

Some Topics in Computational Topology

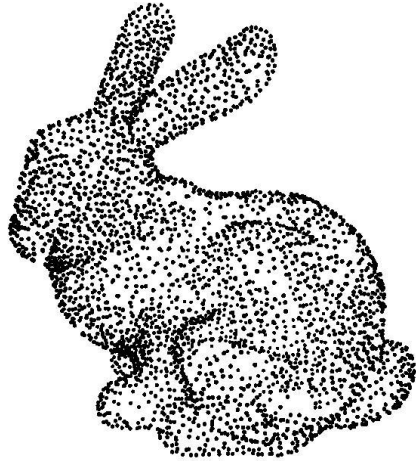
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AMS Short Course 2014

Introduction

- ▶ Much recent developments in computational topology
 - ▶ Both in theory and in their applications
 - ▶ E.g, the theory of persistence homology
 - ▶ *[Edelsbrunner, Letscher, Zomorodian, DCG 2002], [Zomorodian and Carlsson, DCG 2005], [Carlsson and de Silva, FoCM 2010], ...*
- ▶ This short course:
 - ▶ A computational perspective:
 - ▶ Estimation and inference of topological information / structure from point clouds data



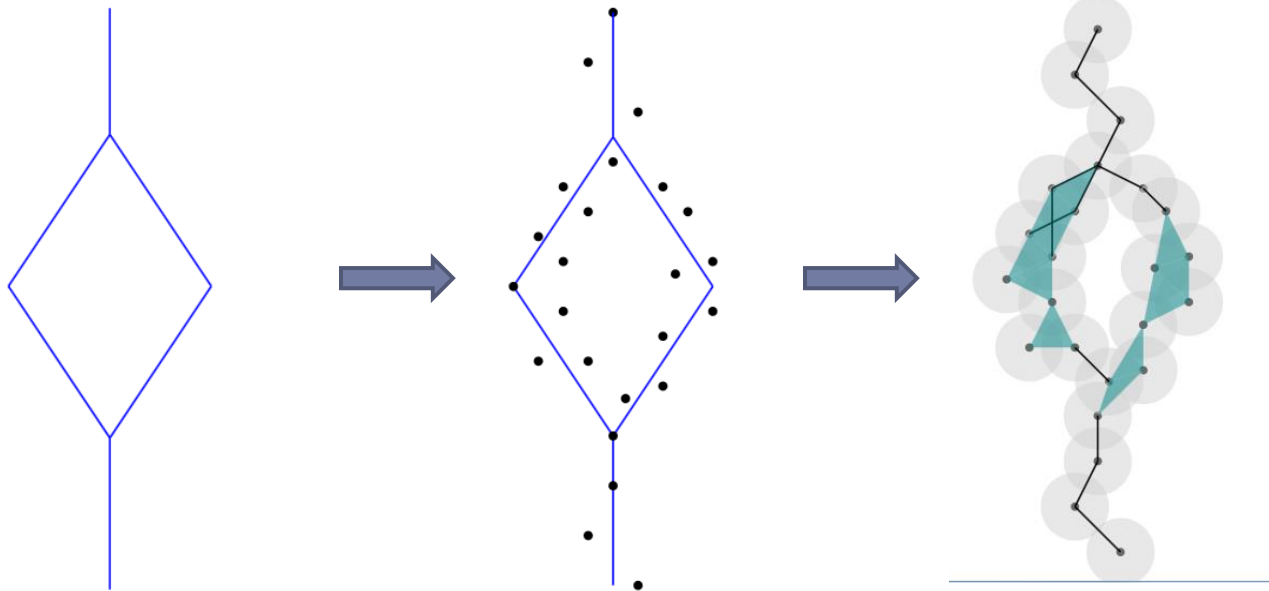


Topological summary
of hidden space

- ▶ Develop discrete analog for the continuous case
- ▶ Approximation from discrete samples with theoretical guarantees
- ▶ Algorithmic issues



Main Topics



- ▶ From PCDs to simplicial complexes
- ▶ Sampling conditions
- ▶ Topological inferences



Outline

- ▶ **From PCDs to simplicial complexes**
 - ▶ Delaunay, Čech, Vietoris-Rips, witness complexes
 - ▶ Graph induced complex

- ▶ **Sampling conditions**
 - ▶ Local feature size, and homological feature size

- ▶ **Topology inference**
 - ▶ Homology inference
 - ▶ Handling noise
 - ▶ *Approximating cycles of shortest basis of the first homology group*
 - ▶ *Approximating Reeb graph*

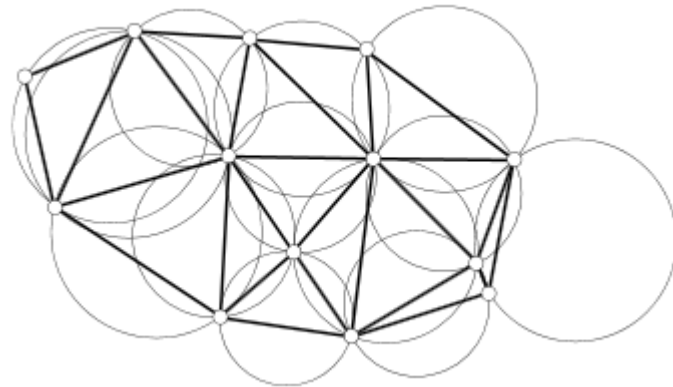


Choice of Simplicial Complexes



Delaunay Complex

- ▶ Given a set of points $P = \{p_1, p_2, \dots, p_n\} \subset R^d$
- ▶ Delaunay complex $Del(P)$
 - ▶ A simplex $\sigma = [p_{i_0}, p_{i_1}, \dots, p_{i_k}]$ is in $Del(P)$ if and only if
 - ▶ There exists a ball B whose boundary contains vertices of σ , and that the interior of B contains no other point from P .



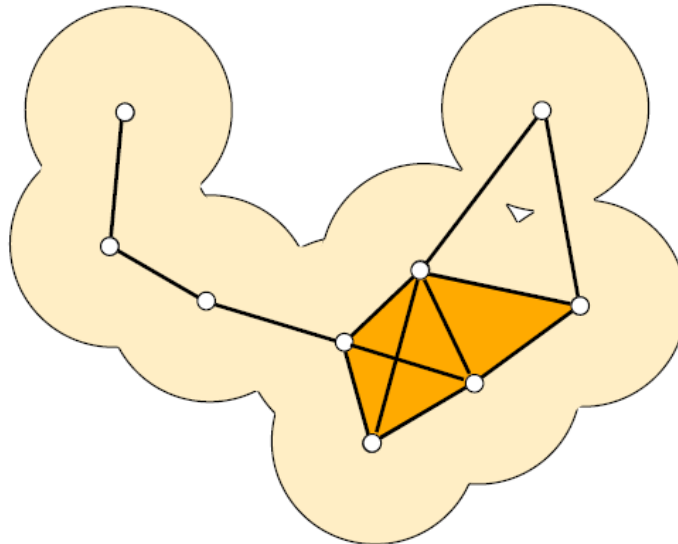
Delaunay Complex

- ▶ Many beautiful properties
 - ▶ Connection to Voronoi diagram
- ▶ Foundation for surface reconstruction and meshing in 3D
 - ▶ *[Dey, Curve and Surface Reconstruction, 2006],*
 - ▶ *[Cheng, Dey and Shewchuk, Delaunay Mesh Generation, 2012]*
- ▶ However,
 - ▶ Computationally very expensive in high dimensions



