Čech filtration $\{C^r\}$ with $\{P^r\}$ through isomorphism
- Rips and Čech are related through interleaving
- Both are related to $\{X^r\}$ through interleaving
- Homology of X can be then inferred from Rips or Čech filtrations of P

Homology inference for manifolds

Hausmann's theorem

- Let M be a Riemannian manifold (i.e., a manifold with a metric structure)

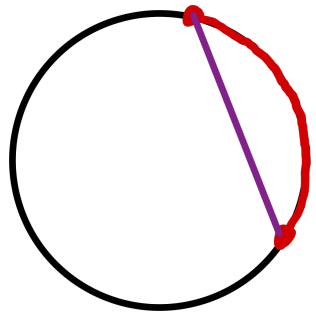


Hausmann's theorem

- Let M be a Riemannian manifold (i.e., a manifold with a metric structure)
- Consider

$$Rips^r(M) = \left\{ (p_0, \ldots, p_k) \,|\, d(p_i, p_j) < r, \forall i, j \text{ and } \forall p_0, \ldots, p_k \in M \right\}$$

- For r sufficiently small, then $Rips^r(M)$ is homotopy equivalent to M



Latschev's theorem - sampling version

- Let M be a Riemannian manifold (i.e., a manifold with a metric structure)
- For any ϵ sufficiently small and any metric space X there exists $\delta > 0$ such that
  - If $d_{GH}(X, M) \leq \delta$, then
  - Then $Rips^{\epsilon}(X)$ is homotopy equivalent to M

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- Let M be a Riemannian manifold (i.e., a manifold with a metric structure)
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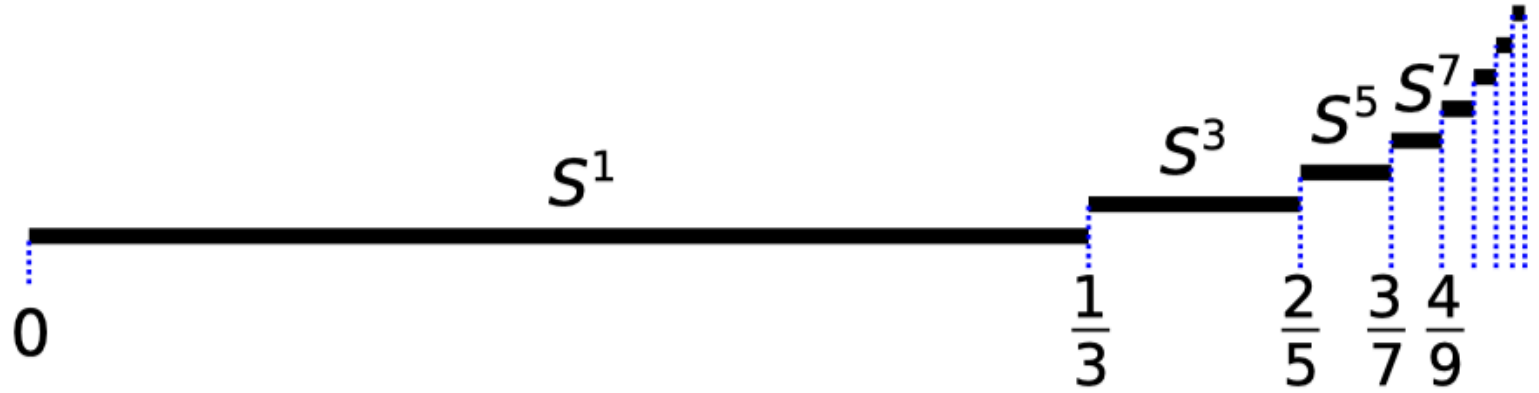
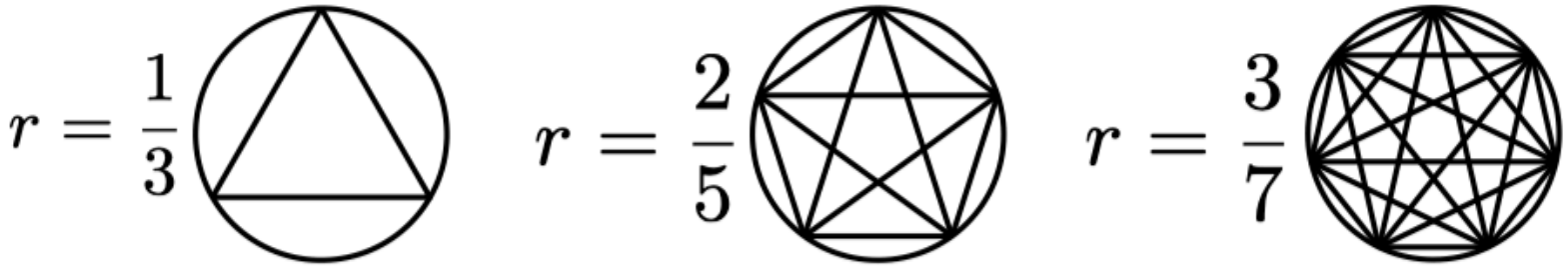
  - Then $Rips^{\epsilon}(X)$ is homotopy equivalent to M

Can we say anything "persistent"?

VR complex of $\mathbb{S}^1$ - circle with unit circumference

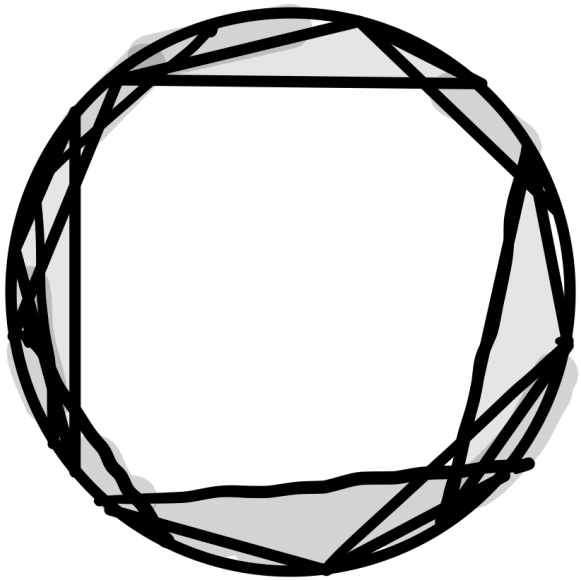
- $Rips^r(\mathbb{S}^1) \simeq \mathbb{S}^{2l+1}, \frac{l}{2l+1} < r \leq \frac{l+1}{2l+3}$



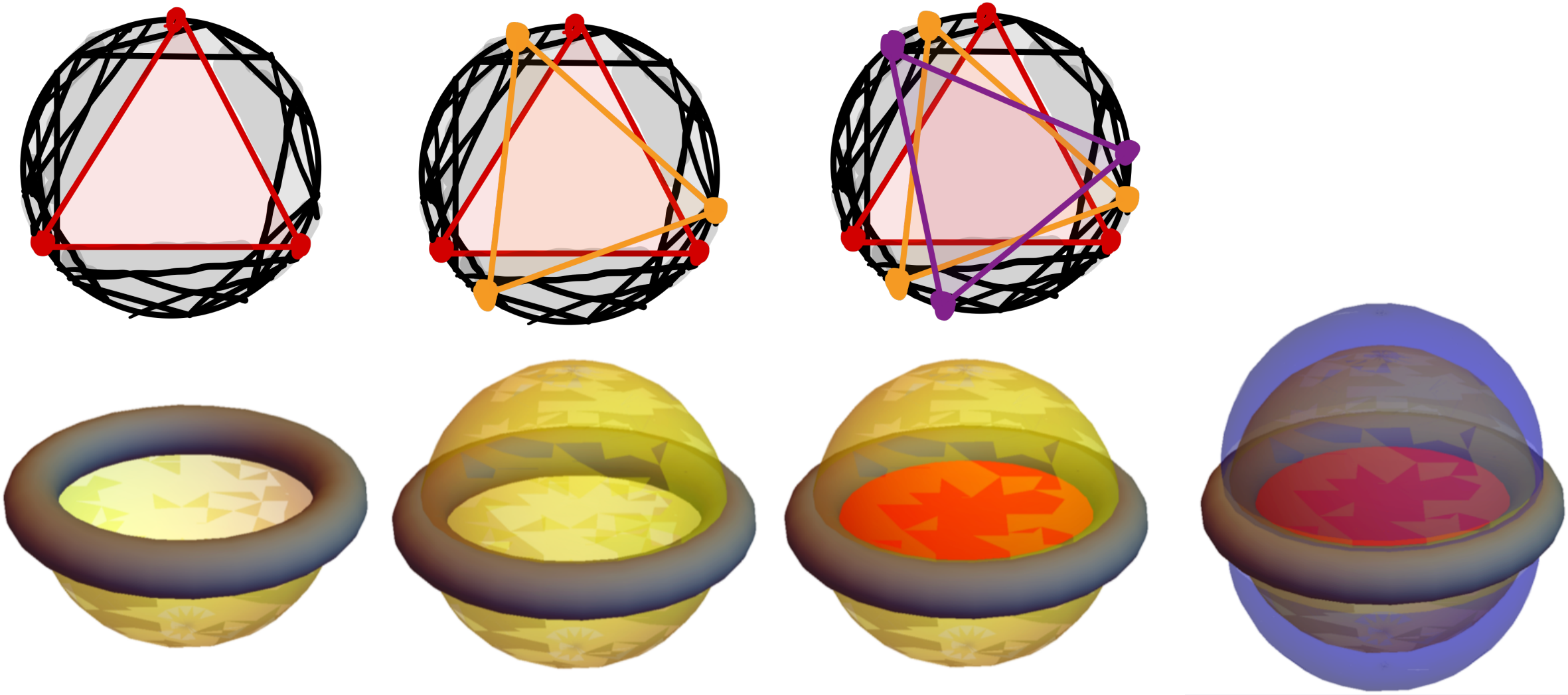


Courtesy of Henry Adams

$r \leq 1/3$

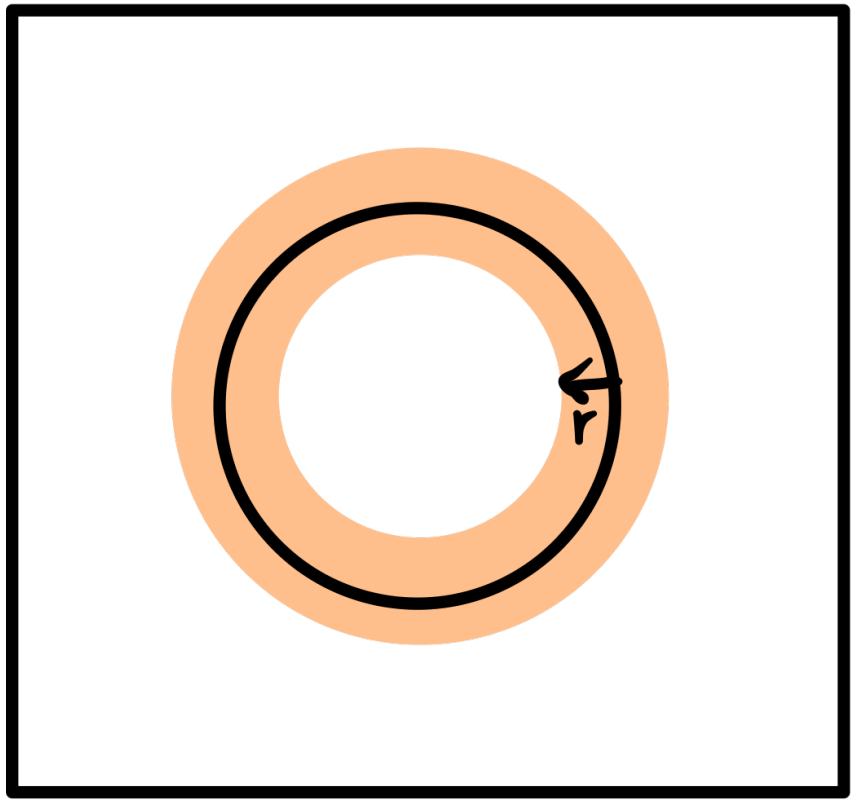


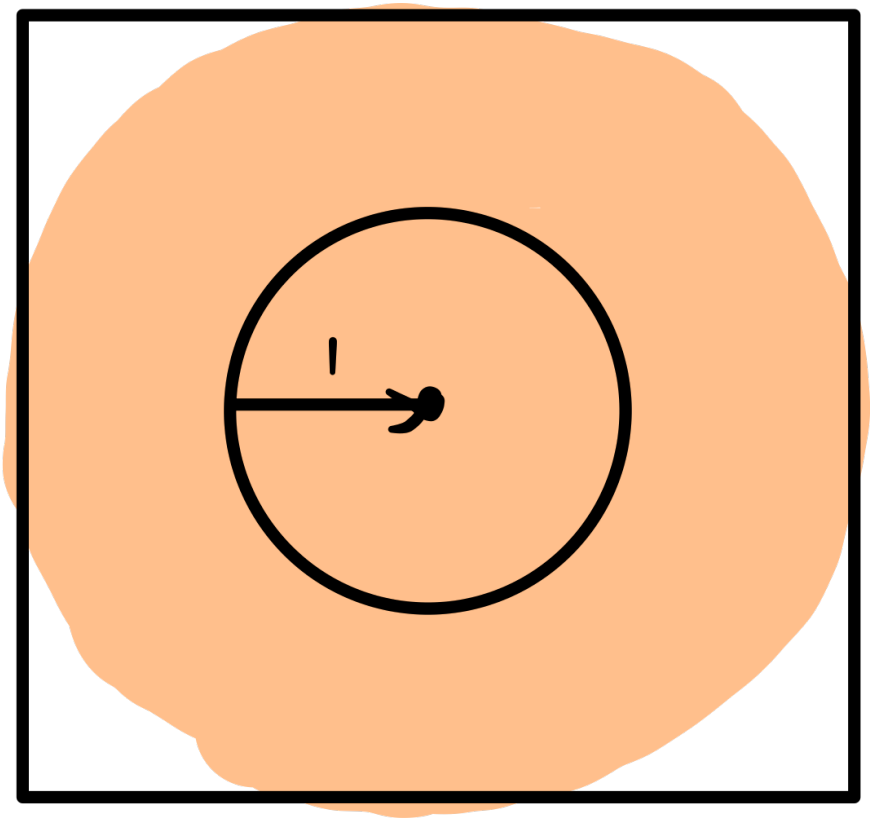
$r > 1/3$



Courtesy of Henry Adams

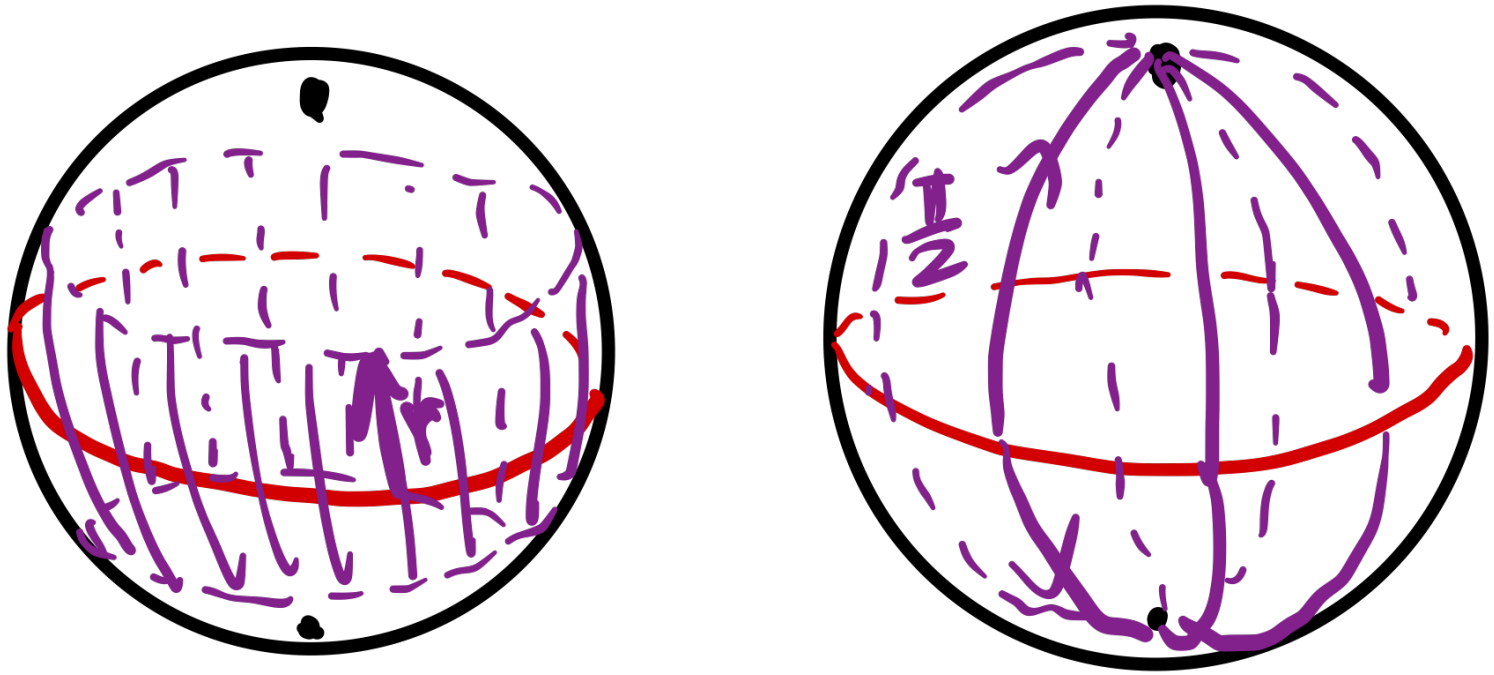
- Can we interpret this using certain offset idea?





