Persistent homology and minimum spanning acycle for random simplicial complexes

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Persistent homology

- Homology theory first appeared around 1900 (Poincaré).
- Persistent homology theory appeared around 2000 independently by
 - Frosini, Ferri et al. in Bologna, Italy.
 - Robins, Colorado, Boulder,
 - Edelsbrunner, at Duke, North Carolina.
- Software for computing persistent homology has also been developed and used for data analysis such as material science, biology etc.

Persistent homology

 \approx time-dependent version of homology

Persistent homology for random object \approx Stochastic process in homology theory

Filtration and persistent homology



 \Downarrow via Čech or Rips-Vietoris complex etc.

Input 2: Filtration = increasing sequence of simplicial complex
 U
 Output: Persistence diagram



Random filtrations

Figure: 20 Poisson points and its filtration $\{X(t), t \ge 0\}$



Figure: Erdös-Rényi random graph process $\{X(t), t \ge 0\}$ for n = 6

• Homology vs. Persistent homology:

- $H_0(X(t)) =$ connected components of X(t).
- $H_1(X(t)) = \text{cycles of } X(t).$
- $PH_0({X(t)}_{t\geq 0}) =$ "death" of connected components.
- $PH_1({X(t)}_{t\geq 0}) =$ "birth and death" of cycles.

Atomic configuration of SiO2



Figure: T. Nakamura, Y. Hiraoka, A. Hirata, et al. http://arxiv.org/abs/1501.03611 and http://arxiv.org/abs/1502.07445

1-dim. Persistence diagram



Figure: T. Nakamura, Y. Hiraoka, A. Hirata, et al. http://arxiv.org/abs/1501.03611 and http://arxiv.org/abs/1502.07445

Minimum spanning tree (MST)



Figure: Weighted graph K_4

Minimum spanning tree (MST)



Figure: All possible 16 spanning trees on K_4

Minimum spanning tree (MST)



Figure: Minimum spanning tree (MST) on a weighted graph K_4

Frieze' result on MST

- Let K_n = (V_n, E_n) be the complete graph with n vertices, and for each edge e ∈ E_n, a uniform random variable t(e) on [0, 1] is assigned independently.
- Minimum spanning tree is the spanning tree T which minimizes the weight

$$wt(T) = \sum_{e \in T} t(e), \quad W_n := \min_{T \in S_n} wt(T),$$

where S_n is the set of spanning trees in K_n . Remark that

$$|\mathcal{S}_n| = n^{n-2}$$

by Cayley's theorem (1889).

• Frieze (1985): As $n \to \infty$,

$$\mathbb{E}[W_n] \to \zeta(3) = 1.20206 \dots$$

• Janson (1995): the CLT:

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$$\frac{\sqrt{n}(W_n - \zeta(3))}{\sqrt{n}(W_n - \zeta(3))} \rightarrow N(0, \sigma^2), \quad \sigma^2 = 6\zeta(4) - 4\zeta(3) \approx 1.68571....$$

A generalization of the problem of MST

- The purpose of this talk is to extend Frieze's result to higher dimensions.
 - (random) graph \implies (random) simplicial complex
 - spanning tree \implies spanning acycle
- We interpret the weight of the minimum spanning tree in terms of persistent homology.
- Kruskal's algorithm of finding MST \implies Erdös-Rényi graph process.



Figure: Erdös-Rényi random graph process for n = 6

Simplicial complex

- V: a finite set
- X: a collection of non-empty subsets of V.

Definition

- X is said to be a (n abstract) simplicial complex on V if
 - $\{v\} \subset X \text{ for all } v \in V.$
 - 2 X is closed under the operation of taking nonempty subsets, i.e.,

$$\sigma \in X, \ \emptyset \neq \tau \subset \sigma \Longrightarrow \tau \in X.$$

- $\sigma \subset V$ with $|\sigma| = k + 1$ is called *k*-simplex or *k*-face.
- We write $\dim(\sigma) = k$ if σ is a k-face.
- When d = max_{σ∈K} dim(σ), we say that X is a d-dimensional simplicial complex or just d-complex.