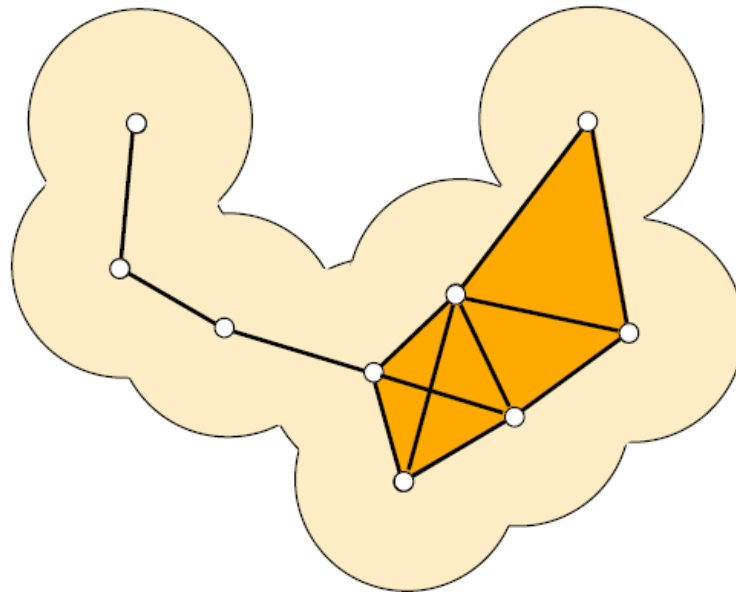
Čech Complex

- ▶ Given a set of points $P = \{p_1, p_2, \dots, p_n\} \subset R^d$
- ▶ Given a real value $r > 0$, the **Čech complex** $C^r(P)$ is the nerve of the set $\{B(p_i, r)\}_{i \in [1, n]}$
 - ▶ where $B_r(p_i) = B(p_i, r) = \{x \in R^d \mid d(p_i, x) < r\}$
- ▶ The definition can be extended to a finite sample P of a metric space.



Rips Complex

- ▶ Given a set of points $P = \{p_1, p_2, \dots, p_n\} \subset R^d$
- ▶ Given a real value $r > 0$, the *Vietoris-Rips (Rips) complex* $R^r(P)$ is:
 - ▶ $\{(p_{i_0}, p_{i_1}, \dots, p_{i_k}) \mid B_r(p_{i_l}) \cap B_r(p_{i_j}) \neq \emptyset, \forall l, j \in [0, k]\}$.



Rips and Čech Complexes

- ▶ **Relation in general metric spaces**
 - ▶ $C^r(P) \subseteq R^r(P) \subseteq C^{2r}(P)$
 - ▶ Bounds better in Euclidean space
- ▶ **Simple to compute**
- ▶ **Able to capture geometry and topology**
 - ▶ We will make it precise shortly
 - ▶ One of the most popular choices for topology inference in recent years

- ▶ **However:**
 - ▶ Huge sizes
 - ▶ Computation also costly



Witness Complexes

- ▶ A simplex $\sigma = \{q_0, \dots, q_k\}$ is *weakly witnessed* by a point x if $d(q_i, x) \leq d(q, x)$ for any $i \in [0, k]$ and $q \in Q \setminus \{q_0, \dots, q_k\}$.
- ▶ Given a set of points $P = \{p_1, p_2, \dots, p_n\} \subset R^d$ and a subset $Q \subseteq P$
- ▶ The *witness complex* $W(Q, P)$ is the collection of simplices with vertices from Q whose all subsimplices are weakly witnessed by a point in P .
 - ▶ *[de Silva and Carlsson, 2004] [de Silva 2003]*
 - ▶ Can be defined for a general metric space
 - ▶ P does not have to be a finite subset of points



Witness Complexes

- ▶ **Greatly reduce size of complex**
 - ▶ Similar to Delaunay triangulation, remove redundancy
- ▶ **Relation to Delaunay complex**
 - ▶ $W(Q, P) \subseteq Del Q$
 - ▶ $W(Q, R^d) = Del Q$
 - ▶ $W(Q, M) = Del|_M Q$ if $M \subseteq R^d$ is a smooth 1- or 2-manifold
 - ▶ *[Attali et al, 2007]*
- ▶ **However,**
 - ▶ Does not capture full topology easily for high-dimensional manifolds

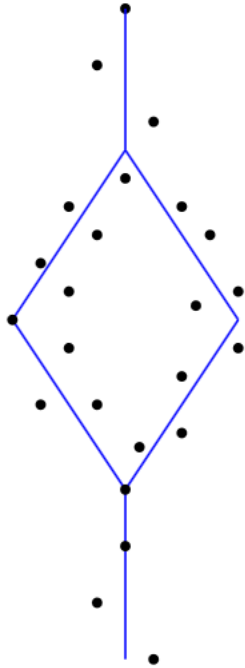


Remark

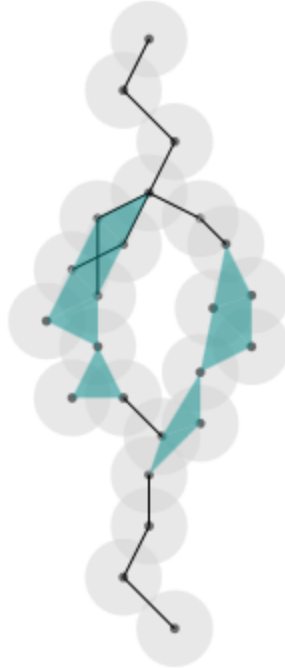
- ▶ **Rips complex**
 - ▶ Capture homology when input points are sampled dense enough
 - ▶ But too large in size
- ▶ **Witness complex**
 - ▶ Use a subsampling idea
 - ▶ Reduce size tremendously
 - ▶ May not be easy to capture topology in high-dimensions
- ▶ **Combine the two ?**
 - ▶ Graph induced complex