Filling radius

- $FillRad(M, X) = \inf\{\epsilon : M^{\epsilon} \subset X \text{ has trivial top dim homology}\}$



$$FillRad(\mathbb{S}^1, \mathbb{S}^2) = \pi/2$$

Filling radius

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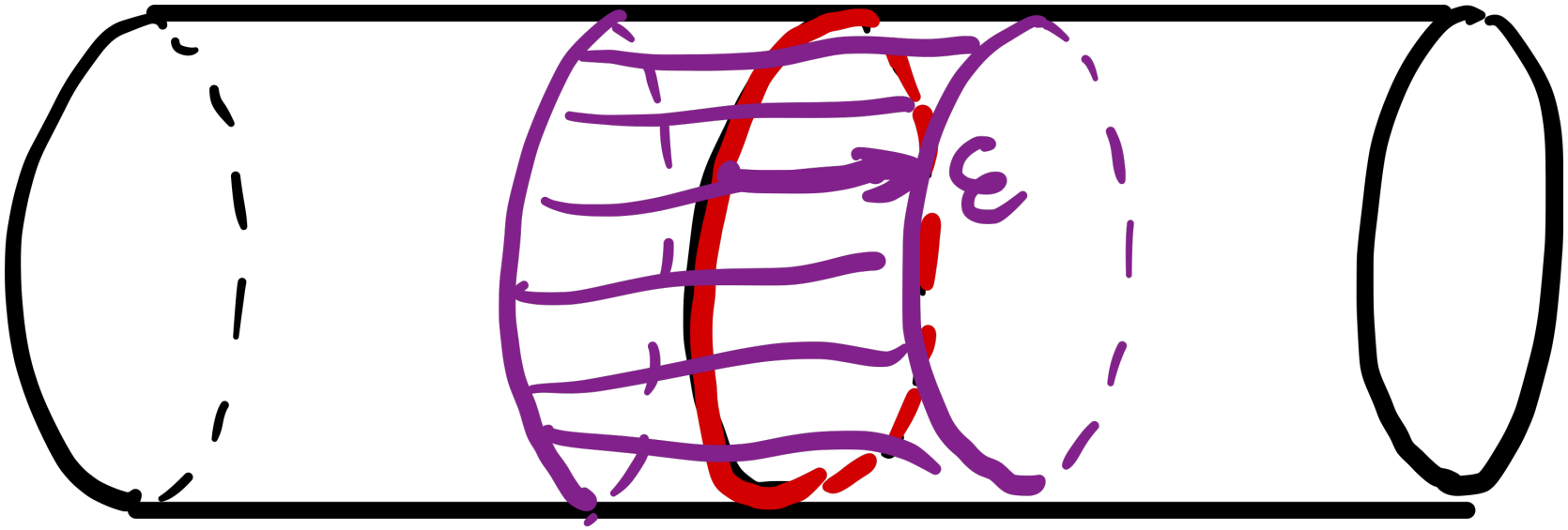


$$FillRad(\mathbb{S}^1, X) = \infty$$

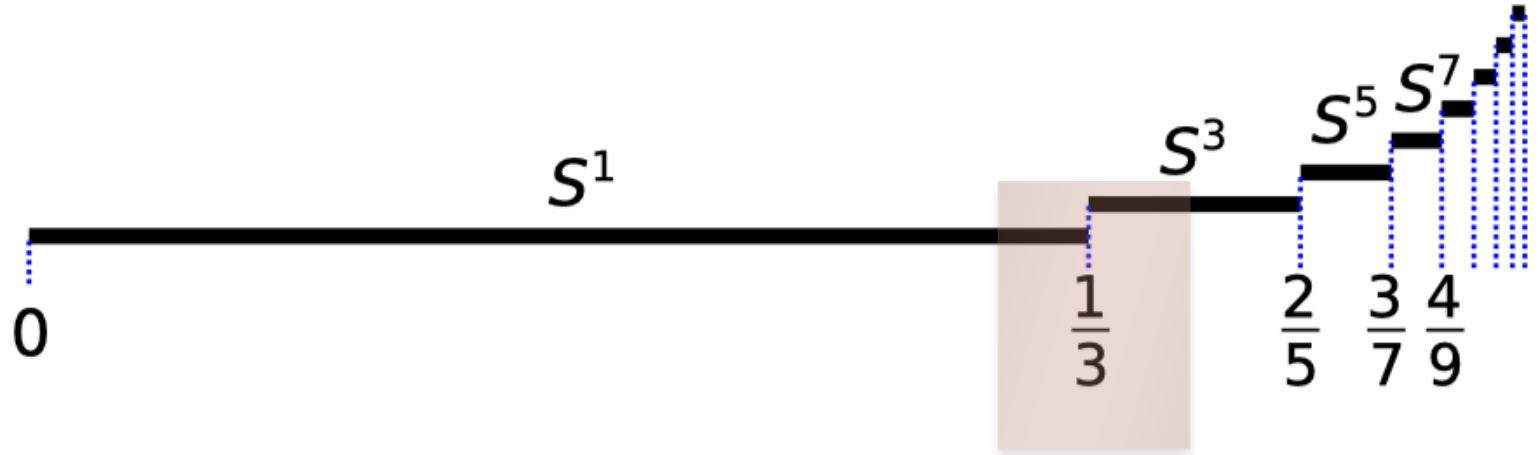
Filling radius

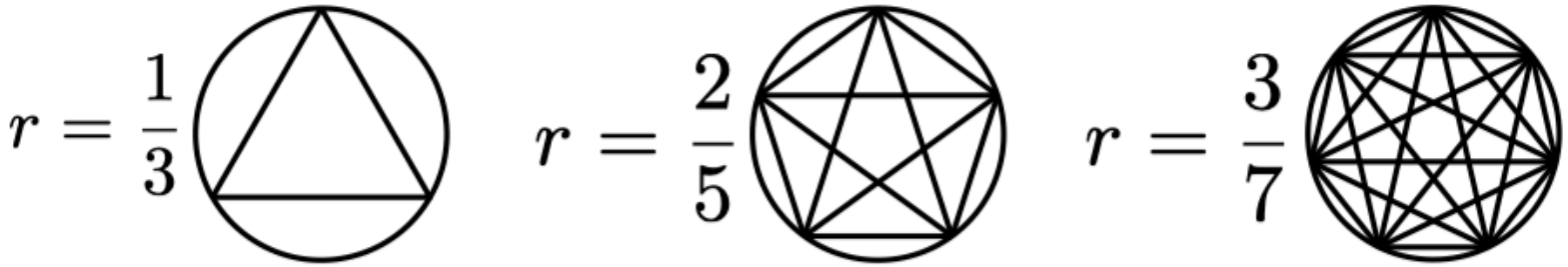
- $FillRad(M, X) = \inf\{\epsilon : M^{\epsilon} \subset X \text{ has trivial top dim homology}\}$
- Filling radius of M: $FillRad(M) := \inf_{X} FillRad(M, X)$

- $FillRad(\mathbb{S}^1) = \pi/3$ and $FillRad(\mathbb{S}^1_1) = 1/6$

VR complex of $\mathbb{S}^1$

- $Rips^r(\mathbb{S}^1) \simeq \mathbb{S}^{2l+1}, \frac{l}{2l+1} < r \leq \frac{l+1}{2l+3}$

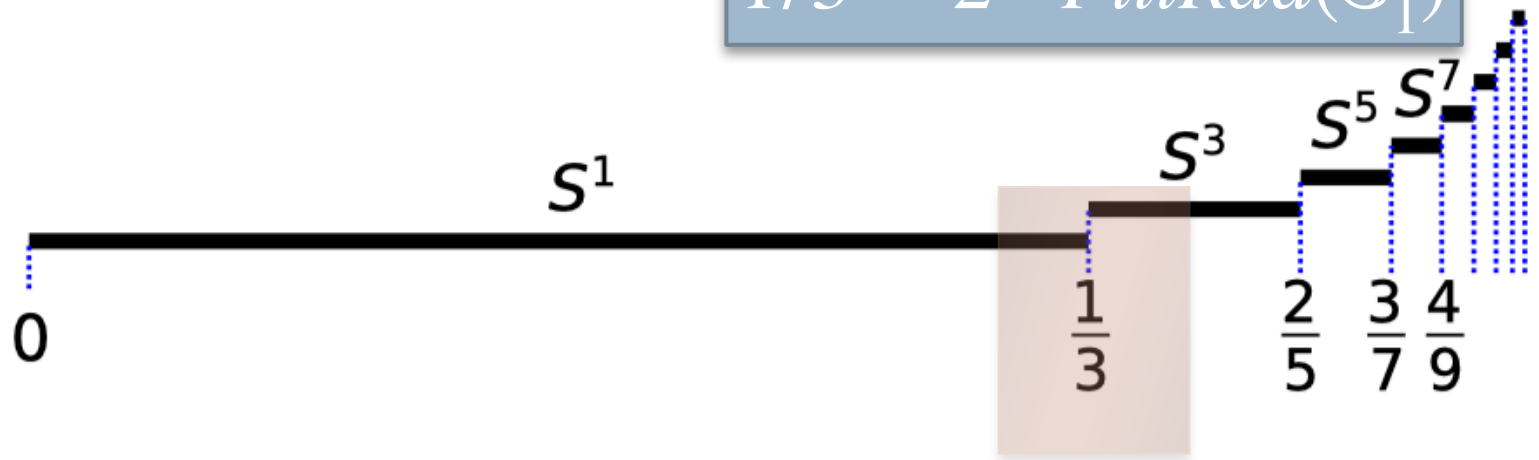


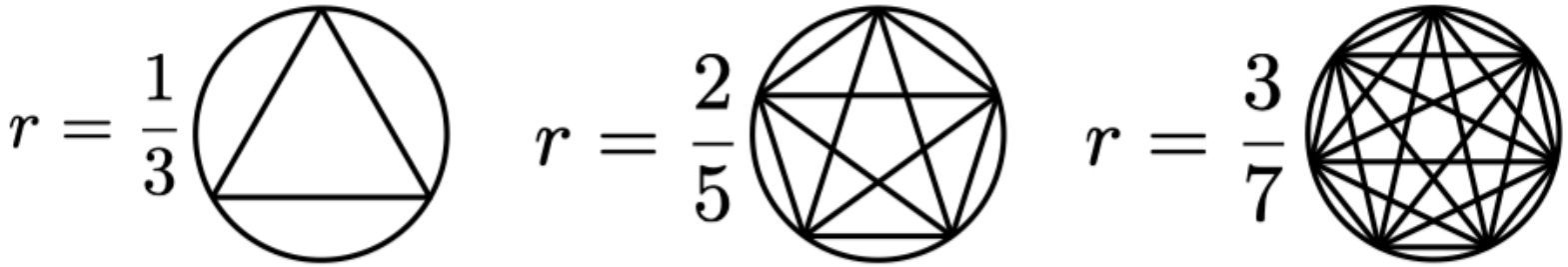


Courtesy of Henry Adams

VR complex of $\mathbb{S}^1$

- $Rips^r(\mathbb{S}^1) \simeq \mathbb{S}^{2l+1}, \frac{l}{2l+1} < r \leq \frac{l+1}{1/3 = 2 * FillRad(\mathbb{S}^1_1)}$





Courtesy of Henry Adams

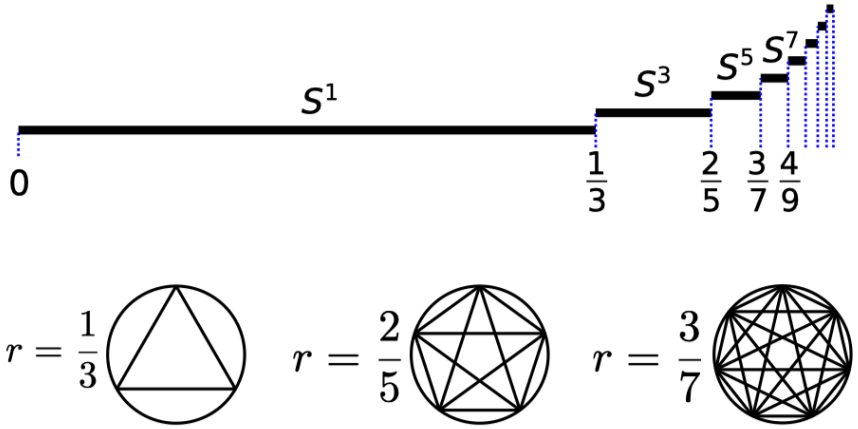
Filling radius and VR filtration

- [Lim et al. 2022]

Proposition 9.4. *Let M be a closed connected n-dimensional Riemannian manifold. Then,*

$$(0, 2\,\mathrm{FillRad}(M)] \in \mathrm{barc}_n^{\mathrm{VR}}(M;\mathbb{F}),$$

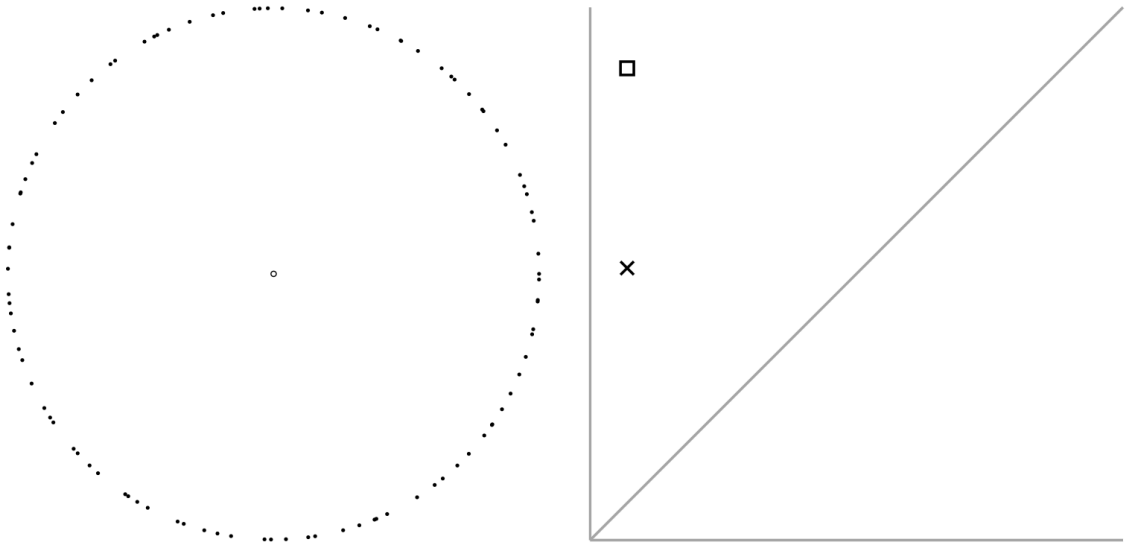
where $\mathbb{F}$ is an arbitrary field if M is orientable, and $\mathbb{F} = \mathbb{Z}_2$ if M is non-orientable. Moreover, this is the unique *interval in $\mathrm{barc}_n^{\mathrm{VR}}(M;\mathbb{F})$ starting at 0.*



Section 2:
Handling of Noise

Noise

- Previous approach can handle Hausdorff type noise
  - Where noise is within a tubular neighborhood of X
- How about more general noise?
  - E.g, Gaussian noise, background noise, outliers



(a) Samples (b) Diagrams

Courtesy of Bendich et al.