Example of simplicial complex



- X = {1,2,3,4,12,13,<u>14</u>,23,<u>34</u>,<u>123</u>} is a 2-dimensional simplicial complex.
- X is determined by facets {14, 34, 123}, i.e. maximal faces w.r.t. inclusion.

$$X = \{\underbrace{\underbrace{1, 2, 3, 4}_{X_0}, \underbrace{12, 13, 14, 23, 34}_{X_1}, \underbrace{123}_{X_2}\}}_{X^{(1): \text{ a graph}}}, \underbrace{X^{(1): \text{ a graph}}}_{X_1}\}$$

X⁽ⁱ⁾ = {σ ∈ X : dim(σ) ≤ i} : i-skeleton.
 X_i = {σ ∈ X : dim(σ) = i} : i-faces of X.

Homology group

- Chain group: for oriented *i*-faces $\langle \sigma \rangle = \langle v_0 v_1 \dots v_i \rangle$, we set $C_i(X, \mathbb{Z}) := \{ \sum a_\sigma \langle \sigma \rangle : a_\sigma \in \mathbb{Z} \}$
 - σ :*i*-faces of X
- Boundary operator: $\partial_i : C_i(X,\mathbb{Z}) \to C_{i-1}(X,\mathbb{Z})$

$$\partial_i \langle \mathbf{v}_0 \mathbf{v}_1 \dots \mathbf{v}_i \rangle := \sum_{j=0}^i (-1)^j \langle \mathbf{v}_0 \mathbf{v}_1 \dots \mathbf{v}_{j-1} \mathbf{v}_{j+1} \dots \mathbf{v}_i \rangle.$$

• Chain complex: $\partial_i \circ \partial_{i+1} = 0$ and

$$\cdots \stackrel{\partial_{i+2}}{\to} C_{i+1}(X,\mathbb{Z}) \stackrel{\partial_{i+1}}{\to} C_i(X,\mathbb{Z}) \stackrel{\partial_i}{\to} C_{i-1}(X,\mathbb{Z}) \stackrel{\partial_{i-1}}{\to} \cdots$$

• Structure theorem for homology groups:

$$H_i(X,\mathbb{Z}) := Z_i(X,\mathbb{Z})/B_i(X,\mathbb{Z}) = \ker \partial_i/\mathrm{Im}\partial_{i+1} \cong \mathbb{Z}^{\beta_i} \oplus \bigoplus_{j=1}^p \mathbb{Z}_{\gamma_j},$$

where $\beta_i = \beta_i(X)$ is the *i*-th Betti number.

Matrix representation of boundary operator





Filtration

• $\mathbb{X} = (X(t))_{t \ge 0}$: an increasing sequence of simplicial complexes.



$$\begin{array}{ll} \bullet \ X(0) = \{1,2,3,4,12,23\}, & T(1) = \cdots = T(23) = 0, \\ \bullet \ X(1) = \{1,2,3,4,12,23,14,34\} & T(14) = T(34) = 1, \\ \bullet \ X(2) = \{1,2,3,4,12,23,14,34,13\} & T(13) = 2, \\ \bullet \ X(3) = \{1,2,3,4,12,23,14,34,13,123\} & T(123) = 3, \\ \bullet \ X(4) = \{1,2,3,4,12,23,14,34,13,123,134\} & T(134) = 4. \end{array}$$

• $T(\sigma)$ denotes the *birth time* of σ .

Persistent homology group (I)

• Given a filtration $\mathbb{X} := \{X(t)\}_{t \ge 0}$, and then the birth times $\{T(\sigma)\}$. Suppose that the filtration is *saturated* in the sense that

$$\exists au \geq 0 ext{ s.t. } X(t) = X(au) \quad \forall t \geq au$$

• ℓ -th chain group as a graded module on the polynomial ring $\mathbb{F}[x]$:

$$C_\ell(\mathbb{X}) := igoplus_{t\geq 0} C_\ell(X(t),\mathbb{F}) = \{(c_t)_{t\geq 0}: c_t\in C_\ell(X(t),\mathbb{F})\}$$

with the right-shift actions

$$x^{s} \cdot (c_0, c_1, \dots) := (\underbrace{0, \dots, 0}_{s\text{-times}}, c_0, c_1, \dots)$$