Subsampling



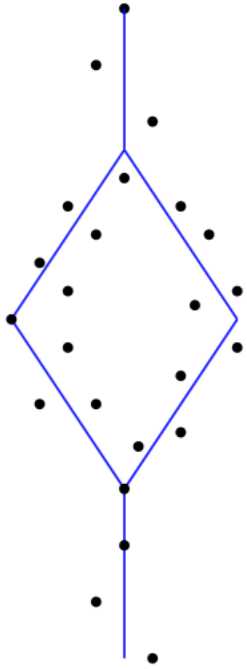
P



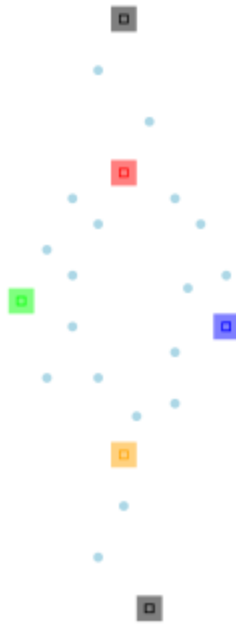
$R^\epsilon(P)$



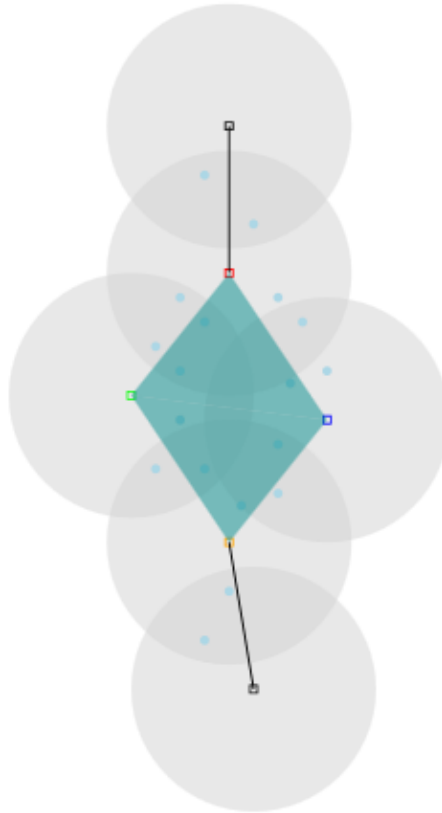
Subsampling -cont



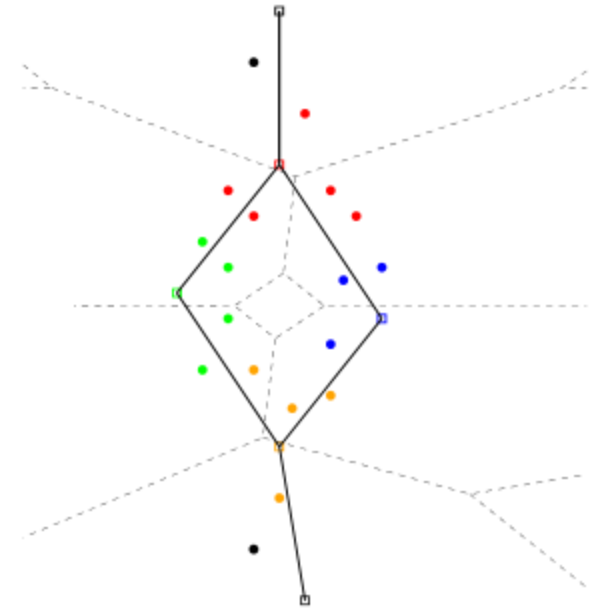
P



$Q \subseteq P$



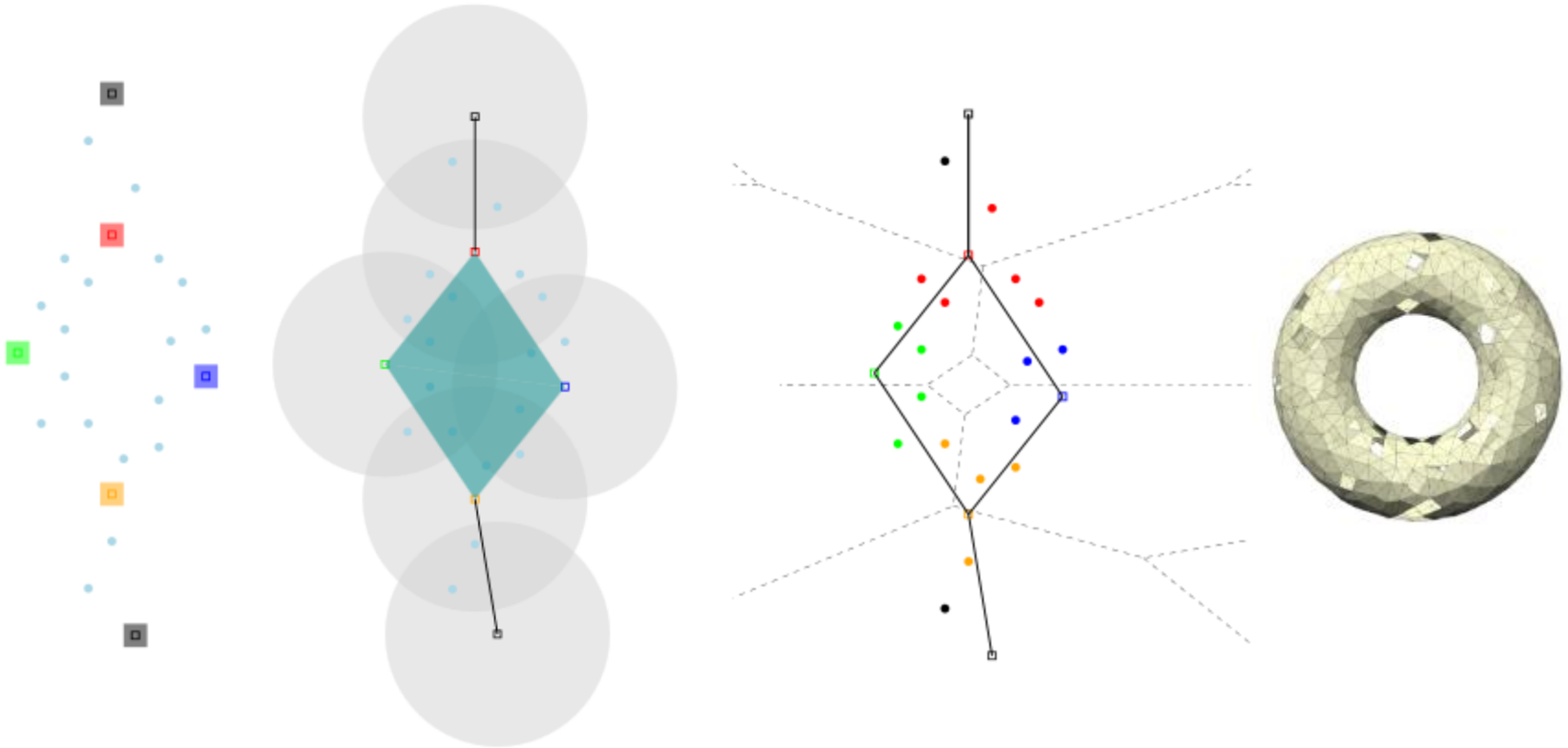
$R^r(Q)$



$W(Q, P)$



Subsampling -cont



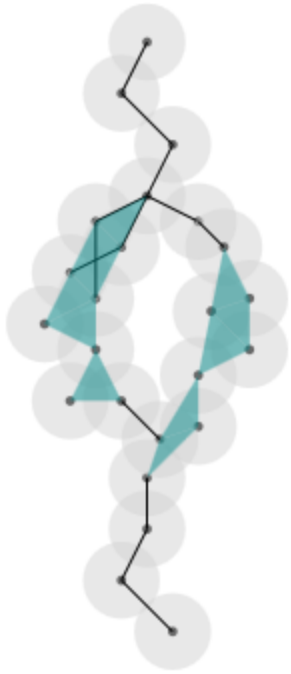
$Q \subseteq P$

$R^r(Q)$

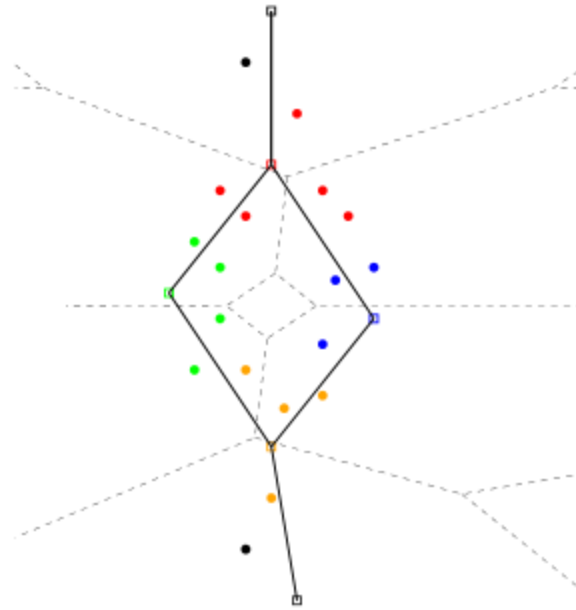
$W(Q, P)$



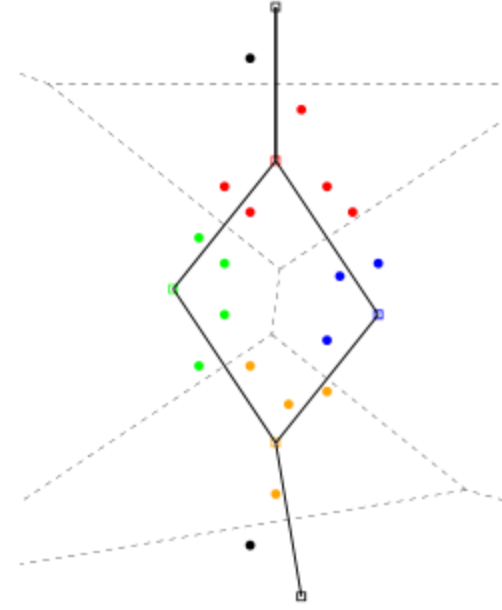
Subsampling - cont



$R^\epsilon(P)$



$W(Q, P)$