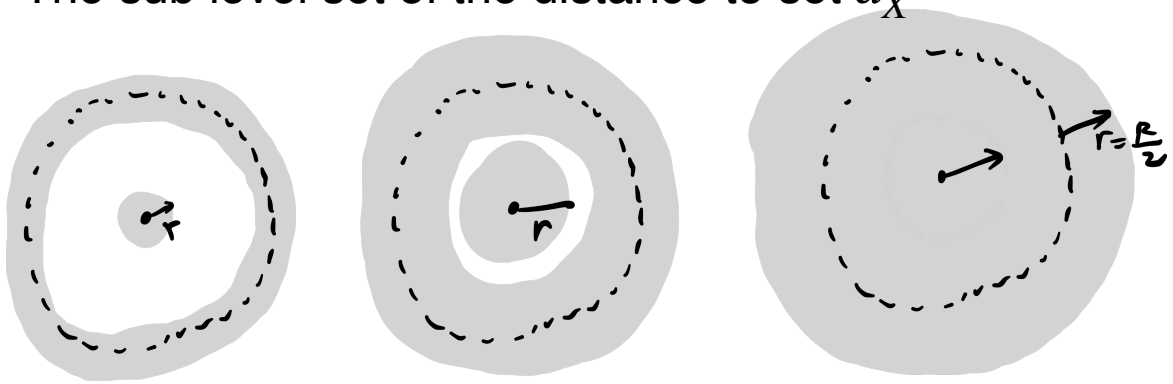
Noise

- Previous approach can handle Hausdorff type noise
  - Where noise is within a tubular neighborhood of X
- How about more general noise?
  - E.g, Gaussian noise, background noise

- Distance to measure framework
  - *[Chazal, Cohen-Steiner, Mérigot, 2011]*

Main idea

The sub level set of the distance to set d_X



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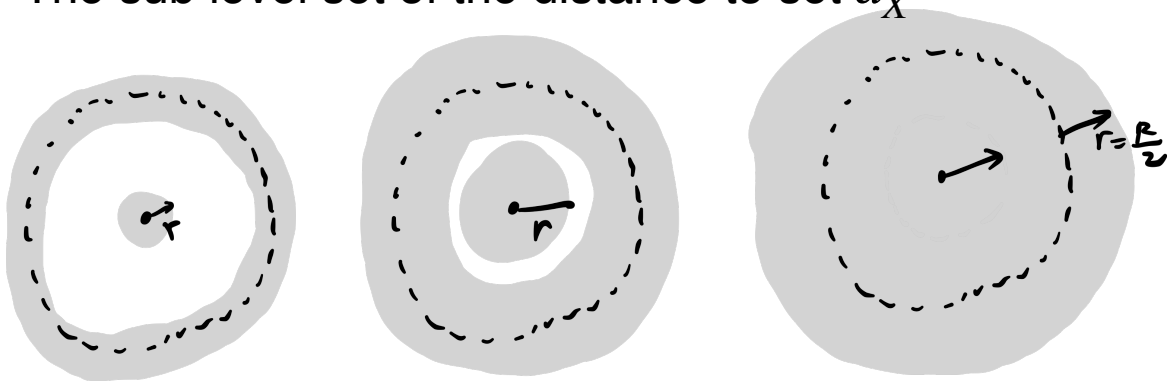

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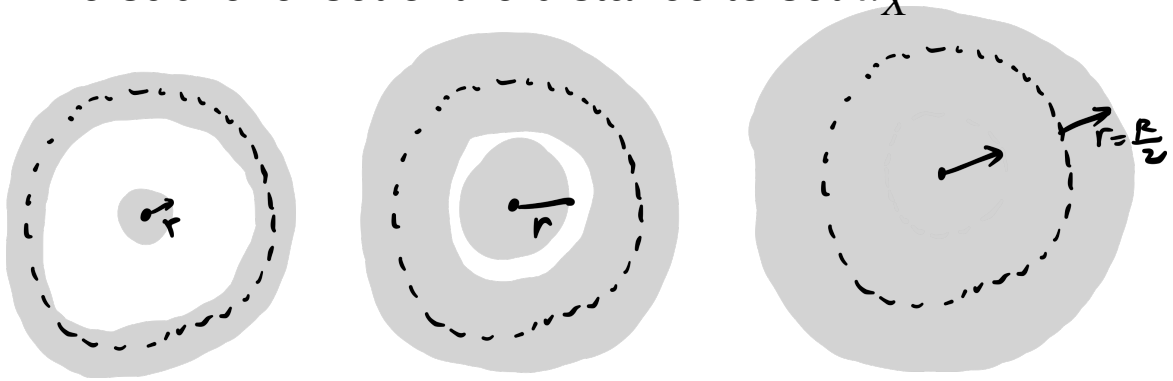
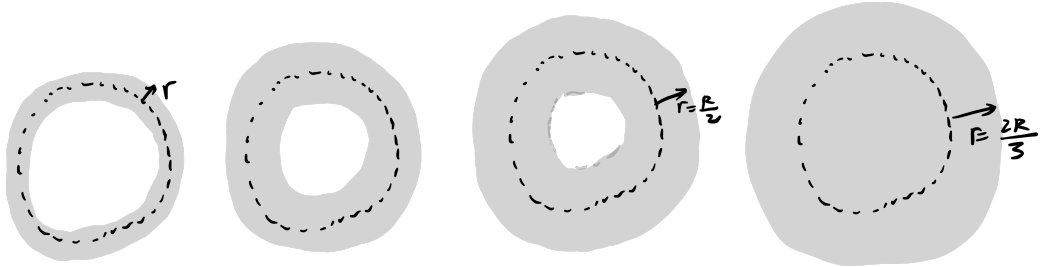


The sub level set of the “distance to measure”



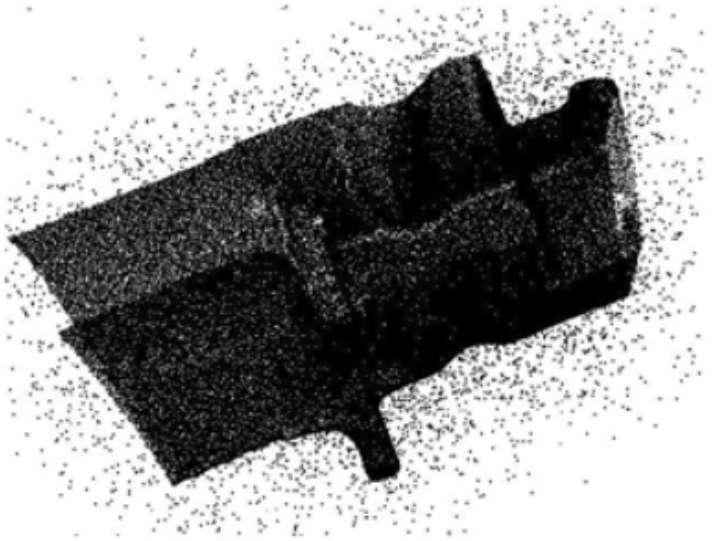
Main Idea

- The work of *[Chazal, Cohen-Steiner, Mérigot, 2011]*

- A new distance function $d_{\mu,m}$ to a probability measure μ (ie., distance to measures) to replace the role of distance function d_X.
- Show that the two distance functions are close (in L_∞ norm)
- Topological inference follows from some stability results or the interleaving sequences

Overview

- Input:
  - A set of points P sampled from a probabilistic measure μ on R^d potentially concentrated on a hidden compact (e.g, manifold) X.
- Goal:
  - Approximate topological features of X



Courtesy of Chazal et al 2011

Definitions

- μ: a probability measure on $\mathbb{R}^d$; $\mu(\mathbb{R}^d) = 1$
- $0 < \ m, m_0 < 1$: *mass* parameters
- $\delta_{\mu,m}(\mathrm{x}) := \inf\{\mathrm{r} > 0; \mu\left(\bar{B}(x,\ r)\right) > m\ \}$

  where $\bar{B}(x,\ r)$ is the closed Euclidean ball at x

- That is, $\delta_{\mu,m}(\mathrm{x})$ is the radius of the ball necessary in order to enclose mass m

Discrete setting

- Given a set of points $P \subset \mathbb{R}^d$, consider the empirical probability measure $\mu_P = \frac{1}{n} \sum_{p \in P} \delta_p$ where intuitively every point has measure $\frac{1}{n}$
- For any integer k, we let $kNN(x)$ denote the set of k nearest neighbors of x in P
  - Denote $kNN(x) = \{x_1, \ldots, x_k\}$ such that $\|x - x_i\| \leq \|x - x_{i+1}\|$
- In this case if $\frac{k-1}{n} \leq m < \frac{k}{n}$, then
- $\delta_{\mu_P, m} = \|x - x_k\|$

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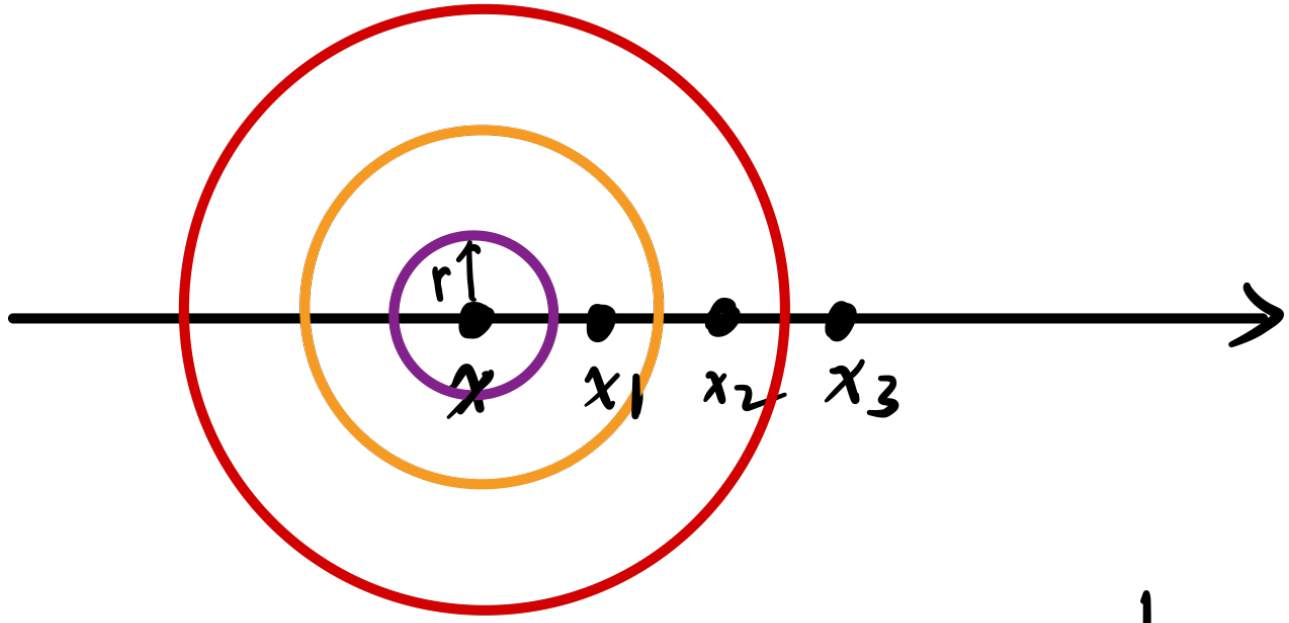

$$\delta_{\mu,m}(x) = \begin{cases} \|x - x_1\| & 0 < m < \frac{1}{3} \\ \|x - x_2\|, & \frac{1}{3} \leq m < \frac{2}{3} \\ \|x - x_3\|, & \frac{2}{3} \leq m < 1 \end{cases}$$

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- That is, $\delta_{\mu,m}(\mathrm{x})$ is the radius of the ball necessary in order to enclose mass m
  - $\delta_{\mu,m}$ is not continuous and hence not a good substitute for d_X
- *Distance to measure* d_{μ,m_0}:

$$d^2_{\mu,m_0}(x) = \frac{1}{m_0} \int_0^{m_0} \delta_{\mu,m}(x)^2 \, dm$$

Distance to Measures

- *Distance to measure* d_{μ,m_0}:

$$d^2_{\mu,m_0}(x) = \frac{1}{m_0}\int_0^{m_0} \delta_{\mu,m}(x)^2\, dm$$

- Intuitive, $d_{\mu,m}(\mathrm{x})$ averages distance within a range and is more robust to noise.
- Note this distance depends on a mass parameter m_0

Discrete setting

- Given a set of points $P \subset \mathbb{R}^d$, consider the empirical probability measure $\mu_P = \frac{1}{n} \sum_{p \in P} \delta_p$ where intuitively every point has measure $\frac{1}{n}$

- In this case, if $m = k/n$, then
- $$d_{\mu_P, m}(x) = \sqrt{\frac{1}{k} \sum_{q \in kNN(x)} \|x - q\|^2} =: d_{\mu_P, k}(x)$$

Wasserstein Distance

- A *transport plan* between two probability measures $\mu,\ \nu$ on $\mathbb{R}^d$ is a probability measure π on $\mathbb{R}^d \times \mathbb{R}^d$ such that for every $A, B \subseteq \mathbb{R}^d$, $\pi(A \times \mathbb{R}^d) = \mu(A)$ and $\pi(\mathbb{R}^d \times B) = \mu(B)$.
- The p-cost of a transport plan π is:

$$C_p(\pi) = \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^p \pi(dx \times dy) \right)^{1/p}$$

- The *Wasserstein distance* of order p between $\mu,\ \nu$ on $\mathbb{R}^d$ with finite p -moment
  - $W_p(\mu,\ \nu) =$ the minimum p-cost $C_p(\pi)$ of any transport plan π between μ and ν.