• Boundary operator $\partial_{\ell}(x): C_{\ell}(\mathbb{X}) \to C_{\ell-1}(\mathbb{X})$:

$$\partial_{\ell}(x)\langle\!\langle v_0v_1\ldots v_{\ell}\rangle\!\rangle = \sum_{j=0}^{\ell} (-1)^j x^{\mathcal{T}(\sigma)-\mathcal{T}(\sigma_j)} \langle\!\langle v_0v_1\ldots v_{j-1}v_{j+1}\ldots v_{\ell}\rangle\!\rangle.$$

Matrix representation of boundary operator



• We can see that $\partial_\ell(x) \circ \partial_{\ell+1}(x) = 0$ and

$$\cdots \stackrel{\partial_{\ell+2}}{\to} C_{\ell+1}(\mathbb{X}) \stackrel{\partial_{\ell+1}}{\to} C_{\ell}(\mathbb{X}) \stackrel{\partial_{\ell}}{\to} C_{\ell-1}(\mathbb{X}) \stackrel{\partial_{\ell-1}}{\to} \cdots$$

Random simplicial complex

Persistent homology group (II)

• Structure theorem for persistent homology for $\mathbb{X} = \{X(t)\}_{t \geq 0}$:

$$PH_k(\mathbb{X}) := Z_k(\mathbb{X})/B_k(\mathbb{X}) \cong \bigoplus_{i=1}^s (x^{b_i})/(x^{d_i}) \oplus \bigoplus_{i=s+1}^{s+r} (x^{b_i})$$

• $(x^{b_i})/(x^{d_i}) \iff$ persistent interval $[b_i, d_i)$ for an *i*-th homology class • b_i : birth time, d_i : death time, $\ell_i := d_i - b_i$: lifetime.



Figure: Persistence diagram

- For simplicity, we suppose *r* = 0, i.e., *finite* lifetimes.
- The sum of lifetimes of *k*-dimensional homology classes:

$$L_k = \sum_{i=1}^s \ell_i.$$

Persistent homology for random s.c.

deterministic

• $\mathbb{X} = (X(t))_{t \ge 0} \Rightarrow k$ -th persistence diagram \Rightarrow the sum of lifetimes L_k stochastic

Let X = (X(t))_{t≥0} be an increasing stochastic process of simplicial complexes, e.g., the Erdös-Rényi graph process

 $\mathbb{X} = (X(t))_{t \ge 0} \implies \text{random } k\text{-th persistence diagram, } k = 0, 1, 2, \dots$ $\iff \text{point process } \xi \text{ on } \Delta = \{(x, y) \in \mathbb{R}^2 : x \le y\}$ $\implies \text{the sum of lifetimes } L_k(\xi)$

Proposition

When $\mathbb{X} = (X(t))_{0 \le t \le 1}$ is the Erdös-Rényi graph process,

 $L_0(\xi)$ = the weight of the minimum spanning tree

Persistence diagram



Figure: Persistence diagram for Erdös-Rényi clique complex n = 40

ℓ -Linial-Meshulam process

$$\begin{aligned} [n] &= \{1, 2, \dots, n\} \\ \mathcal{F}_{\ell} &:= \binom{[n]}{\ell+1}: \text{ the set of } \ell\text{-faces or } (\ell+1)\text{-subsets of } [n]. \\ \{t(\sigma) : \sigma \in \mathcal{F}_{\ell}\}: \text{ i.i.d. uniform r.v.'s on } [0,1]: \text{ birth times.} \\ X^{(\ell)}(t) &= \bigcup_{\substack{j=0\\j=0\\\text{all } j(<\ell)\text{-faces}}^{\ell-1} \mathcal{F}_{j} \quad \cup \quad \underbrace{\{\sigma \in \mathcal{F}_{\ell} : t(\sigma) \leq t\}}_{\ell\text{-faces born before } t}. \end{aligned}$$

- $(\ell = 1) X^{(1)}(t)$ is the Erdös-Rényi graph process $(X^{(1)}(t) \stackrel{d}{=} G(n, t))$.
- $(\ell = 2) X^{(2)}(t)$ starts from K_n at time 0, a 2-face is attached at random birth time, and ends up with complete 2-skeleton.