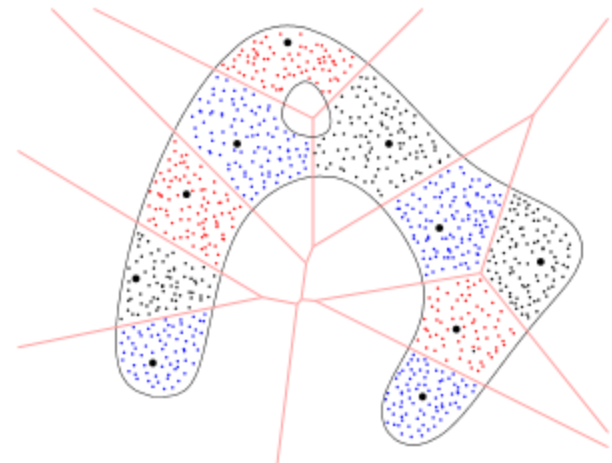
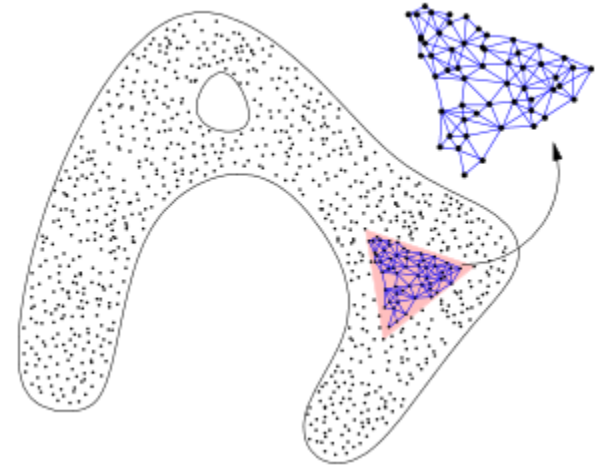


$G^r(Q, P)$



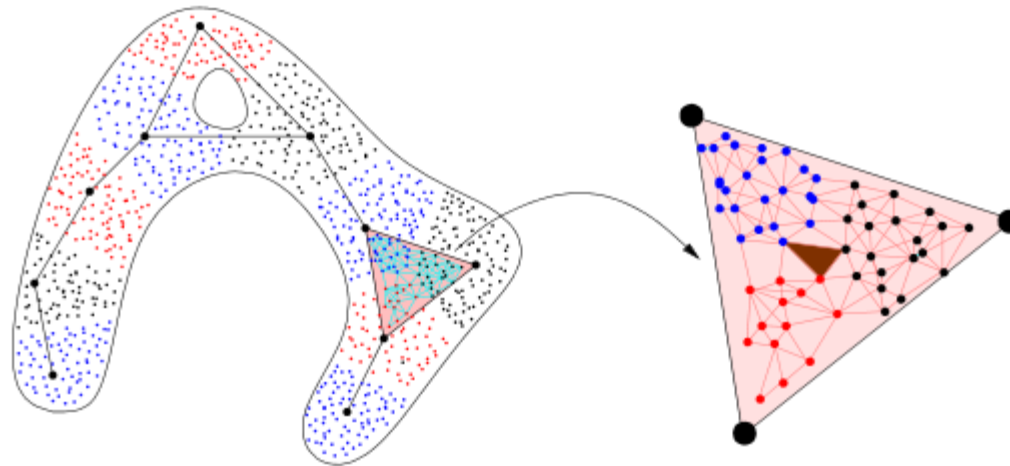
Graph Induced Complex

- ▶ P : finite set of points
 - ▶ (P, d) : metric space
 - ▶ $G(P)$: a graph
-
- ▶ $Q \subset P$: a subset
 - ▶ $\pi(p)$: the closest point of $p \in P$ in Q



Graph Induced Complex

- ▶ **Graph induced complex** $\mathcal{G}(P, Q, d): \{q_0, \dots, q_k\} \subseteq Q$
 - ▶ if and only if there is a $(k+1)$ -clique in $G(P)$ with vertices p_0, \dots, p_k such that $\pi(p_i) = q_i$, for any $i \in [0, k]$.