Wasserstein Distance

- The Wasserstein distance can be generalized to compare two measures μ and ν with the same total mass (not necessarily =1)
- A measure ν is a submeasure of μ if $\nu(B) \leq \mu(B)$ for any measurable set B. Let $Sub_m(\mu)$ denote the set of all submeasures of μ with total mass m
- $$d_{\mu,m_0}(x) = \min_{\nu \in Sub_{m_0}(\mu)} \frac{1}{\sqrt{m_0}} W_2(m_0\delta_x, \nu)$$

Properties

Properties

- Theorem [Stability] [Chazal et al 2011]

  Let $\mu,\ \mu'$ be two probability measures on $\mathbb{R}^d$ and $m_0 > 0$. Then

  $$\left\| d_{\mu,\, m_0} - d_{\mu', m_0} \right\|_\infty \leq \frac{1}{\sqrt{m_0}} W_2(\mu,\ \mu')$$

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- Theorem [Stability of PD] [Buchet et al 2016]

  Let $\mu,\ \mu'$ be two probability measures on $\mathbb{R}^d$ and $m_0 > 0$. Then,

  $$d_B(Dgm(d_{\mu,m_0}), Dgm(d_{\mu',m_0})) \leq \|d_{\mu,m_0} - d_{\mu,m_0}\|_\infty \leq \frac{1}{\sqrt{m_0}} W_2(\mu, \mu')$$

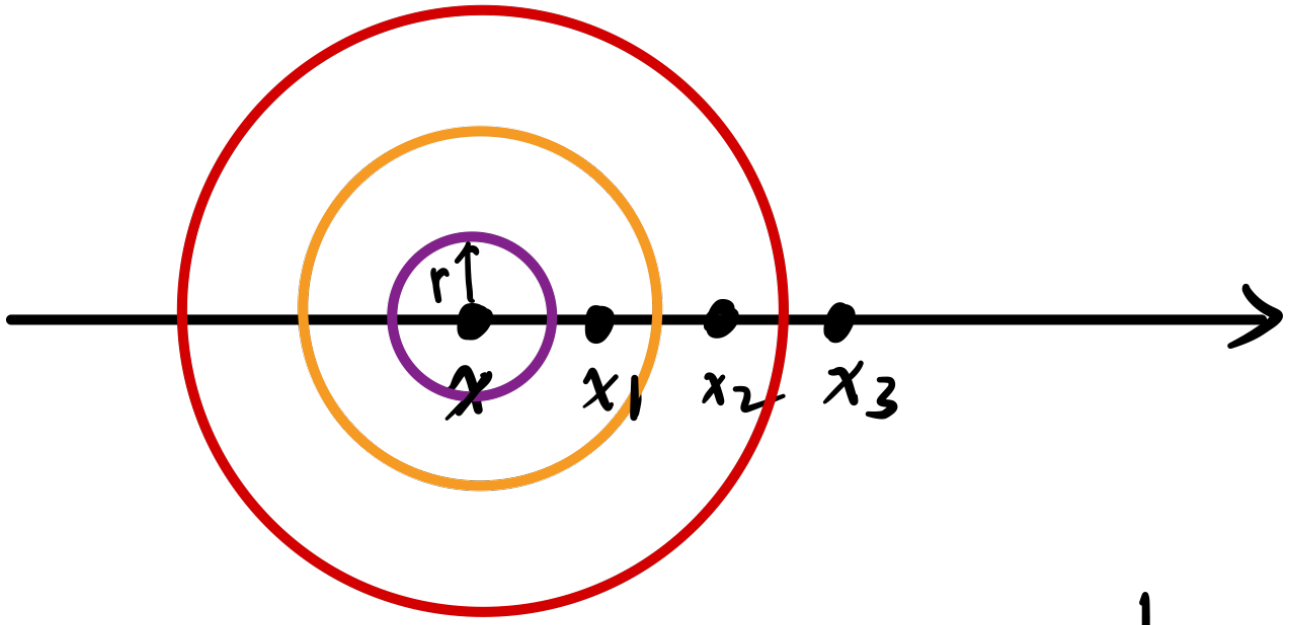
Relation to Distance Function

- Let ν_X denote the uniform measure on a manifold X

> - Theorem [Approximation Distance]:
>
> $\|d_X - d_{\nu_X, m_0}\|_\infty \leq C(X)^{-1/k} m_0^{1/k}$
>
> where X is a k-dimensional smooth manifold and $C(X)$ is a quantity depending on X and k .

- In particular, $\lim_{m \to 0} d_{\nu_X, m} = d_X$

Relation to Distance Function



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- $d^2_{\mu,m_0}(x) = \|x - x_1\|^2 = d_X(x)$ when $m_0 \in (0,1/3)$

Relation to Distance Function

- Now suppose P is sampled from, not compact X, but a probabilistic measure μ on $\mathbb{R}^d$ concentrated on X.
  - Consider P as a noisy sample of X
- Let ν_X denote the uniform measure on X

- Theorem [Approximation Distance]:

$$\left\| d_X - d_{\mu,m_0} \right\|_\infty \leq C(X)^{-\frac{1}{k}} m_0^{\frac{1}{k}} + \frac{1}{\sqrt{m_0}} W_2(\mu, \nu_X)$$

where X is a k-dimensional smooth manifold and $C(X)$ is a quantity depending on X and k .

Topological inference

Theorem [Niyogi, Smale, Weinberger]

Let $P \subset X$ be such that $d_H(X,\ P) \leq \epsilon$. If $2\epsilon \leq \alpha \leq \sqrt{\frac{3}{5}}\rho(X)$, there is a deformation retraction from P^{α} to X .

Topological inference

Corollary 4.11 *Let μ be a measure and K its support. Suppose that μ has dimension at most k and that $\mathrm{reach}_\alpha(d_K) \geq R$ for some $R > 0$. Let μ' be another measure, and let ε be an upper bound on the uniform distance between d_K and d_{μ',m_0}. Then, for any $r \in [4\varepsilon/\alpha^2, R - 3\varepsilon]$, the r-sublevel sets of d_{μ',m_0} and the offsets K^η, for $0 < \eta < R$, are homotopy equivalent, as soon as*

$$\mathrm{W}_2(\mu, \mu') \leq \frac{R\sqrt{m_0}}{5 + 4/\alpha^2} - C(\mu)^{-1/k} m_0^{1/k+1/2}.$$

Noisy sample

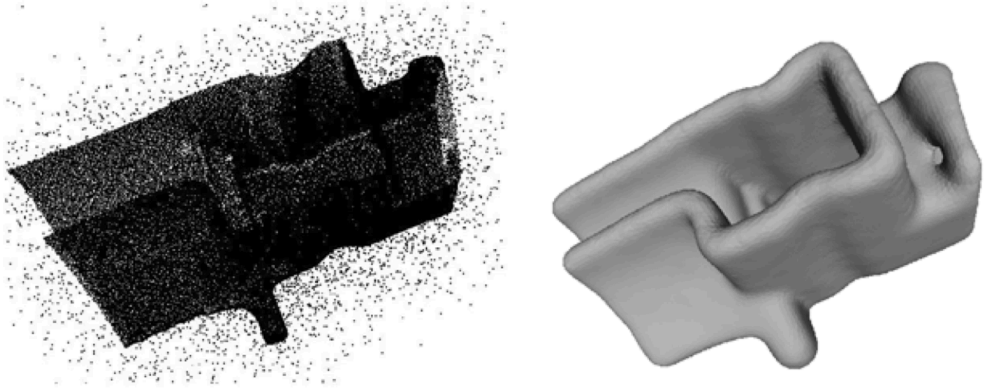


Fig. 1 *Left*: a point cloud sampled on a mechanical part to which 10% of outliers (uniformly sampled in a box enclosing the model) have been added. *Right*: the reconstruction of an isosurface of the distance function d_{μ_C,m_0} to the uniform probability measure on this point cloud

Properties

- Theorem [Distance-Likeness] [Chazal et al 2011]

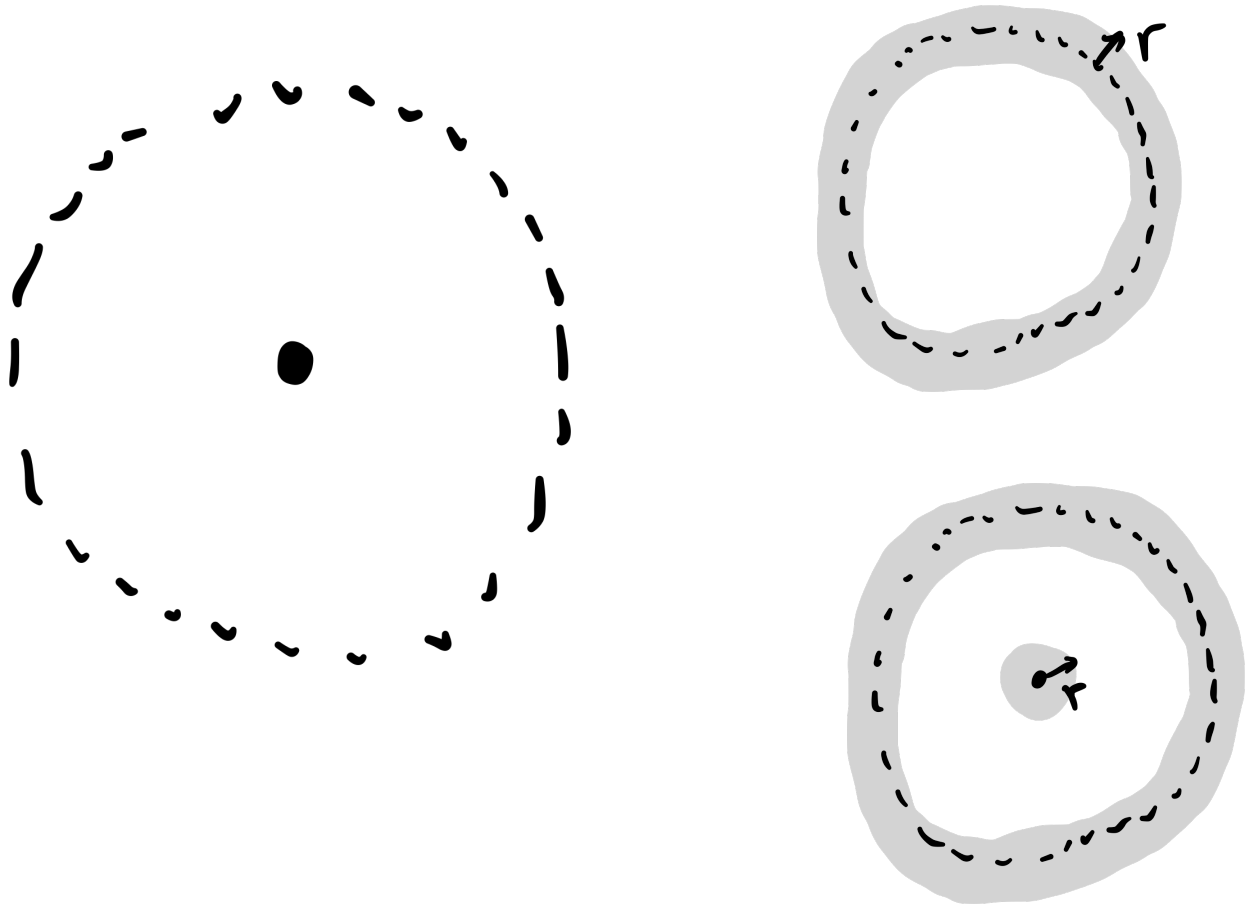
  d_{μ,m_0} is distance like. That is:

  - The function d_{μ,m_0} is 1-Lipschitz.
  - The function d^2_{μ,m_0} is 1-semiconcave, meaning that the map $x \rightarrow d^2_{\mu,\, m_0}(x) - \|x\|^2$ is concave.

- Theorem [Isotopy Lemma]:

  Let ϕ be a distance-like function and $r_1 < r_2$ be two positive numbers such that ϕ has no critical points in the subset $\phi^{-1}\Big(\big[r_1, r_2\big]\Big)$. Then all the sublevel sets $\phi^{-1}\Big(\big[0, r\big]\Big)$ are isotopic for $r \in [r_1, r_2]$.

Sublevel set of distance to measure



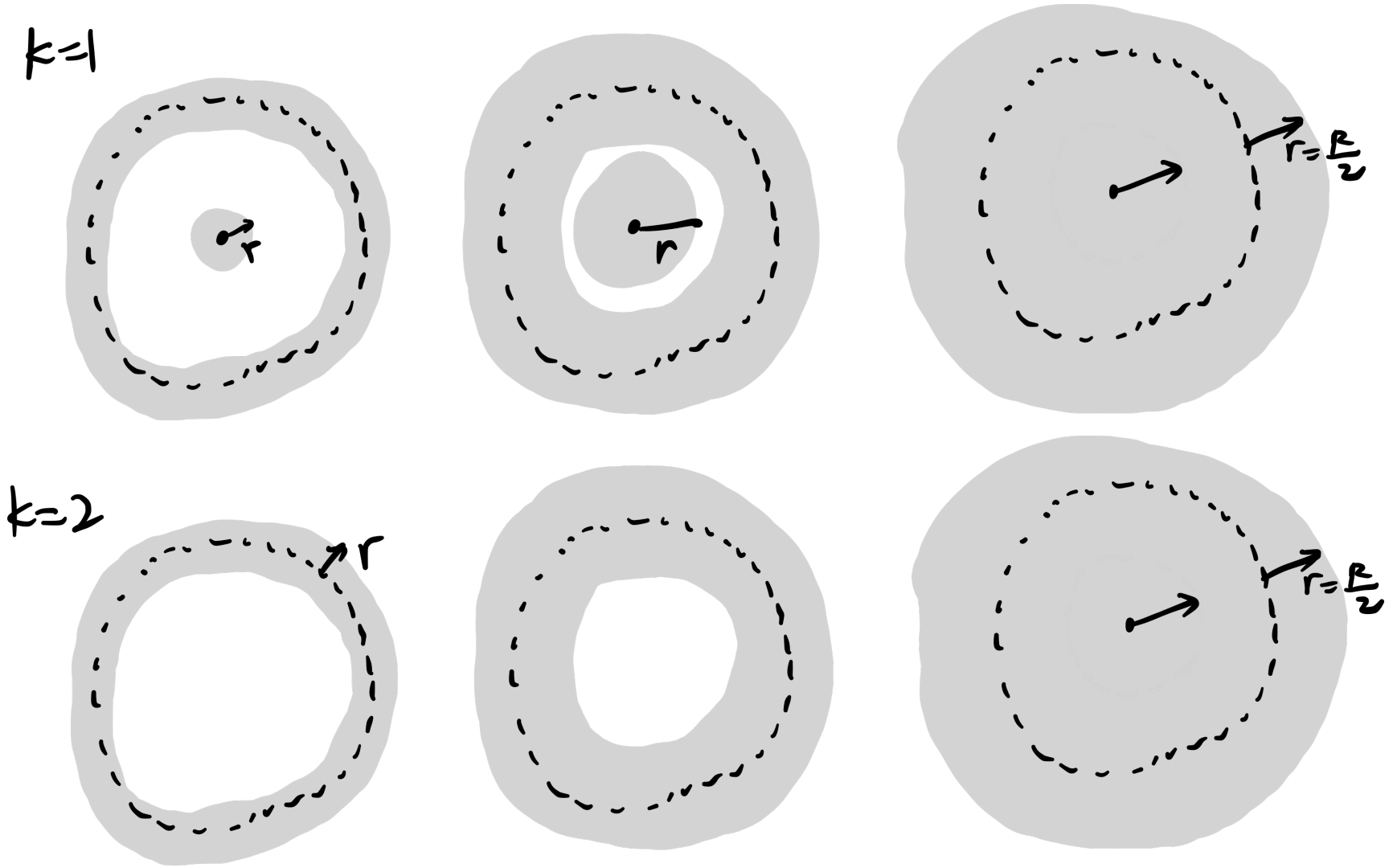
$k=3$

$$d_{\mu,k}(x) = \sqrt{\frac{1}{k}\sum_{q \in kNN(x)} d^2(x,q)} \leq r$$

$$d_X^{-1}(-\infty, r]$$

Sublevel set of distance to measure

$$d_{\mu_P,m}(x) = \sqrt{\frac{1}{k} \sum_{q \in kNN(x)} \|x - q\|^2} =: d_{\mu_P,k}(x)$$