Threshold for connectivity for Erdös-Rényi graph

- $X^{(1)}(t)$: Erdös-Rényi graph.
 - $(\ell = 1)$ Erdös-Rényi (1960)

$$\mathbb{P}(G(n,t) \text{ is connected}) = \mathbb{P}(\tilde{H}_0(X^{(1)}(t)) = 0) \rightarrow \begin{cases} 0 & t = \frac{\log n - \omega_n}{n} \\ 1 & t = \frac{\log n + \omega_n}{n} \end{cases}$$

•
$$(\ell = 1)$$
 Pittel (1988)
 $\mathbb{P}(G(n, t) \text{ has no cycle}) = \mathbb{P}(\tilde{H}_1(X^{(1)}(t)) = 0)$
 $\rightarrow \begin{cases} \sqrt{1-c} \exp(\frac{c}{2} + \frac{c^2}{4}) & t = \frac{c}{n} \ (0 < c < 1) \\ 0 & t = \frac{c}{n} \ (c > 1) \end{cases}$

Threshold for connectivity for the Linial-Meshulam process

• $(\ell = 1)$ Erdös-Rényi (1960)

$$\mathbb{P}(G(n,t) \text{ is connected}) = \mathbb{P}(\tilde{H}_0(X^{(1)}(t)) = 0) \rightarrow \begin{cases} 0 & t = \frac{\log n - \omega_n}{n} \\ 1 & t = \frac{\log n + \omega_n}{n} \end{cases}$$

•
$$(\ell = 2, p = 2)$$
 Linial-Meshulam(2006)
 $(\ell \ge 2, \forall p)$ Meshulam-Wallach (2009)
 $\mathbb{P}(\tilde{H}_{\ell-1}(X^{(\ell)}(t), \mathbb{Z}_p) = 0) \rightarrow \begin{cases} 0 & t = \frac{\ell \log n - \omega_n}{n} \\ 1 & t = \frac{\ell \log n - \omega_n}{n} \end{cases}$

- Remark that the threshold for $\tilde{H}_{\ell-1}(X^{(\ell)}(t),\mathbb{Z}) = 0$ is still open. Hoffman-Kahle-Paquette obtained a partial result.
- They obtained the same threshold for " $\pi_1(X^{(2)}(t))$ has property (T)".

Betti number $\beta_1(X^{(2)}(t))$ in the case $\ell = 2$

$$ilde{eta}_1(X^{(2)}(0))=inom{n-1}{2}\searrow 0= ilde{eta}_1(X^{(2)}(1))$$



Figure: $\beta_1(X^{(2)}(t))$ for 2-Linial-Meshulam process when n = 15.

Spanning *l*-acycle

Spanning tree T in the complete graph K_n satisfies the following:
1 |T| = n − 1 = (^{n−1}₁). *H*₀(T) = 0 ⇔ connected. *H*₁(T) = 0 ⇔ no cycle.

Definition

- A subset T of ℓ -faces is a spanning ℓ -acycle over [n] if
- $|T| = \binom{n-1}{\ell}$. • $\tilde{H}_{\ell-1}(X_T) = \text{finite group}$ • $\tilde{H}_{\ell}(X_T) = 0 \iff no \ \ell \text{-dim. cycles.}$ • $X_T = \Delta_{n-1}^{(\ell-1)} \sqcup T$
 - This definition was given by G. Kalai(1983).
 - Any two of the above three conditions implies the third.

Spanning ℓ -acycle in general simplicial complex

Definition

Let X be a simplicial complex. For $\ell \leq \dim X$, a subset T of ℓ -faces in X is a spanning ℓ -acycle if

In this case, $|T| = |X_{\ell}| - \tilde{\beta}_{\ell}(X)$.