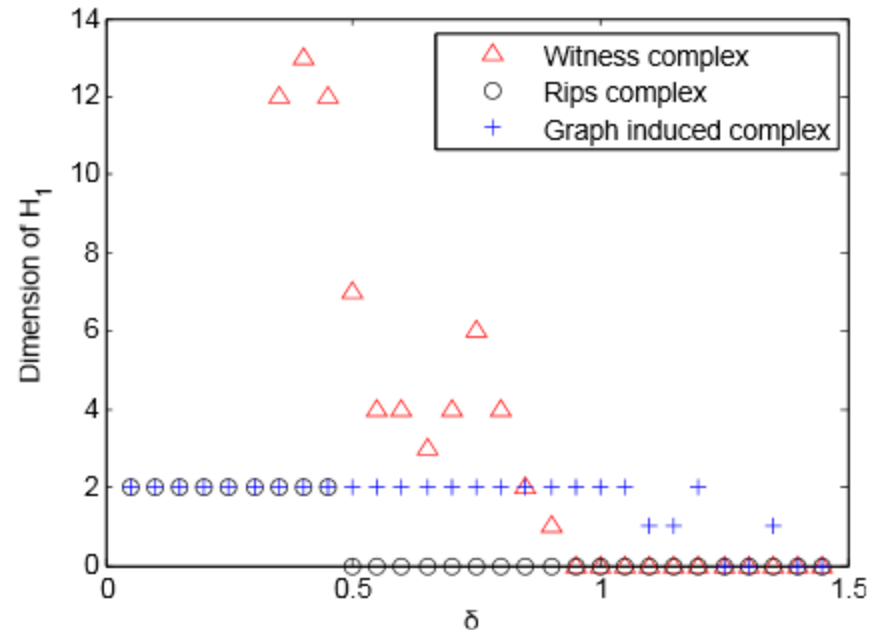
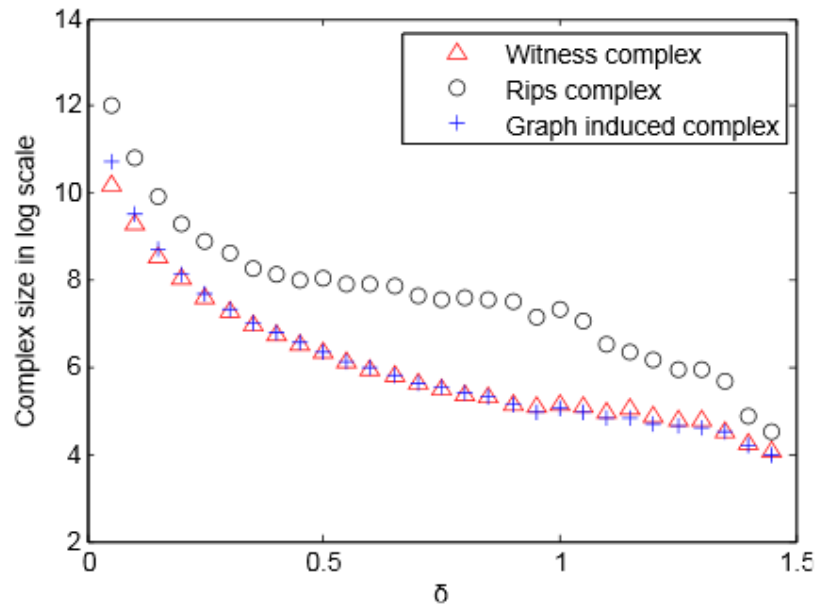


- ▶ Graph induced complex depends on the metric d :
 - ▶ Euclidean metric
 - ▶ Graph based distance d_G



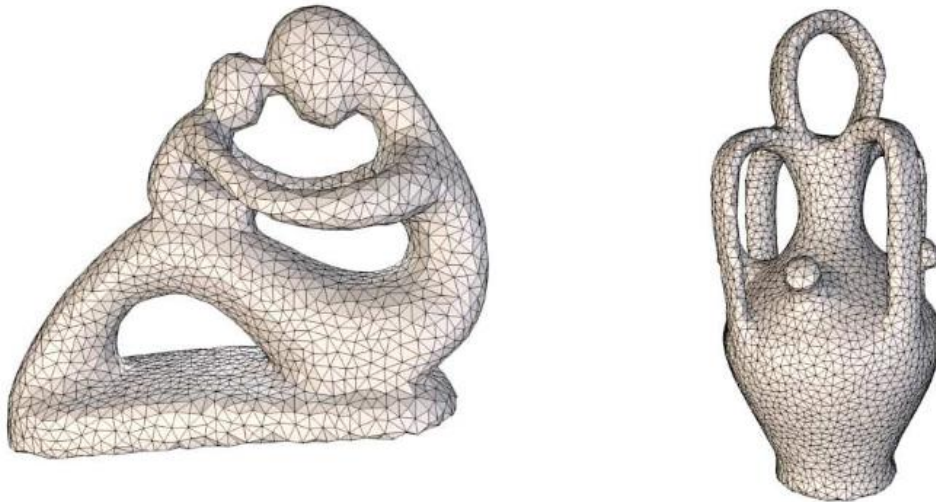
Graph Induced Complex

- ▶ Small size, but with homology inference guarantees
- ▶ In particular:
 - ▶ H_1 inference from a lean sample



Graph Induced Complex

- ▶ Small size, but with homology inference guarantees
- ▶ In particular:
 - ▶ H_1 inference from a lean sample
 - ▶ Surface reconstruction in R^3



- ▶ Topological inference for compact sets in R^d using persistence



Outline

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Sampling Conditions



Motivation

- ▶ Theoretical guarantees are usually obtained when input points P sampling the hidden domain “well enough”.
- ▶ Need to quantize the “wellness”.
- ▶ Two common ones based on:
 - ▶ Local feature size
 - ▶ Weak feature size