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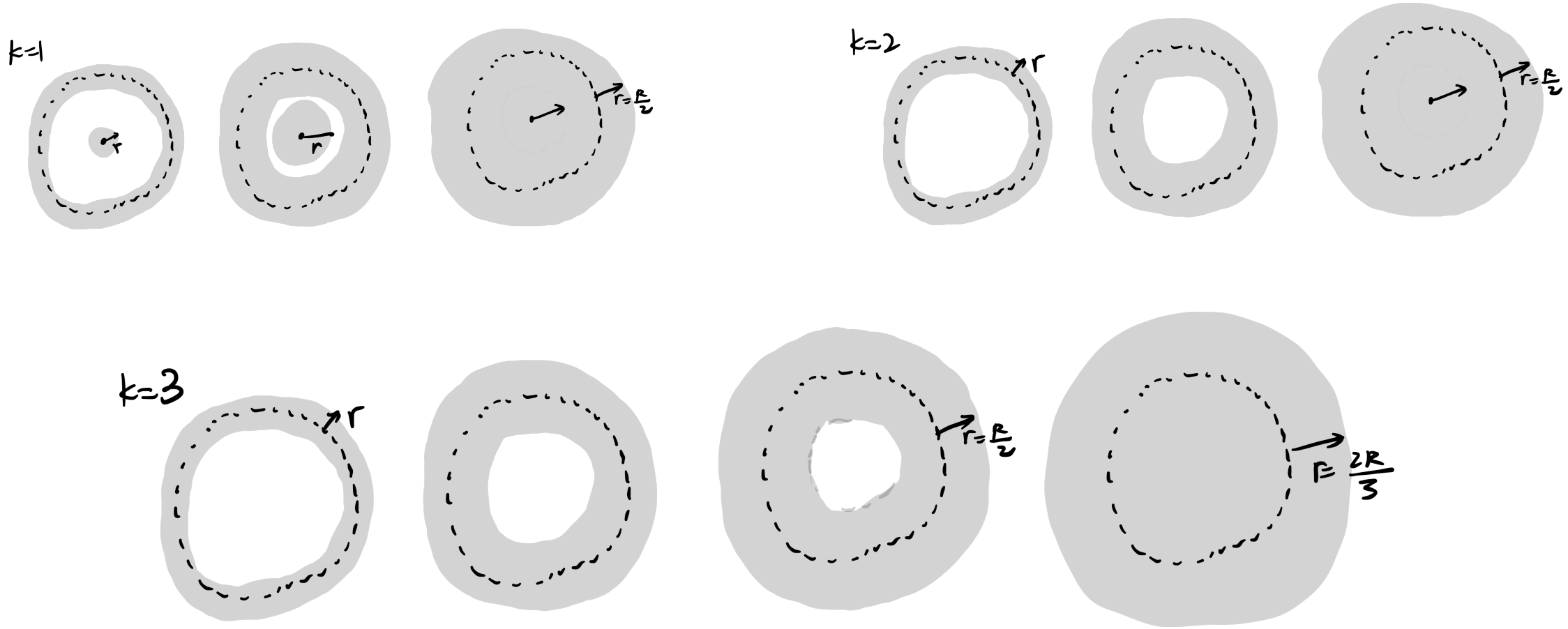


Approximate distance to measure using weighted Rips

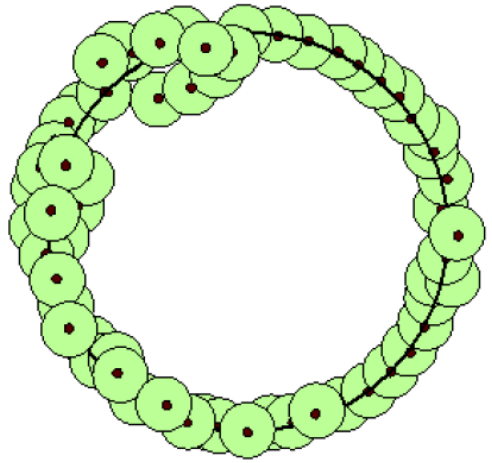
How to use the distance to measures?

- Previous theorem suggests that using distance-to-measure, instead of distance can be used to approximate topology.

Nerve Lemma

- Nerve Lemma (a simplified version):
  - Let $\mathcal{U}$ be a finite collection of closed, convex subsets in R^d. Then $Nrv(\mathcal{U}) \simeq \cup_{\alpha \in A} U_\alpha \subset \mathbb{R}^d$.

- Given a set of points P
  - approximating a hidden domain M
  - $U^r(P) = \bigcup_{p \in P} B(p,\ r)$ approximates M
  - $C^r(P)$ approximates $U^r(P)$



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- Corollary:
  - $C^r(P) \simeq \bigcup_{p \in P} B(p,\ r)$, i.e, $C^r(P)$ is homotopy equivalent to the union of r-balls around points in P

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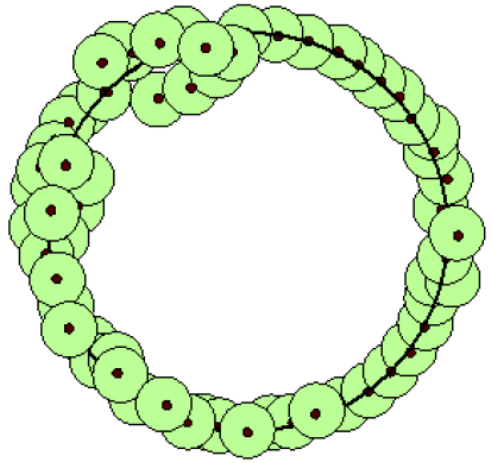

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- In practice, using union of weighted balls of non-uniform radius to approximate hidden space, so that bad points have lower contribution!
- One way to achieve this is through the power-distance
  - [Buchet et al., 2016]

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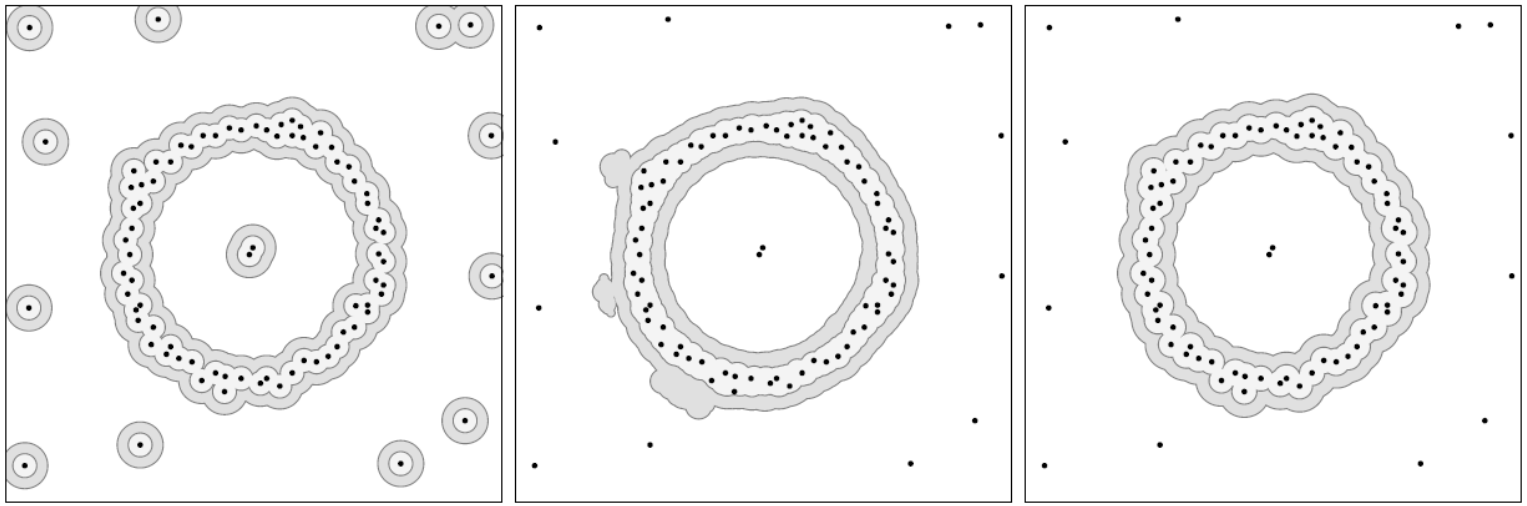

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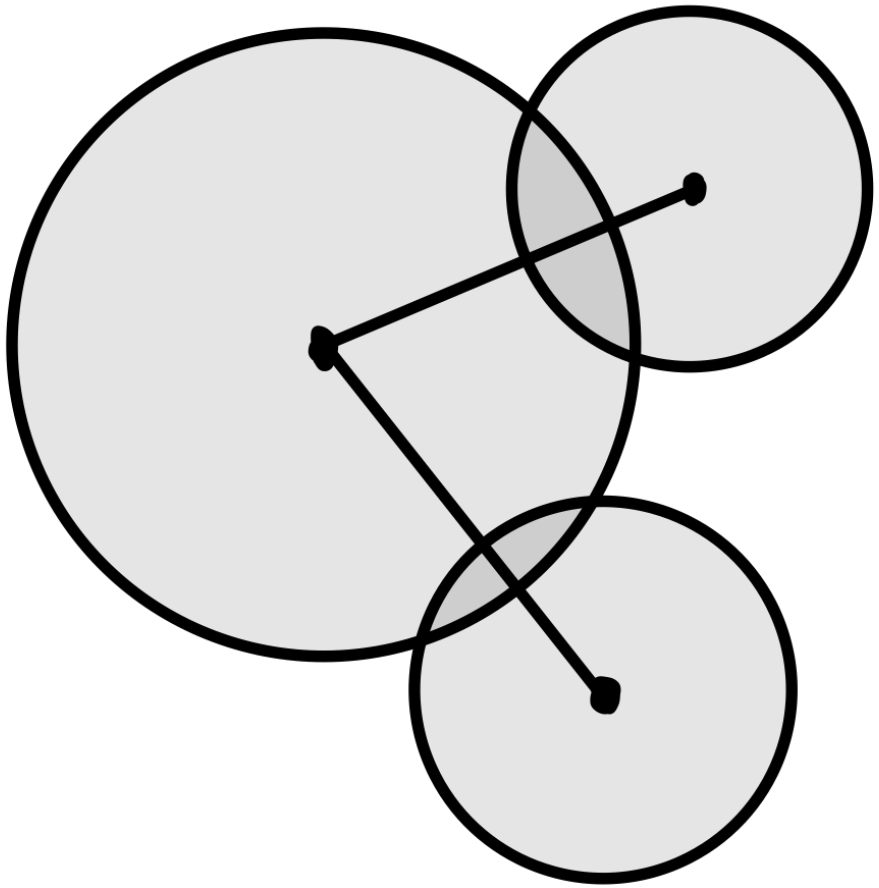
- $wR^{\alpha}(P) = \{\sigma = \left(p_{i_0}, \ \ldots, \ p_{i_s}\right) \mid d\left(p_{i_j}, \ p_{i_{j'}}\right) \leq r_{p_{i_j}}(\alpha) + r_{p_{i_{j'}}}(\alpha), \ \ \forall j \neq j' \in \left[0, s\right]\}$



Weighted Rips Filtration

- Weighted Rips filtration
  - $w\mathcal{F}: \ wR^{\alpha_0}(P) \hookrightarrow \ wR^{\alpha_1}(P) \hookrightarrow \cdots \hookrightarrow \ wR^{\alpha_m}(P)$
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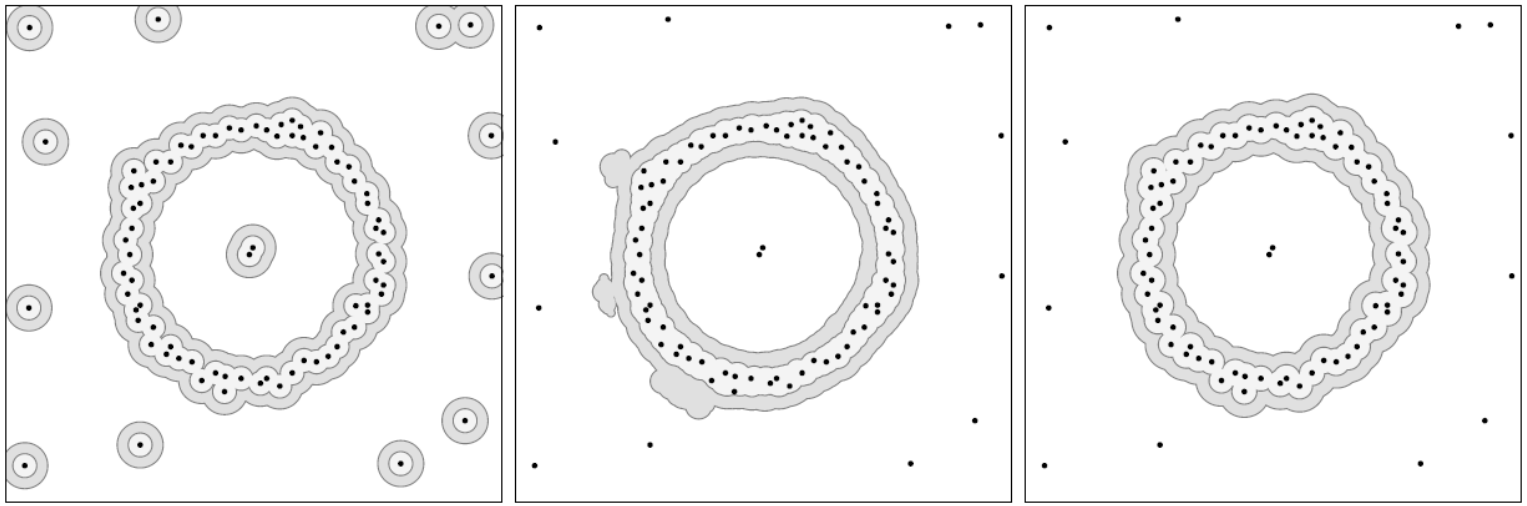

