Some Topics in Computational Topology

Yusu Wang

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
- 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, Cech, 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 \( P = \{ p_1, p_2, ..., p_n \} \subset R^d \)
- Delaunay complex \( Del(P) \)
  - A simplex \( \sigma = [p_{i_0}, p_{i_1}, ..., p_{i_k}] \) is in \( Del(P) \) if and only if
    - There exists a ball \( B \) whose boundary contains vertices of \( \sigma \), 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 $P = \{ p_1, p_2, ..., p_n \} \subset R^d$
- 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 $B_r(p_i) = B(p_i, r) = \{ x \in R^d | d(p_i, x) < r \}$
- The definition can be extended to a finite sample $P$ of a metric space.
Rips Complex

- Given a set of points $P = \{ p_1, p_2, ..., p_n \} \subset \mathbb{R}^d$
- Given a real value $r > 0$, the Vietoris-Rips (Rips) complex $R^r(P)$ is:

  \[ \{ (p_{i_0}, p_{i_1}, ..., p_{i_k}) \mid B_r(p_{i_l}) \cap B_r(p_{i_j}) \neq \emptyset, \forall \ l, j \in [0, k] \} \]
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 $\sigma = \{q_0, ..., q_k\}$ is **weakly witnessed** by a point $x$ if $d(q_i, x) \leq d(q, x)$ for any $i \in [0, k]$ and $q \in Q \setminus \{q_0, ..., q_k\}$.

- Given a set of points $P = \{p_1, p_2, ..., p_n\} \subset \mathbb{R}^d$ 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

$P$

$R^\varepsilon(P)$
Subsampling - cont

\[ P \quad Q \subseteq P \quad R^r(Q) \quad W(Q, P) \]
Subsampling - cont

\[ Q \subseteq P \quad R^r(Q) \quad W(Q, P) \]
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** $G(P, Q, d)$: $\{q_0, \ldots, q_k\} \subseteq Q$
  - if and only if there is a $(k+1)$-clique in $G(P)$ with vertices $p_0, \ldots, p_k$ 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 $\mathbb{R}^3$
  - Topological inference for compact sets in $\mathbb{R}^d$ using persistence
Outline

- From PCDs to simplicial complexes
  - Delaunay, Cech, 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
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

- $X \subseteq R^d$: a compact subset of $R^d$
- Distance function $d_X: R^d \to R^+ \cup \{0\}$
  - $d_X(x) = \min_{y \in X} d(x,y)$
  - $d_X$ is a 1-Lipschitz function

- $X^\alpha$: $\alpha$-offset of $X$
  - $X^\alpha = \{ y \in R^d \mid d(y,X) \leq \alpha \}$

- Given any point $x \in X$
  - $\Gamma(x) := \{ y \in X \mid d(x,y) = d_X(x) \}$
The *medial axis* $\Sigma$ of $X$ is the closure of the set of points $x \in \mathbb{R}^d$ 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 $\Sigma$ 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 \( x \in \mathbb{R}^d \setminus X \),
  - 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 \textit{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 $\Sigma$. 

![Diagram showing critical points and medial axis]
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 $\alpha$ such that $A \subseteq B^\alpha$ and $B \subseteq A^\alpha$

- No noise version:
  - A set of points $P$ is an $\epsilon$-sample of $X$ if $P \subseteq X$ and $d_H(P, X) \leq \epsilon$

- With noise version:
  - A set of points $P$ is an $\epsilon$-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 $X^\alpha$. In particular, $H(X^\alpha) \cong H(X^{\alpha'})$.

- **Remarks:**
  
  - For the case of compact set $X$, note that it is possible that $X^\alpha$, 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 $\alpha$ from a thickened version (offset) of $X^\alpha$.
  
  - The sampling condition makes sure that the discrete sample is sufficient to recover the offset homology.
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Homology Inference from PCD
Problem Setup

- A hidden compact $X$ (or a manifold $M$)
- An $\epsilon$-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, $P^\alpha$ approximates offset $X^\alpha$

- The Čech complex $C^\alpha(P)$ is the Nerve of $P^\alpha$

- By Nerve Lemma, $C^\alpha(P)$ is homotopy equivalent to $P^\alpha$
Smooth Manifold Case

- Let $X$ be a smooth manifold embedded in $\mathbb{R}^d$

**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 $P^\alpha$ 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 $X^\alpha$
Lemma A [Chazal and Oudot, 2008]:

The following diagram commutes:

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

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 $A \to B \to C \to D \to E$ of homomorphisms between finite dimensional vector spaces, if $rank(A \to E) = rank(C)$, 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**
  
  \[
  rank(H(R^\alpha) \to H(R^{2\alpha})) = rank(H(C^{2\alpha})) = rank(H(X))
  \]
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 $\epsilon < \frac{1}{4} \text{wfs}(X)$. Then for all $\alpha, \beta \in [\epsilon, \text{wfs}(X) - \epsilon]$ such that $\beta - \alpha \geq 2\epsilon$, and for all $\lambda \in (0, \text{wfs}(X))$, we have $H(X^\lambda) \cong \text{image}(i_*)$, where $i_*: H(P^\alpha) \to H(P^\beta)$ is the homomorphism between homology groups induced by the canonical inclusion $i: P^\alpha \to P^\beta$. 
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 $\epsilon < \frac{1}{9} wfs(X).$ Then for all $\alpha \in \left[2\epsilon, \frac{1}{4} (wfs(X) - \epsilon)\right]$ all $\lambda \in (0, wfs(X))$, 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]:

Let $P \subset \mathbb{R}^d$ 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 $j: \mathbb{R}^\alpha \rightarrow \mathbb{R}^{4\alpha}$. 
Summary of Homology Inference

- $X^\alpha$ homotopy equivalent to $X^\beta$
  - Critical points of distance field
- $P^\alpha$ approximates $X^\alpha$ (may be interleaving)
  - E.g. [Niyogi, Smale, Weinberger, 2006], [Chazal and Oudot 2008]
- $C^\alpha$ homotopy equivalent to $P^\alpha$
  - Nerve Lemma
- $H(C^\alpha)$ interleaves $H(X^\alpha)$ at homology level
  - [Chazal and Oudot 2008]
- $R^\alpha$ and $C^\alpha$ interleave
- Derive homology inference from the interleaving sequence of homomorphisms
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  - Handling noise
    - Approximating cycles of shortest basis of the first homology group
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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 $\mu$ on $R^d$ potentially concentrated on a hidden compact (e.g., manifold) $X$.

- **Goal:**
  - Approximate topological features of $X$
Main Idea

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

- A new distance function $d_{\mu,m}$ to a probability $\mu$ measure (i.e., distance to measures) to replace the role of distance function $d_X$.

- Show that the two distance fields are close (in $L_\infty$ norm)

- Topological inference follows from some stability results or the interleaving sequences
Definitions

- \( \mu \): 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
  \[
  \delta_{\mu,m}(x) := \inf\{r > 0; \mu(\overline{B}(x,r)) > m\}
  \]
  where \( \overline{B}(x,r) \) 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** \( d_{\mu,m_0} \):
  \[
  d^2_{\mu,m_0}(x) = \frac{1}{m_0} \int_0^{m_0} \delta_{\mu,m}(x)^2 \, dm
  \]
Distance to Measures

- **Distance to measure** $d_{\mu,m_0}$:
  
  $$d_{\mu,m_0}^2(x) = \frac{1}{m_0} \int_0^{m_0} \delta_{\mu,m}(x)^2 \, dm$$

- 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 \( \mu, \nu \) on \( \mathbb{R}^d \) is a probability measure \( \pi \) 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 \( \pi \) is:

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

- The Wasserstein distance of order \( p \) between \( \mu, \nu \) on \( \mathbb{R}^d \) with finite \( p \)-moment

\[
W_p(\mu, \nu) = \text{the minum p-cost } C_p(\pi) \text{ of any transport plan } \pi \text{ between } \mu \text{ and } \nu.
\]
Properties

- **Theorem [Distance-Likeness] [Chazal et al 2011]**
  \(d_{\mu,m_0}^2\) is distance like. That is:
  - The function \(d_{\mu,m_0}\) is 1-Lipschitz.
  - The function \(d_{\mu,m_0}^2\) is 1-semiconcave, meaning that the map \(x \to d_{\mu,m_0}^2(x) - \|x\|^2\) is concave.

- **Theorem [Stability] [Chazal et al 2011]**
  Let \(\mu, \mu'\) be two probability measures on \(\mathbb{R}^d\) and \(m_0 > 0\). Then
  \[
  \|d_{\mu,m_0} - d_{\mu',m_0}\|_\infty \leq \frac{1}{\sqrt{m_0}} W_2(\mu, \mu')
  \]
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 $\phi$ be a distance-like function and $r_1 < r_2$ be two positive numbers such that $\phi$ 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 $\mu$ on $R^d$ concentrated $X$.
  - Consider $P$ as a noisy sample of $X$
- Let $\nu_X$ denote the uniform measure on $X$

Theorem [Approximation Distance]:

$$\|d_X - d_{\mu,m_0}\|_\infty \leq C(X) \frac{1}{km_0^k} + \frac{1}{\sqrt{m_0}} W_2(\mu, \nu_X)$$

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]
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    - *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?
References


References – cont.


- **Topological estimation using witness complexes.** V. de Silva, G. Carlsson, Symposium on Point-Based Graphics,, 2004


References – cont.


References – cont.