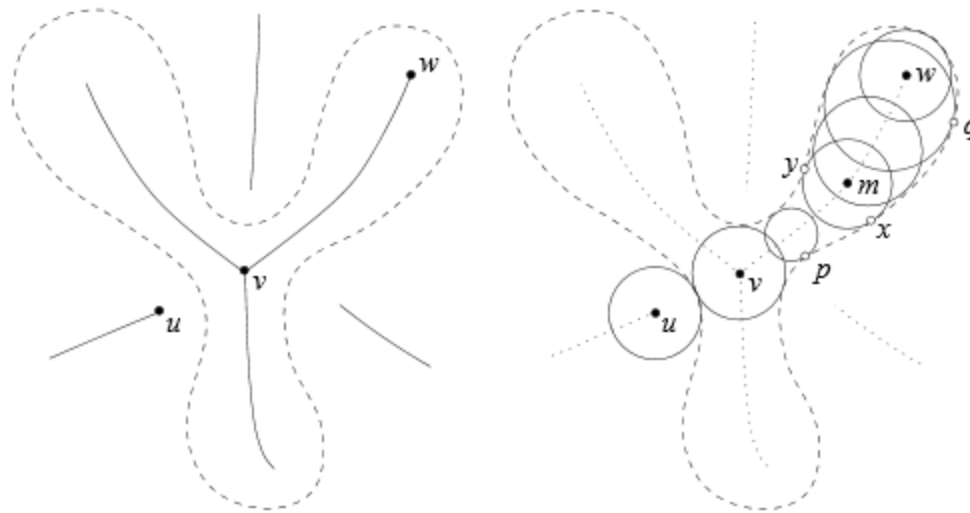
Distance Function

- ▶ $X \subset R^d$: a compact subset of R^d
- ▶ Distance function $d_X: R^d \rightarrow R^+ \cup \{0\}$
 - ▶ $d_X(x) = \min_{y \in X} d(x, y)$
 - ▶ d_X is a 1-Lipschitz function
- ▶ X^α : α -offset of X
 - ▶ $X^\alpha = \{y \in R^d \mid d(y, X) \leq \alpha\}$
- ▶ Given any point $x \in X$
 - ▶ $\Gamma(x) := \{y \in X \mid d(x, y) = d_X(x)\}$



Medial Axis

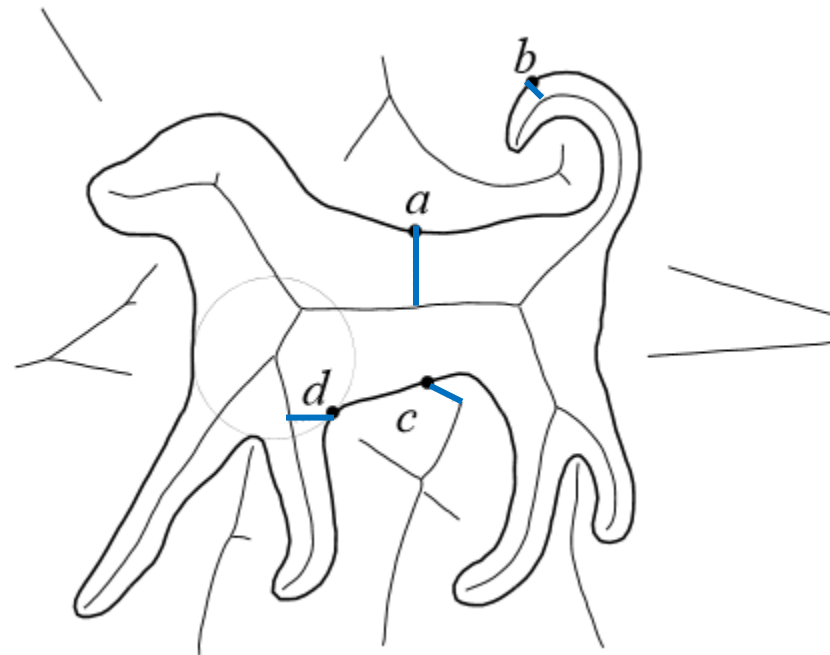
- ▶ The *medial axis* Σ of X is the closure of the set of points $x \in R^d$ such that $|\Gamma(x)| \geq 2$
- ▶ $|\Gamma(x)| \geq 2$ means that there is a medial ball $B_r(x)$ touching X at more than 1 point and whose interior is empty of points from X .



Courtesy of [Dey, 2006]

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



Courtesy of [Dey, 2006]

Gradient of Distance Function

- ▶ Distance function not differentiable on the medial axis
- ▶ Still can define a generalized concept of gradient
 - ▶ *[Lieutier, 2004]*
- ▶ For $x \in R^d \setminus X$,
 - ▶ 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

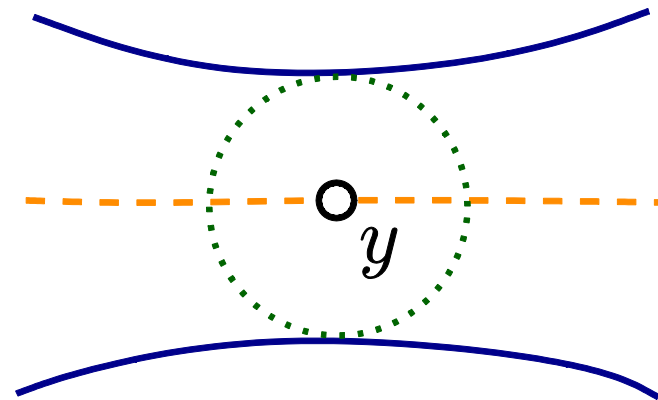
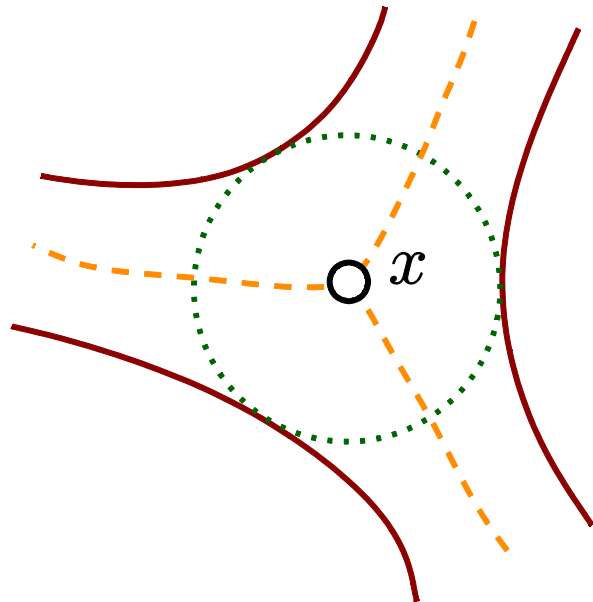
$$\nabla_X(x) = \frac{x - c_X(x)}{r_X(x)}$$

- ▶ Examples:
-



Critical Points

- ▶ A critical point of the distance function is a point whose generalized gradient $\nabla_X(x)$ vanishes
- ▶ A critical point is either in X or in its medial axis Σ



Weak Feature Size

- ▶ Given a compact $X \subset R^d$, let $C \subset R^d$ denote
 - ▶ the set of critical points of the distance function d_X that are not in X
- ▶ 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
- ▶ $\rho(X) \leq wfs(X)$



Typical Sampling Conditions

- ▶ Hausdorff distance $d_H(A, B)$ between two sets A and B
 - ▶ infimum 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 $d_H(P, X) \leq \epsilon$



Why Distance Field?