- Gudhi tutorial
- Youtube videos

Section 3:
Data Sparsification

Rips Filtration

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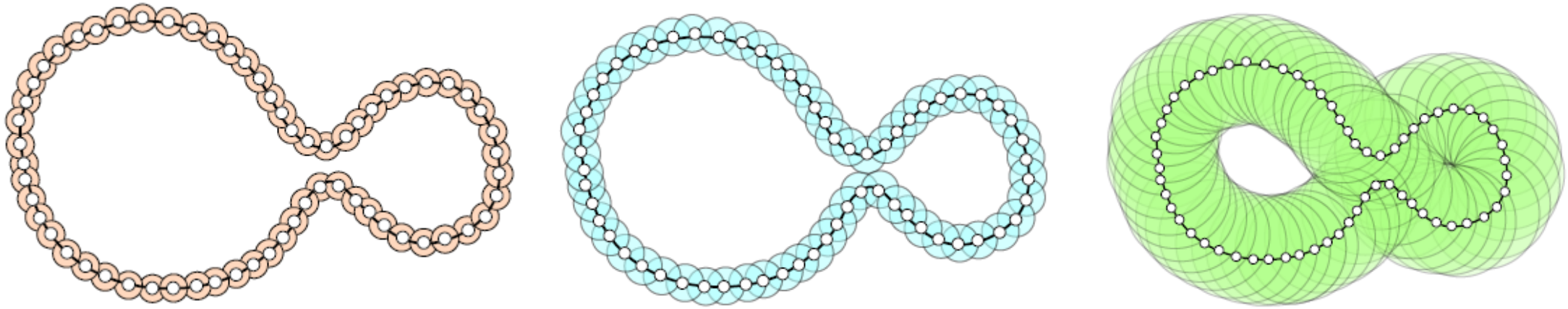
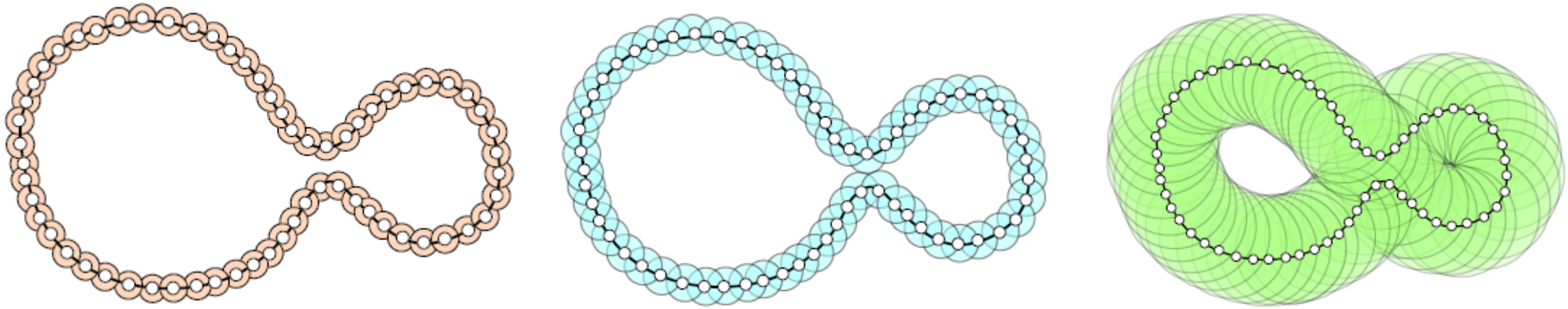


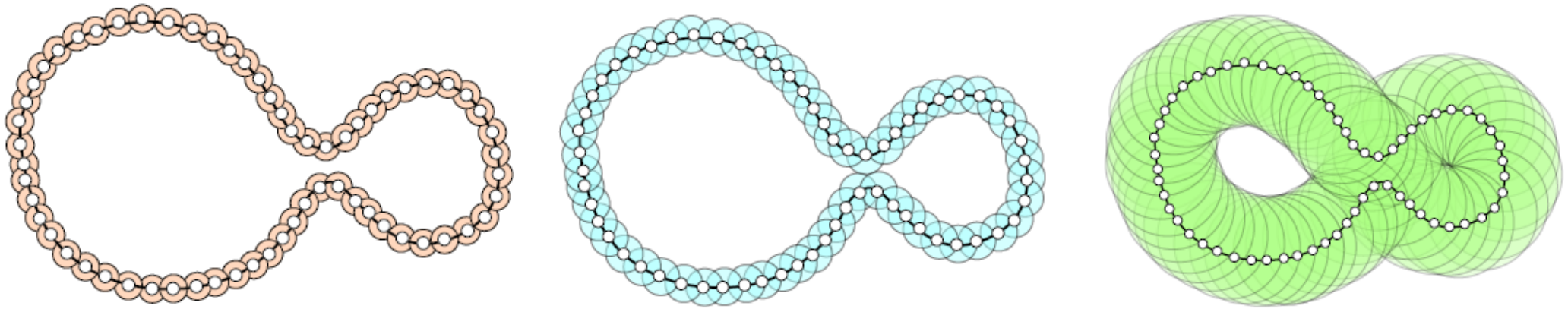
Rips Filtration

- Size becomes huge quickly
- But not all simplices are needed, especially at large scales!



Rips Filtration

- Size becomes huge quickly
- But not all simplices are needed, especially at large scales!
- Idea:
  - Use fewer number of points (balls) at larger scales



- Sheehy 2012
- Cavanna et al. 2015
- Buchet et al. 2016
- A video explanation by *Cavanna, Jahanseir and Sheehy*
  - https://vimeo.com/119603608

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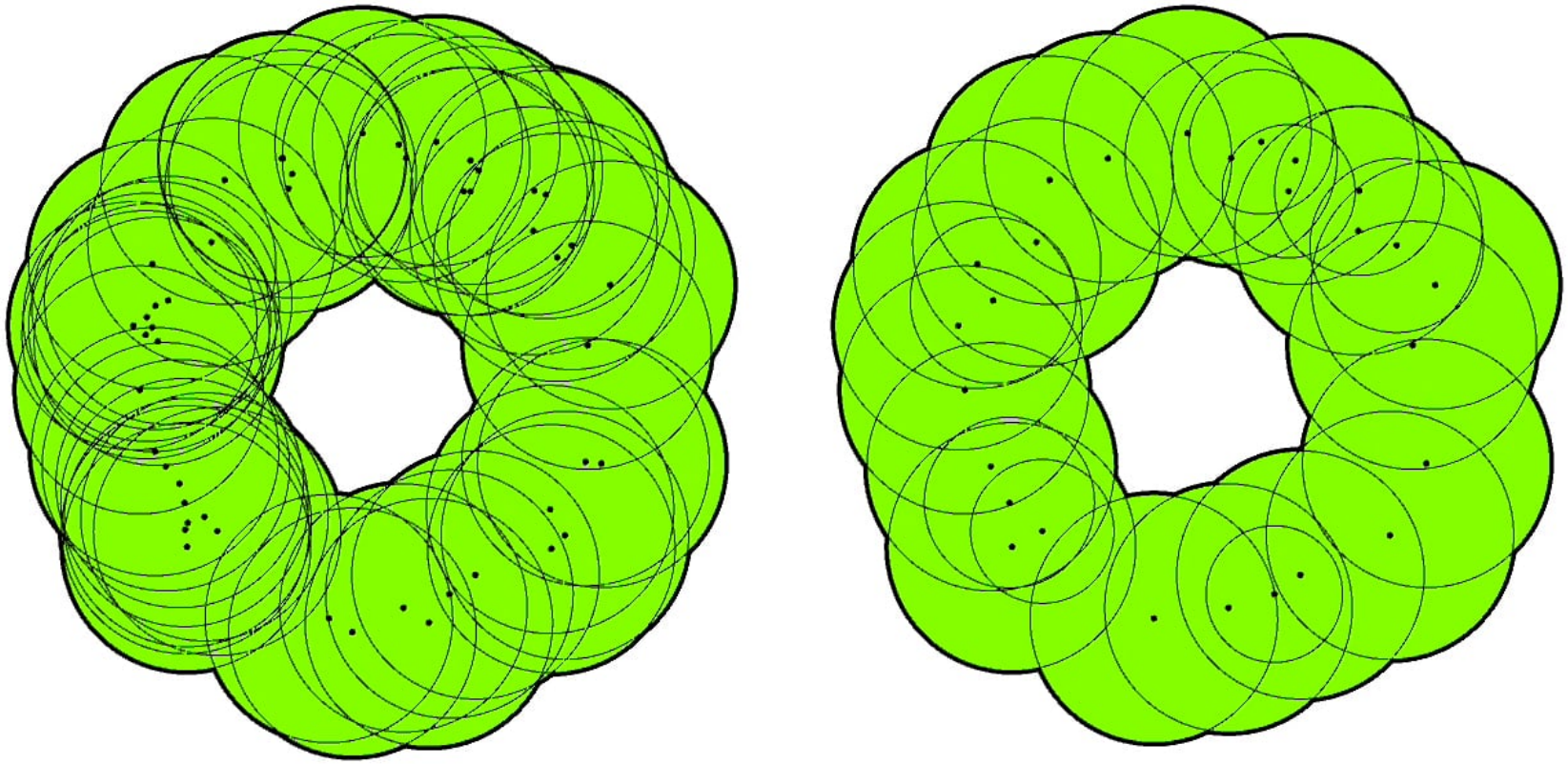

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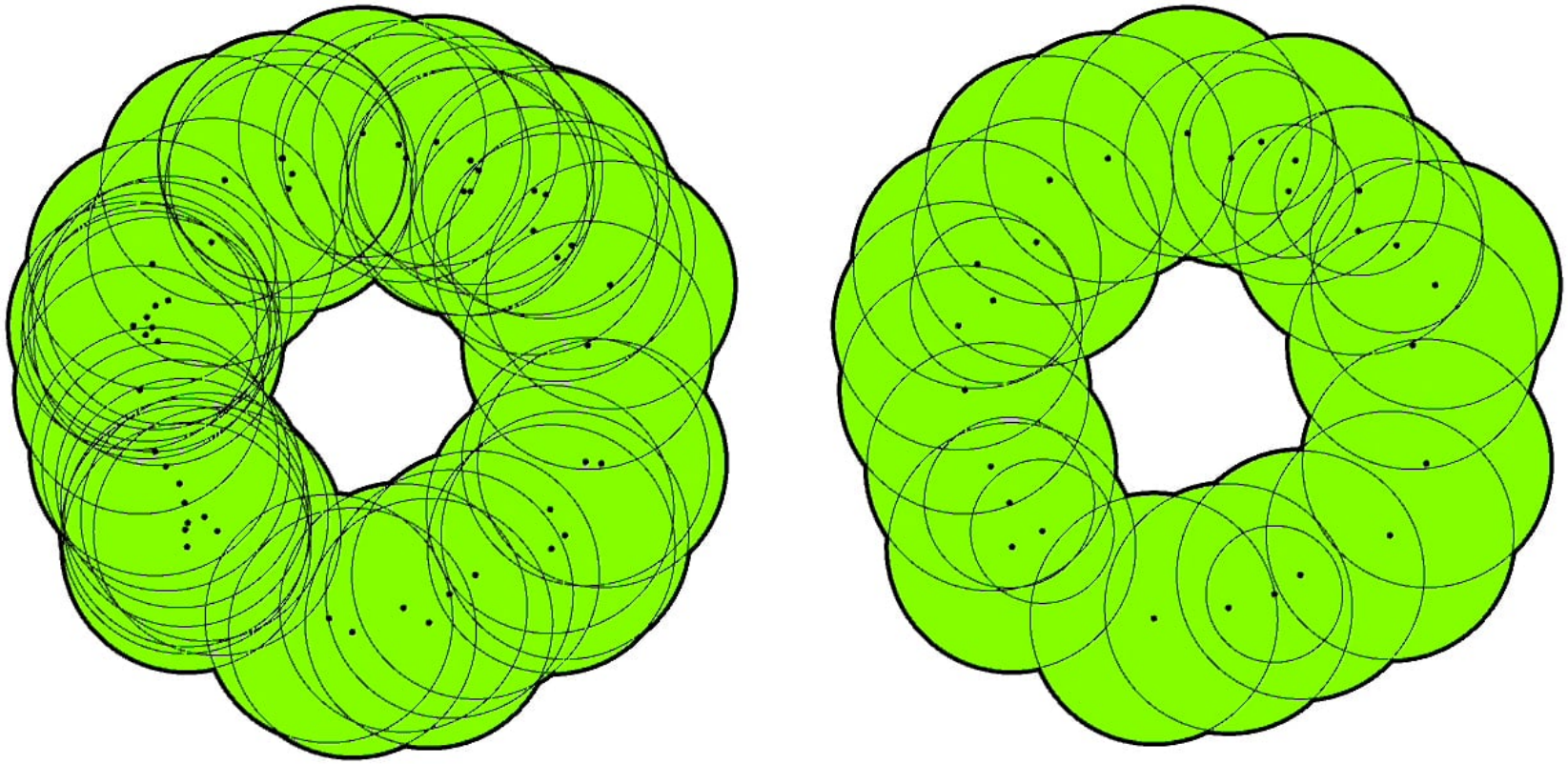

A good subsample

- Given a set of points P, a subset $Q \subseteq P$ is a ε-net of P if
  - (covering-condition): Q is a ε-dense, i.e., for any $p \in P, d(p, Q) \leq \epsilon$, i.e., $d_H(P, Q) \leq \epsilon$
  - (sparsity-condition): Q is a ε-sparse, i.e., for every $q \neq q' \in Q$, $d\left(q,\ q'\right) \geq \varepsilon$

- Covering-condition guarantees that Q represents P well at scale ε
- Sparsity-condition makes sure Q is not overly dense, thus is of small cardinality

How to generate an ϵ-net?

- Given input point set $P \subset R^d$
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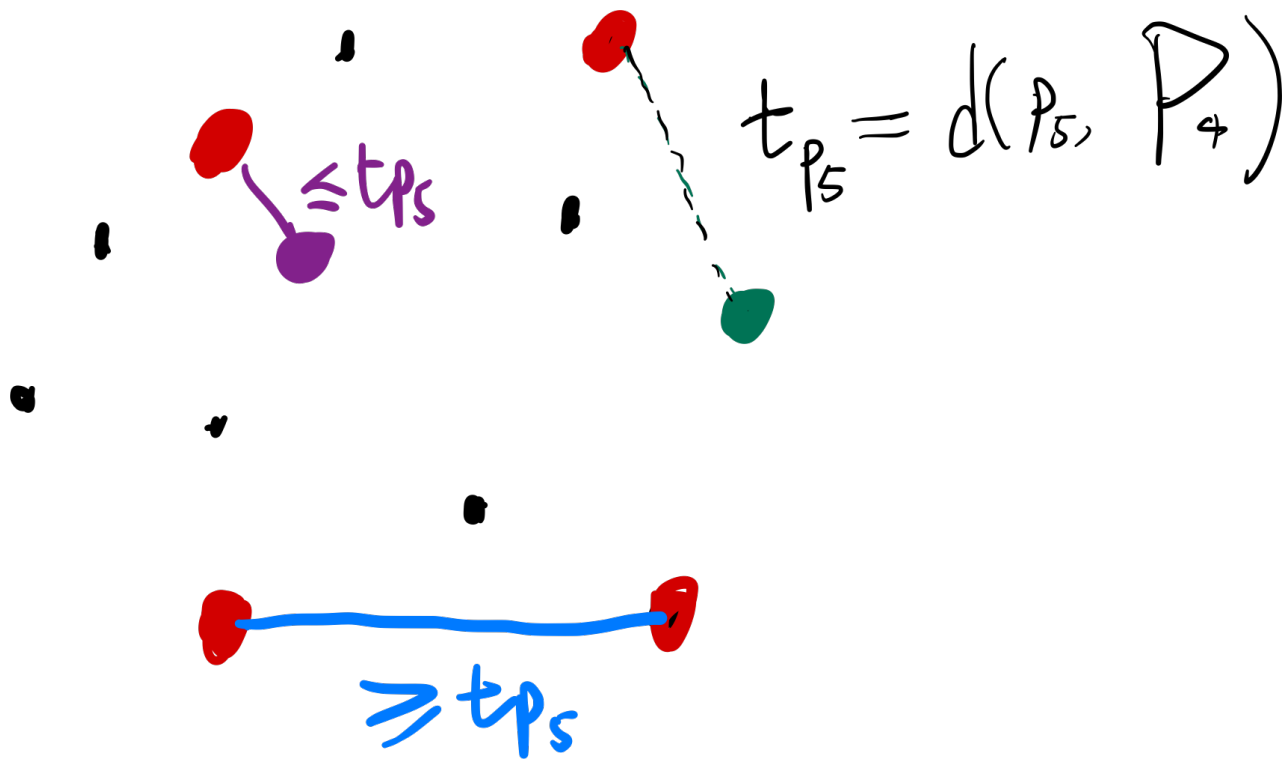