- Any two of the above three conditions implies the third.
- k-spanning acycle exists only if $|\tilde{H}_{k-1}(X^{(k)})| < \infty$.
- A triangulation of 2-sphere minus one 2-face is a spanning 2-acycle.
- So For a triangulation X_g of a compact oriented surface of g ≥ 1, since $\tilde{H}_1(X_g) = 2g$, there is no spanning 2-acycle in our definition.

Theorem (Kalai '83)

Let $S^{(\ell)}(n)$ be the set of spanning ℓ -acycle with $(\ell - 1)$ -complete skeleton on n-vertices. Then,

$$\sum_{T\in\mathcal{S}^{(\ell)}(n)}|\tilde{H}_{\ell-1}(T)|^2=n^{\binom{n-2}{\ell}}.$$

• For
$$\ell = 2$$
, since $\tilde{H}_1(T)$ is trivial for $n = 4, 5$,
 $|S^{(2)}(4)| = 4^{\binom{4-2}{2}} = 4$, $|S^{(2)}(5)| = 5^{\binom{5-2}{2}} = 125$

• For $\ell = 2$ and n = 6, since $\tilde{H}_1(T) \cong \mathbb{Z}_2$ for 12 spanning 2-acycles, $|S^{(2)}(6)| = 46620 \neq 6^{\binom{6-2}{2}} = 6^6 = 46656$

Such a 2-complex is a triangulation of the projective plane.

e.g. $\{123, 124, 135, 146, 156, 236, 245, 256, 345, 346\}$

Determinantal formula

X: a simplicial complex with $ilde{H}_{\ell-2}(X^{(\ell-1)}) = 0.$

• L: an $(\ell - 1)$ -acycle, S: ℓ -faces with |S| = |K|.

• det $\partial_{KS} \neq 0$ iff S is an ℓ -acycle.

Proposition (Matrix-Tree type theorem)

Let $L \in S^{(\ell-1)}$ and set $K = X_{\ell-1} \setminus L$. Then,

$$\det(\partial_{\mathcal{K}}\partial_{\mathcal{K}}^{\mathcal{T}}) = \sum_{S\in\mathcal{S}^{(\ell)}} (\det\partial_{\mathcal{K}S})^2 = \sum_{S\in\mathcal{S}^{(\ell)}} |\tilde{H}_{\ell-1}(X_S)|^2$$

When $\ell = 1$, $|\tilde{H}_{\ell-1}(X_S)| = 1$, this gives us $\det(\partial_K \partial_K^T) = |S^{(1)}|$.

Sum of lifetimes of homology generators



Theorem

1 Let $\tilde{\beta}_{\ell-1}(t)$ be the (reduced) Betti number at time t. Then,

$$L_{\ell-1} = \int_0^\infty \widetilde{eta}_{\ell-1}(t) dt.$$

2 Let $T_{min}^{(\ell)}$ be the minimum spanning ℓ -acycle. Then,

$$L_{\ell-1} = \mathsf{wt}(\mathsf{T}_{\mathsf{min}}^{(\ell)}) - \mathsf{wt}(\mathsf{X}_{\ell-1} \setminus \mathsf{T}_{\mathsf{min}}^{(\ell-1)}),$$

Betti number $ilde{eta}_1(t)$ in the case $\ell=2$

• For the 2-Linial-Meshulam process, $L_1 = \sum_{\Delta \in \mathcal{T}_{min}^{(2)}} t(\Delta)$.



Figure: $\tilde{\beta}_1(t)$ for 2-Linial-Meshulam process when n = 15.

$$L_1 = \int_0^1 \beta_1(t) dt = wt(T_{\min}^{(2)})$$

Main result

Theorem (Y.Hiraoka-T.S.)