▶ Theorem [Offset Homotopy]

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 .
- ▶ The sampling condition makes sure that the discrete sample is sufficient to recover the offset homology.



Outline

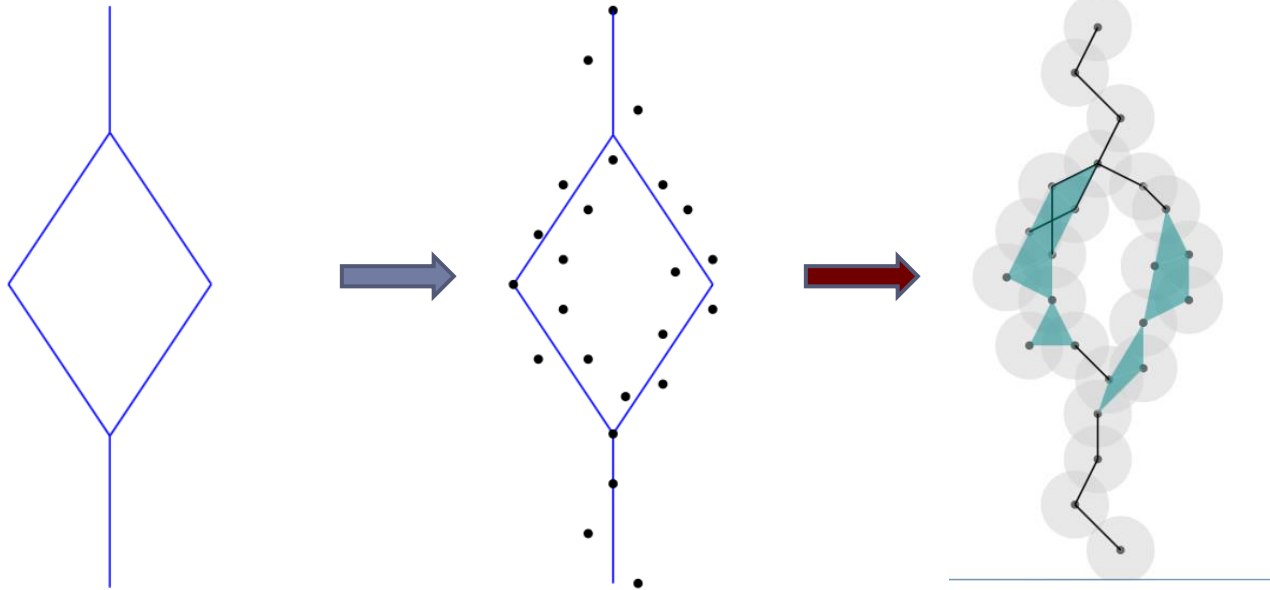
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Homology Inference from PCD



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

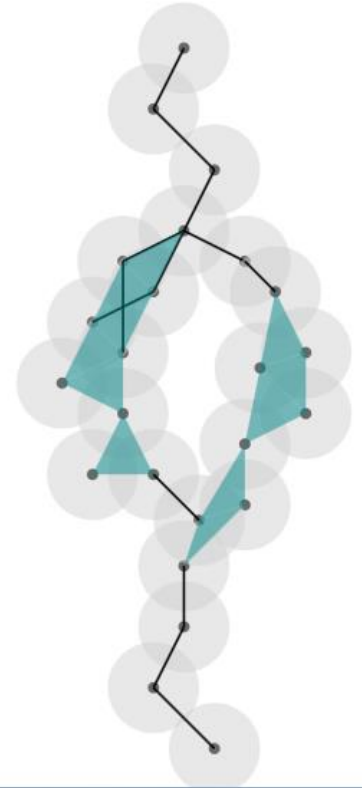


Union of Balls

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

- ▶ 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

$$H(X) \cong H(P^\alpha) \cong H(C^\alpha(P)).$$



-
- ▶ 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



Convert to Cech Complexes

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

$$\begin{array}{ccc} H(P^\alpha) & \xrightarrow{i_*} & H(P^\beta) \\ h_* \downarrow & & \downarrow h_* \\ H(C^\alpha) & \xrightarrow{i_*} & H(C^\beta) \end{array}$$

Corollary B

Let $P \subset X$ be s.t. $d_H(X, P) \leq \epsilon$. If $2\epsilon \leq \alpha \leq \alpha' \leq \sqrt{\frac{3}{5}}\rho(X)$,
 $H(X) \cong H(C^\alpha) \cong H(C^\beta)$ where the second isomorphism is induced by inclusion.

From Rips Complex

▶ **Lemma B:**

Given a sequence $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E$ of homomorphisms between finite dimensional vector spaces, if $\text{rank}(A \rightarrow E) = \text{rank}(C)$, then $\text{rank}(B \rightarrow D) = \dim C$.

▶ **Rips and Čech complexes:**

$$\begin{aligned} C^\alpha(P) &\subseteq R^\alpha(P) \subseteq C^{2\alpha}(P) \subseteq R^{2\alpha}(P) \subseteq C^{4\alpha}(P) \\ \Rightarrow H(C^\alpha) &\rightarrow H(R^\alpha) \rightarrow H(C^{2\alpha}) \rightarrow H(R^{2\alpha}) \rightarrow H(C^{4\alpha}) \end{aligned}$$

▶ **Applying Lemma B**

$$\text{rank}(H(R^\alpha) \rightarrow H(R^{2\alpha})) = \text{rank}(H(C^{2\alpha})) = \text{rank}(H(X))$$



The Case of Compact

▶ In contrast to Corollary A, now we have the follow (using Lemma B).

▶ Lemma C [*Chazal and Oudot 2008*]:

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



The Case of Compacts

- ▶ One more level of interleaving.
- ▶ Use the following extension of Lemma B:

Given a sequence $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E \rightarrow F$ of homomorphisms between finite dimensional vector spaces, if $\text{rank}(A \rightarrow F) = \text{rank}(C \rightarrow D)$, then $\text{rank}(B \rightarrow E) = \text{rank}(C \rightarrow D)$.