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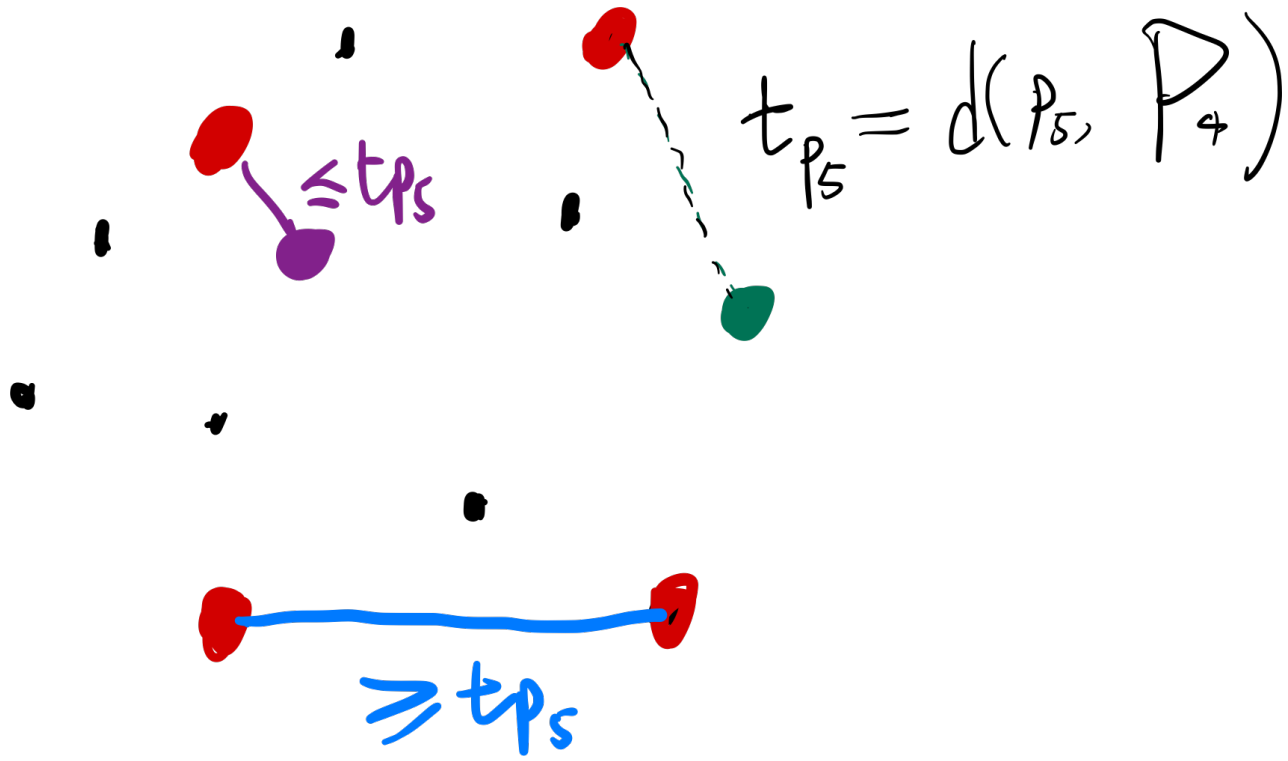

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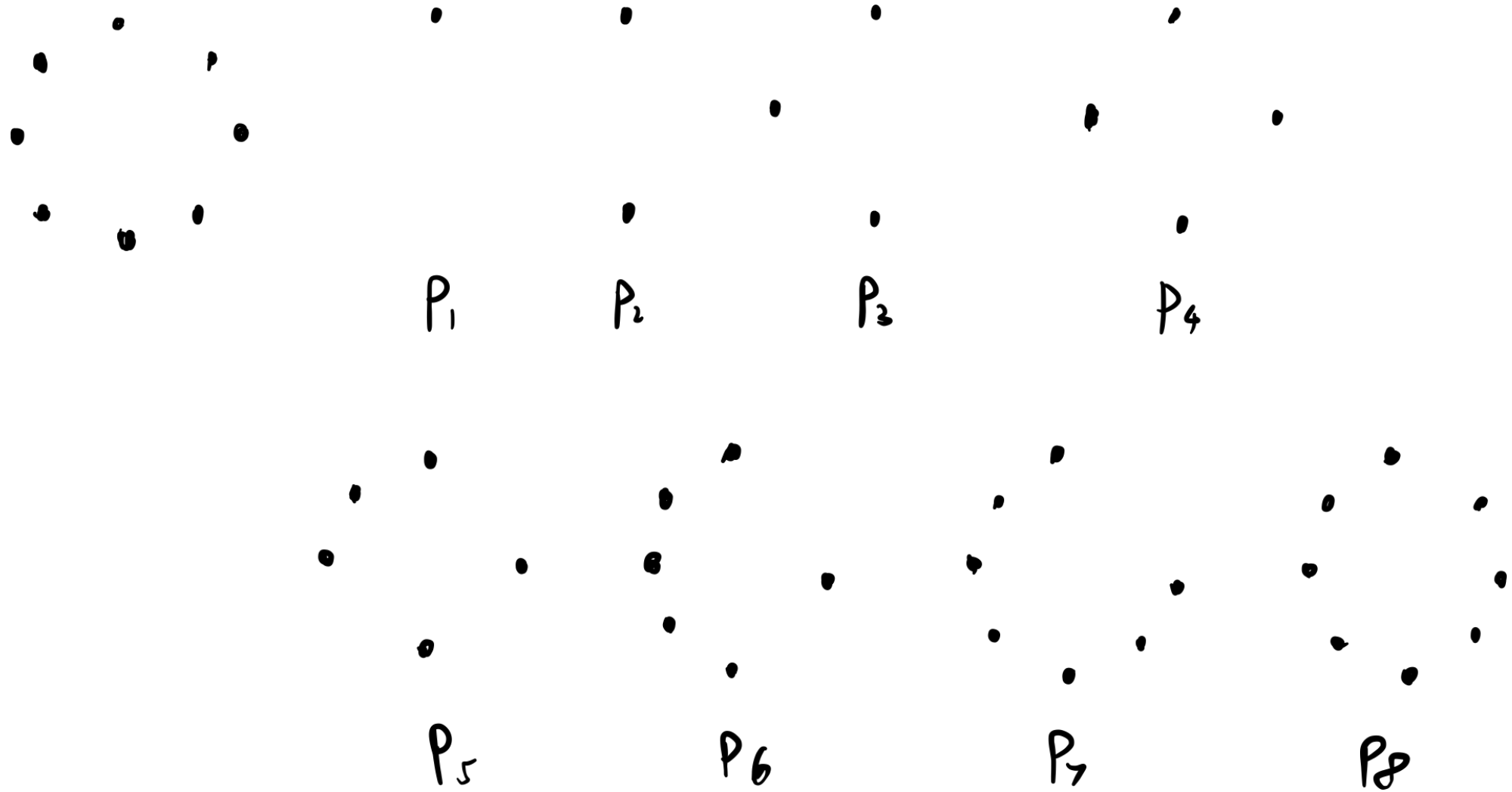
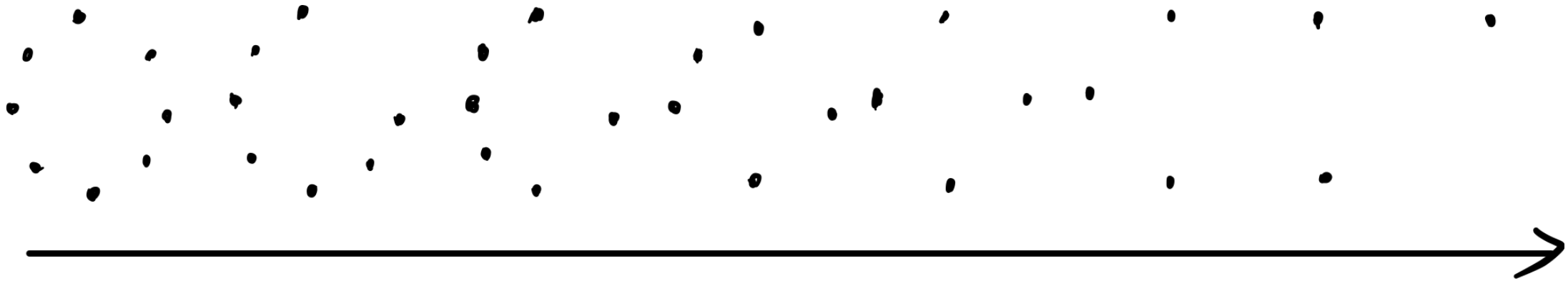
- Exit-time of $p = p_i$ is set to be $t_{p_i} := d(p_i, P_{i-1})$
- Construct two families of γ-nets:

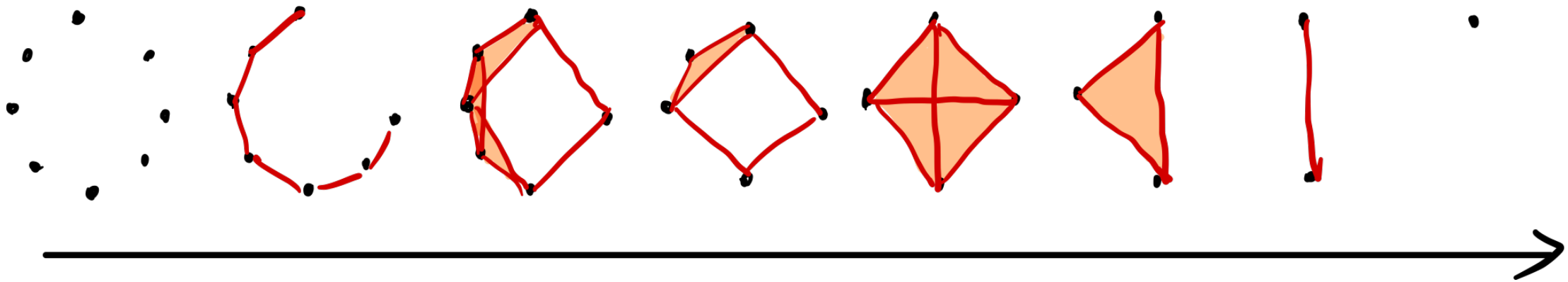
$$\textit{Open net-tower } \mathcal{N} = \{N_\gamma\}_{\gamma \in \mathbb{R}} \text{ where } N_\gamma := \{p \in P \mid t_p > \gamma\}.$$

$$\textit{Closed net-tower } \overline{\mathcal{N}} = \{\overline{N}_\gamma\}_{\gamma \in \mathbb{R}} \text{ where } \overline{N}_\gamma := \{p \in P \mid t_p \geq \gamma\}.$$