Let $L_{\ell-1}(n)$ be the lifetime sum of $(\ell - 1)$ -st persistent homology for the ℓ -Linial-Meshulam process on n vertices,

$$\mathbb{E}[L_{\ell-1}(n)] = \mathbb{E}[\min_{T \in \mathcal{S}^{(\ell)}(n)} wt(T)] = O(n^{\ell-1})$$

as $n \to \infty$, where

$$wt(T) := \sum_{\sigma \in T} t(\sigma).$$

See http://arxiv.org/abs/1503.05669

Remark: For ℓ = 1, 𝔼[𝒪₀(n)] → ζ(3).
 We will give a remark on the limiting value

$$\lim_{n\to\infty}\frac{1}{n^{\ell-1}}\mathbb{E}[L_{\ell-1}(n)].$$

Conjecture for the limiting values

Let $L_{\ell-1}(n)$ be the sum of lifetimes of $(\ell - 1)$ -th persistent homology for the ℓ -Linial-Meshulam process on n vertices,

$$\mathbb{E}[L_{\ell-1}(n)] = \mathbb{E}[\min_{T \in \mathcal{S}^{(\ell)}(n)} wt(T)] = O(n^{\ell-1}) \quad \text{as } n \to \infty.$$

Conjecture

$$\lim_{n \to \infty} \frac{1}{n^{\ell-1}} \mathbb{E}[L_{\ell-1}(n)] = \frac{1}{\ell!} \int_0^\infty h_{\ell-1}(c) dc =: I_{\ell-1},$$

where

$$h_d(c) = ct_c(1-t_c)^d + rac{c}{d+1}(1-t_c)^{d+1} + t_c - rac{c}{d+1}$$

and t_c is the minimum positive solution to $t = e^{-c(1-t)^d}$ for $c > c_d^*$ and $t_c = 1$ for $c < c_d^*$.

• Remark. For $\ell = 1$, $I_0 = \zeta(3)$, which recovers Frieze's result.

Clique (Flag) complex process

- The clique complex Cl(G) associated with a graph G is the maximal simplicial complex having G as a 1-dimensional skeleton.
- X⁽¹⁾(t): Erdös-Rényi graph process

$$\mathcal{C}(t) = \operatorname{Cl}(X^{(1)}(t)), \quad 0 \leq t \leq 1,$$

 The process starts from the 0-skeleton, i.e., n isolated vertices, and ends up with Δ_{n-1}. Namely,

$$\Delta_{n-1}^{(0)}=\mathcal{C}(0)\subset \mathcal{C}(t)\subset \mathcal{C}(1)=\Delta_{n-1}.$$

 The main difference from the Linial-Meshulam case is absence of monotonicity of Betti numbers.



Figure: Clique complex process on 5-vertices

Proposition

Let $L_{\ell-1}(n)$ be the lifetime sum for the clique complex process on *n*-vertices. Then, for $\ell = 1, 2$,

$$cn^{\ell-1} \leq \mathbb{E}[L_{\ell-1}(n)] \leq Cn^{\ell-1}\log n$$

and for $\ell \geq 3$,

$$cn^{\frac{(\ell+2)(\ell-1)}{2\ell}} \leq \mathbb{E}[L_{\ell-1}(n)] \leq Cn^{\ell-1}$$

- When $\ell = 1$, L_0 is equal to the lifetime sum of the Erdös-Rényi graph process. Since $\mathbb{E}[L_0] = O(1)$, the *lower* bound is correct.
- When ℓ = 2, the *upper* bound seems to be more appropriate than the lower one by simulation.

- Prove the conjecture for $\mathbb{E}[L_{\ell-1}(n)]$ as $n \to \infty$.
- Give an asymptotic expansion of $\mathbb{E}[L_{\ell-1}(n)]$.
- Give the exact asymptotics of $\mathbb{E}[L_{\ell-1}(n)]$ for clique complex.
- Limit theorem for scaled persistence diagrams (or barcodes, persistent landspaces etc.).
- Random geometric graph version of this problems.

Point process on $\mathbb{R}^d \Longrightarrow k$ -persistence diagram

- Anatomy of *l*-Linial-Meshulam complex as was done for the original Erdös-Rényi random graph. (cf. recent results by Linial-Peled.)
- Extension of Wilson's algorithm of generating a uniform spanning tree.

Filtration and persistent homology