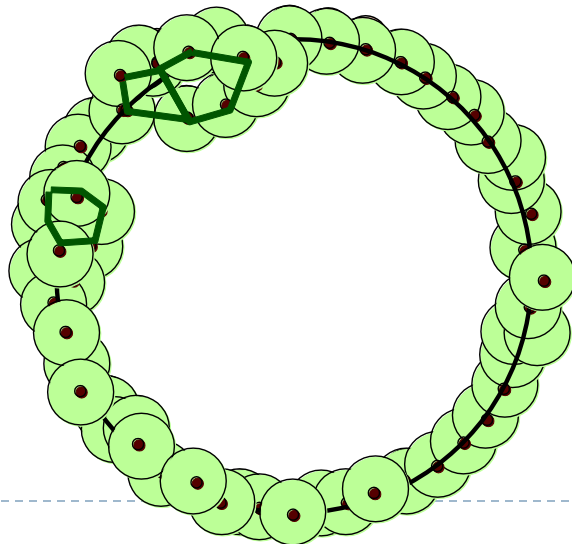
- ▶ **Theorem [Homology Inference] [Chazal and Oudot 2008]:**

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



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

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Summary of Homology Inference

- ▶ X^α homotopy equivalent to X^β
 - ▶ Critical points of distance field
- ▶ P^α approximates X^α (may be interleaving)
 - ▶ E.g, *[Niyogi, Smale, Weinberger, 2006]*, *[Chazal and Oudot 2008]*
- ▶ C^α homotopy equivalent to P^α
 - ▶ Nerve Lemma
- ▶ $H(C^\alpha)$ interleaves $H(X^\alpha)$ at homology level
 - ▶ *[Chazal and Oudot 2008]*
- ▶ R^α and C^α interleave
- ▶ Derive homology inference from the interleaving sequence of homomorphisms



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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
- ▶ Some approaches
 - ▶ Bound the probability that input samples fall in Hausdorff model
 - ▶ Denoise so that fall in Hausdorff model
 - ▶ E.g, *[Niyogi, Smale, Weinberger 2006, 2008]*
- ▶ Distance to measure framework
 - ▶ *[Chazal, Cohen-Steiner, Mérigot, 2011]*



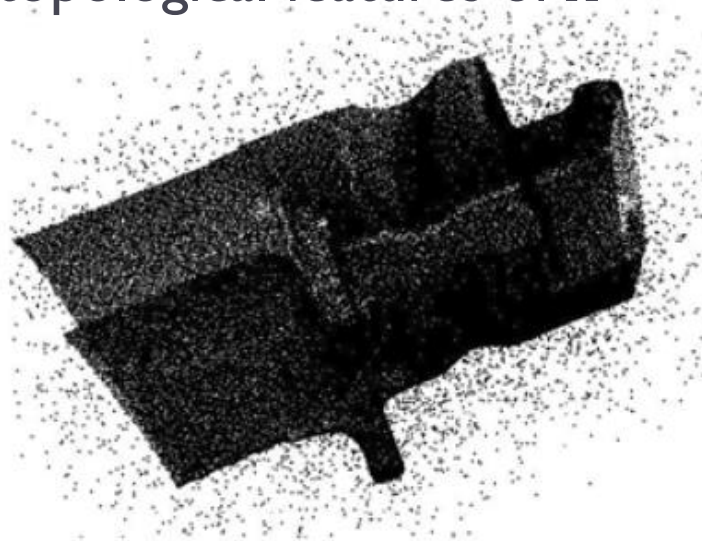
Overview

- ▶ **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

Main Idea

- ▶ The work of [*Chazal, Cohen-Steiner, Mérigot, 2011*]
- ▶ A new distance function $d_{\mu,m}$ to a probability μ measure (ie., distance to measures) to replace the role of distance function d_X .
- ▶ Show that the two distance fields are close (in L_∞ norm)
- ▶ Topological inference follows from some stability results or the interleaving sequences



Definitions

▶ μ : a probability measure on R^d ; $\mu(R^d) = 1$

▶ $0 < m, m_0 < 1$: *mass* parameters

▶ $\delta_{\mu,m}$: a pseudo-distance function such that

$$\delta_{\mu,m}(x) := \inf\{r > 0; \mu(\bar{B}(x, r)) > m\}$$

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

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

▶ *Distance to measure* d_{μ,m_0} :

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



Distance to Measures

- ▶ *Distance to measure* d_{μ, m_0} :

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

- ▶ Intuitive, $d_{\mu, m}(x)$ averages distance within a range and is more robust to noise.
- ▶ Examples.
- ▶ Wasserstein distance:



Wasserstein Distance

- ▶ A **transport plan** between two probability measures μ, ν on R^d is a probability measure π on $R^d \times R^d$ such that for every $A, B \subseteq R^d$, $\pi(A \times R^d) = \mu(A)$ and $\pi(R^d \times B) = \nu(B)$.

- ▶ The **p-cost** of a transport plan π is:

$$C_p(\pi) = \left(\int_{R^d \times R^d} \|x - y\|^p d\pi(x, y) \right)^{\frac{1}{p}}$$

- ▶ The **Wasserstein distance** of order p between μ, ν on 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 .



Properties

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

d_{μ, m_0}^2 is distance like. That is:

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

▶ Theorem [Stability] [Chazal et al 2011]

Let μ, μ' be two probability measures on R^d and $m_0 > 0$. Then

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



Distance-Like Function

- ▶ There are many interesting consequences of [Theorem Distance-Likeness Theorem].
 - ▶ E.g, one can define critical points, weak feature size, etc.

▶ 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 $\phi^{-1}([r_1, r_2])$. Then all the sublevel sets $\phi^{-1}([0, r])$ are isotopic for $r \in [r_1, r_2]$.



Relation to Distance Function

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

▶ Theorem [Approximation Distance]:

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

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



Computational Aspect

- ▶ Distance to measures can be approximated efficiently for a set of points P
 - ▶ *[Guibas, Mérigot and Morozov, DCG 2013]*
- ▶ Can be extended to metric spaces, and build weighted Čech / Rips complexes for reconstruction and homology inference
 - ▶ *[Buchet, Chazal, Oudot, Sheehy, 2013]*



Outline

- ▶ **From PCDs to simplicial complexes**
 - ▶ Delaunay, Čech, Vietoris-Rips, witness complexes
 - ▶ Graph induced complex
- ▶ **Sampling conditions**
 - ▶ Local feature size, and homological feature size
- ▶ **Topology inference**
 - ▶ Homology inference
 - ▶ Handling noise
 - ▶ *Approximating cycles of shortest basis of the first homology group*
 - ▶ *Approximating Reeb graph*



Two Additional Examples

- ▶ **Previously:**
 - ▶ Homology inference: topological information of a space
- ▶ **Approximating cycles of shortest basis of the first homology group**
 - ▶ As an example of combining geometry and topology
- ▶ **Approximating Reeb graph**
 - ▶ As an example of approximating the topology of a scalar field
- ▶ **See separate slides for these two additional topics.**



Summary

- ▶ One example of the pipeline of approximating certain topological structure from discrete samples
- ▶ The components in the pipeline are quite generic

- ▶ Many other issues too:
 - ▶ Stability
 - ▶ Efficiency
 - ▶ Sparsification
 - ▶ etc



Summary – cont.

- ▶ Starting to have more interaction with statistics and probability theory
 - ▶ E.g, [*Balakrishnan et al., AISTATS 2012*], [*Bendich et al., SoDA 2012*]
- ▶ How to develop algorithms that integrating computational geometry / topology ideas with statistics, especially in data analysis?



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