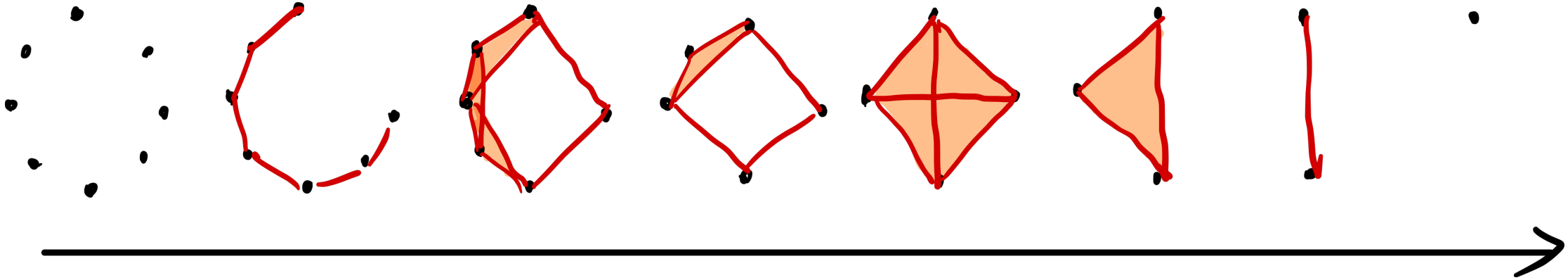
Example

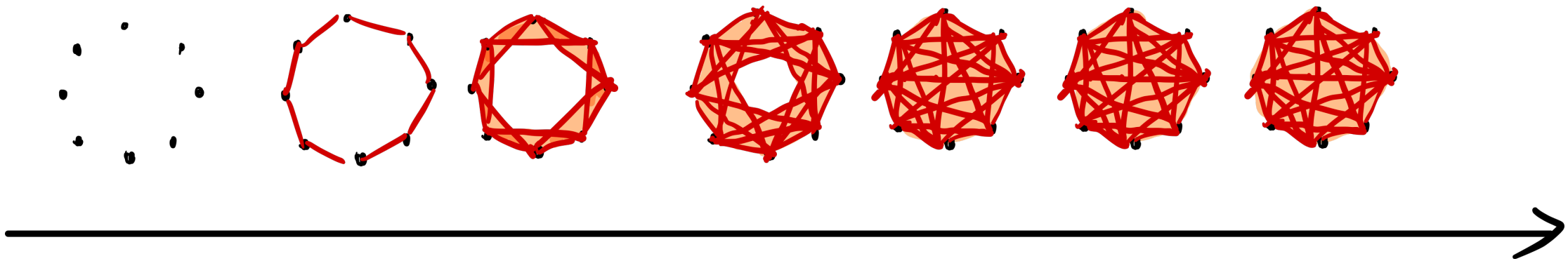




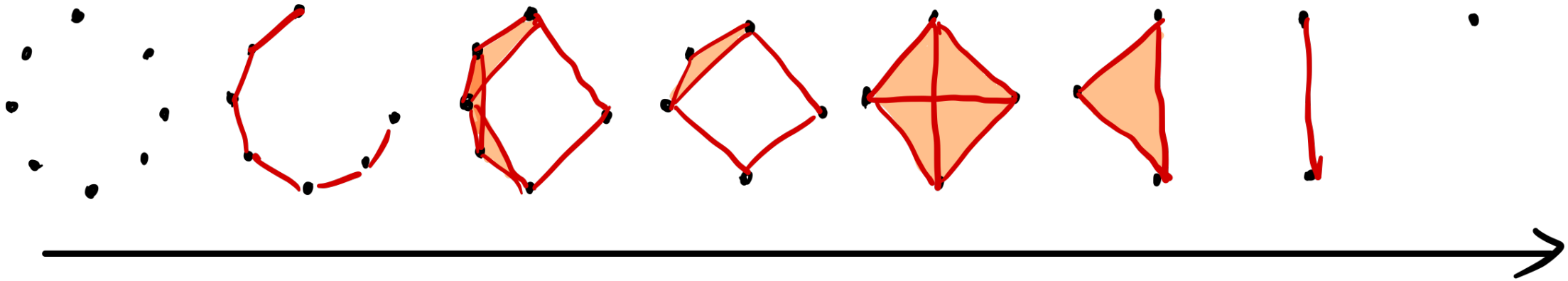


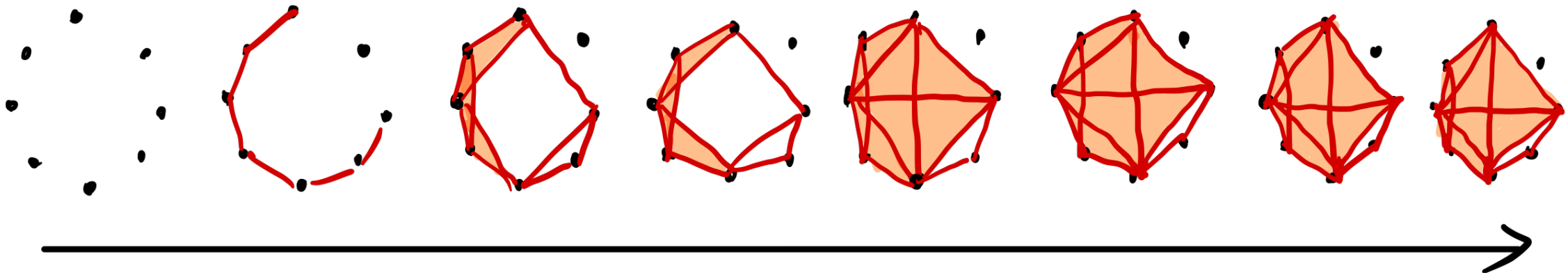
A Sparse Rips filtration





Rips filtration

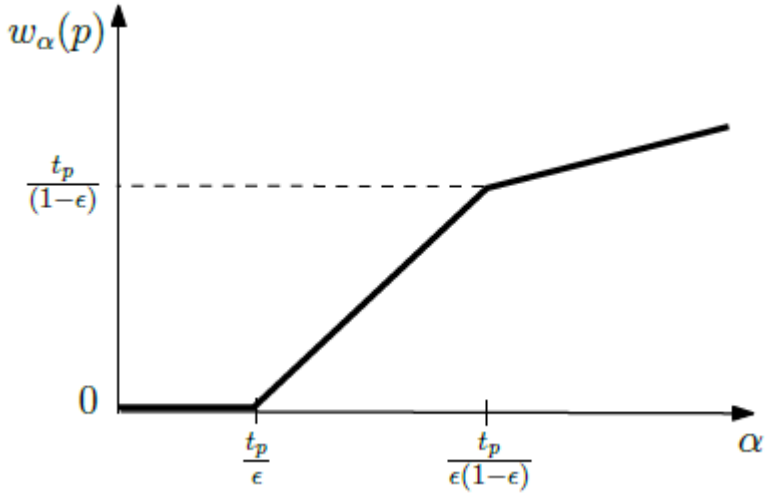




Weights and weighted distance

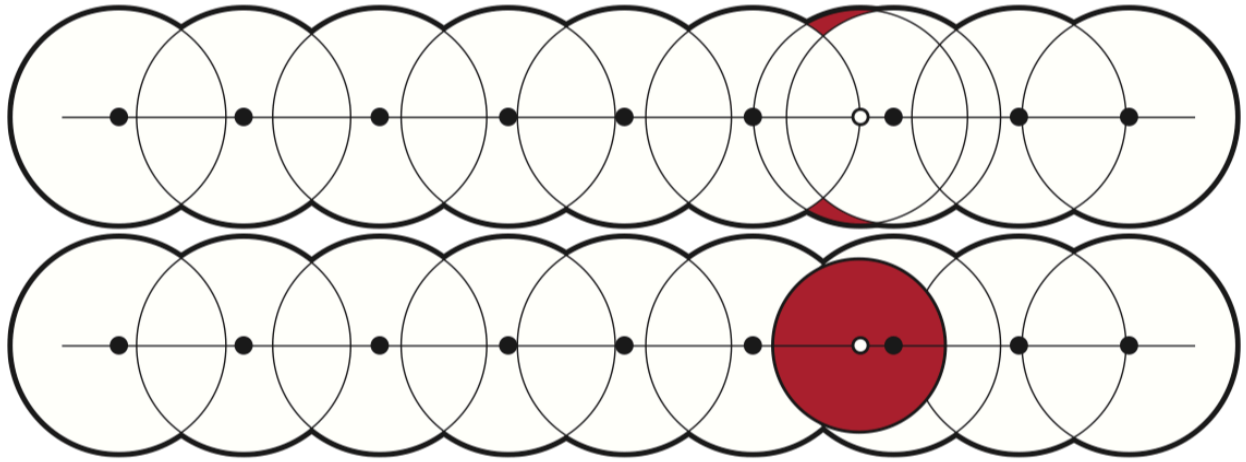
- Using exit-time, we assign a weight $w_p(\alpha)$ for each point p at scale α

$$w_p(\alpha) = \begin{cases} 0 & \frac{t_p}{\varepsilon} \geq \alpha \\ \alpha - \frac{t_p}{\varepsilon} & \frac{t_p}{\varepsilon} < \alpha < \frac{t_p}{\varepsilon(1-\varepsilon)} \\ \varepsilon\alpha & \frac{t_p}{\varepsilon(1-\varepsilon)} \leq \alpha \end{cases}$$

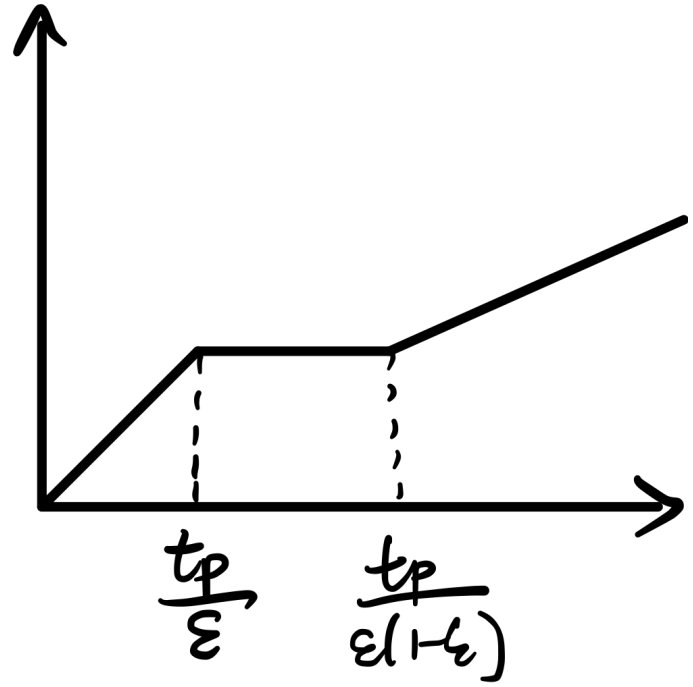


- Net-induced distance at scale α is:
  - $\hat{d}_\alpha(p,\ q) = d(p,\ q) + w_p(\alpha) + w_q(\alpha)$

- $\hat{d}_\alpha(p,q) \leq 2\alpha$ means two balls $B(p, r_p(\alpha))$ and $B(q, r_q(\alpha))$ have intersection where
- $r_p(\alpha) = \alpha - w_p(\alpha)$



Courtesy of Sheehy 2012



- Let $\hat{VR}^{\alpha}(P) = \{\sigma : \hat{d}(p,q) \leq 2\alpha \text{ for } p,q \in \sigma\}$
- $VR^{\alpha(1-\epsilon)}(P) \subseteq \hat{VR}^{\alpha}(P) \subseteq VR^{\alpha}(P)$

Sparse Rips complexes

Definition 6.5 (Sparse (Vietoris-)Rips)**.** Given a set of points $P \subset \mathbb{R}^d$, a constant $0 < \epsilon < 1/3$, and the open net-tower $\{N_\gamma\}$ as well as the closed net-tower $\{\overline{N}_\gamma\}$ for P as introduced above, the *open sparse-Rips complex at scale* α is defined as

$$\mathsf{Q}^\alpha := \{\sigma \subseteq N_{\varepsilon(1-\varepsilon)\alpha} \mid \forall p, q \in \sigma,\ \widehat{\mathsf{d}}_\alpha(p,q) \leq 2\alpha\}; \tag{6.9}$$

while the *closed sparse-Rips at scale* α is defined as

$$\overline{\mathsf{Q}}^\alpha := \{\sigma \subseteq \overline{N}_{\varepsilon(1-\varepsilon)\alpha} \mid \forall p, q \in \sigma,\ \widehat{\mathsf{d}}_\alpha(p,q) \leq 2\alpha\}. \tag{6.10}$$

Set $\mathsf{S}^\alpha := \cup_{\beta \leq \alpha} \overline{\mathsf{Q}}^\alpha$, which we call the *cumulative complex at scale* α. The *(ε-)sparse Rips filtration* then refers to the $\mathbb{R}$-indexed filtration $\mathcal{S} = \{\mathsf{S}^\alpha \hookrightarrow \mathsf{S}^\beta\}_{\alpha \leq \beta}$.

- Larger ϵ corresponds to sparser complexes
- S and $\hat{VR}$ has the same barcodes!!

Guarantee of Sparse Rips Filtration

Theorem 6.4. *Let $P \subset \mathbb{R}^d$ be a set of n points where d is a constant, and $\mathcal{R}(P) = \{\mathbb{VR}^r(P)\}$ be the Vietoris-Rips filtration over P. Given net-towers $\{N_\gamma\}$ and $\{\overline{N}_\gamma\}$ induced by exit-times $\{\mathsf{t}_p\}_{p\in P}$, let $\mathcal{S}(P) = \{\mathsf{S}^\alpha\}$ be its corresponding ε-sparse Rips filtration as defined in Definition 6.5. Then, for a fixed $0 < \varepsilon < \frac{1}{3}$,*

(i) $\mathcal{S}(P)$ and $\mathcal{R}(P)$ are multiplicatively $\frac{1}{1-\varepsilon}$-interleaved at the homology level. Thus, for any $k \geq 0$, the persistence diagram $\mathrm{Dgm}_k\mathcal{S}(P)$ is a $\log\frac{1}{1-\varepsilon}$-approximation of $\mathrm{Dgm}_k\mathcal{R}(P)$ at the log-scale.

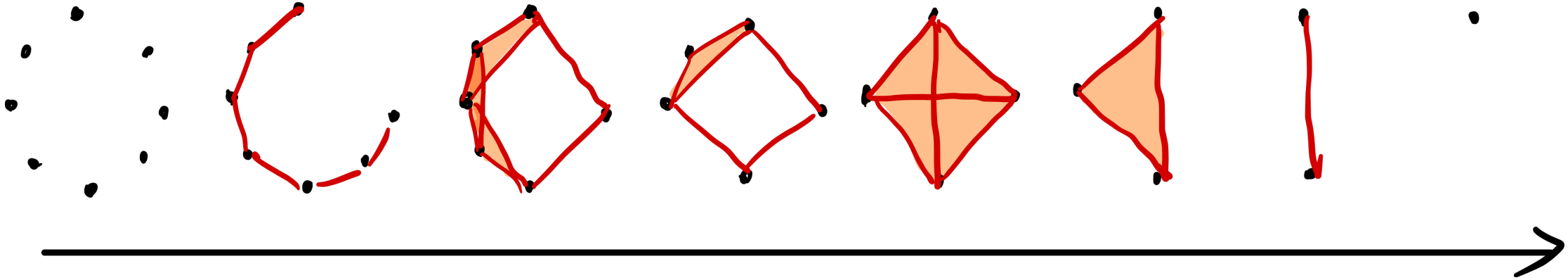
(ii) For any fixed dimension $k \geq 0$, the total number of k-simplices ever appeared in $\mathcal{S}(P)$ is $\Theta((\frac{1}{\varepsilon})^{kd}n)$.

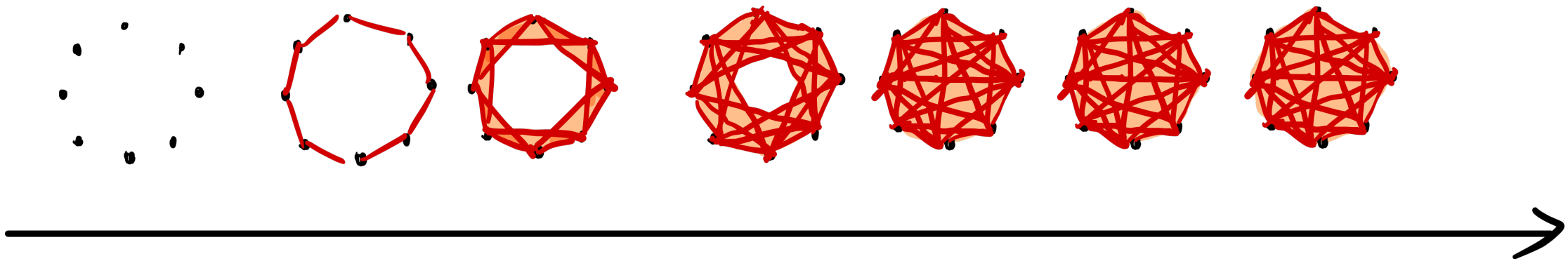
- Finally, this sparsification strategy can be extended to handle weighted Rips filtration w.r.t. distance to measures.
  - [Buchet, Chazal, Oudot, Sheehy, CGTA 2016]

- An implementation in Ripser
- Giotto-TDA

A more aggressive approach

A Sparse Rips filtration





Rips filtration

Approximation via simplicial tower

- Given a set of points $P \subset \mathbb{R}^d$, $\alpha > 0$ and some $0 < \varepsilon < 1$, consider the following filtration, which is a subsequence of standard Rips filtration:

$$\mathbb{VR}^{\alpha}(P) \hookrightarrow \mathbb{VR}^{\alpha(1+\varepsilon)}(P) \hookrightarrow \mathbb{VR}^{\alpha(1+\varepsilon)^2}(P) \hookrightarrow \cdots \hookrightarrow \mathbb{VR}^{\alpha(1+\varepsilon)^m}(P).$$

- We will aim to approximate the above sequence via a sequence of sparsified simplicial complexes connected by simplicial maps (not inclusions)

Nets, and induced Rips complexes

- Set $P_0 := P$. Build a sequence of point sets $P_1, \ldots, P_m$ such that
  - P_{k+1} is a $\left(\frac{\alpha\varepsilon}{2}\right)(1+\varepsilon)^{k-1}$-net of P_k
  - Terminates when P_m is of constant size.

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  - where $\pi_k(p) = argmin_{q \in P_{k+1}} d(p, q)$

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- Claim:
  - π_k induces a simplicial map $\pi_k : \mathbb{VR}^{\alpha(1+\varepsilon)^k}(P_k) \to \mathbb{VR}^{\alpha(1+\varepsilon)^{k+1}}(P_{k+1})$

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- This thus gives rise to the following simplicial tower:

$$\widehat{\mathcal{S}} : \mathbb{VR}^{\alpha}(P_0) \xrightarrow{\pi_0} \mathbb{VR}^{\alpha(1+\varepsilon)}(P_1) \xrightarrow{\pi_1} \cdots \xrightarrow{\pi_{m-1}} \mathbb{VR}^{\alpha(1+\varepsilon)^m}(P_m).$$

Theoretical Guarantee

Theoretical Guarantee

Theorem 6.8. *Given a set of n points $P \subset \mathbb{R}^d$, we can $3\log(1+\varepsilon)$-approximate the persistence diagram of the discrete Rips filtration in Eqn. (6.12) by that of the filtration in Eqn. (6.13) at the log-scale. The number of k-simplices that ever appear in the filtration in Eqn. (6.13) is $O((\frac{1}{\varepsilon})^{O(kd)}n)$.*

- SimBa

FIN