A unified topological approach to data science via high-dimensional structures of graphs

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Motivations of a unified topological approach in data science

Topology of subgraphs

Super Persistent Homology

Pipeline of Current Topological Data Analysis (TDA)

1. input data consisting on a finite set of points coming with a notion of distance;
2. a “continuous shape” is built on top of the data: this results into an structure over the data;
3. topological and geometric information is extracted from the structures;
4. the topological and geometric information are the output of the approach and correspond to the new features of the data.

Our Goal/Hope—provide an unified approach suitable for both point cloud data and graphic data

- In our setting, we explore topological structures on graphic data with scoring schemes.
- The current persistent homology can be obtained as special cases of our more general theory from a natural transformation from point cloud data to graphic data with scoring schemes.
- This is a **theoretical research** on topological approaches in data science for hoping to make a tunnel between topology and data science.

Our Approaches

A. Homology Theory on **any collection** of subgraphs of a working graph. In theory, you choose whatever collection of subgraphs, you get homology on this collection of subgraphs.

B. Assign **any scoring scheme** on the working graph so that there is a **score** for any subgraph in the collection of subgraphs on your hand. Then it creates **persistent homology** as **new feature** for you.

C. Of course the **current persistent homology on point cloud data** should be answered from **A and B**.

Answer to C for Vietoris-Rips persistent homology

Let X be a point cloud data in $\mathbb{R}^N$. Mathematically, X is a finite set located in $\mathbb{R}^N$.

- **Step 1.** The **working graph** G is a **complete graph** by joining one edge for each pair of points in X.—**simple!**
- **Step 2.** The **collection of subgraphs**: any clique (complete subgraph) of G.—**simple!**
- **Step 3.** The **scoring scheme**: Let G' be a subgraph. Define its score

$$\mathfrak{M}^{VR}(G') = \frac{1}{2}\max\{d(v,w) \mid v,w \in V(G')\},$$

the half of the maximal embedded distance in the Euclidean space between pairwise vertices.—**natural!**

Answer to C for Čech persistent homology

Let X be a point cloud data in $\mathbb{R}^N$. Mathematically, X is a finite set located in $\mathbb{R}^N$.

- **Step 1.** The **working graph** G is a **complete graph** by joining one edge for each pair of points in X.—**simple!**
- **Step 2.** The **collection of subgraphs**: any clique (complete subgraph) of G.—**simple!**
- **Step 3.** The **scoring scheme**: Let G' be a subgraph. Define its score

$$\mathfrak{M}^C(G') = \inf_{x \in \mathbb{R}^N} \max\{d(x, v) \mid v \in V(G')\},$$

—also natural!

Answer to C for Witness persistent homology

- The first two steps are the same.

- Only **re-define scoring schemes**: Let $G' \leq G$ be a subgraph of G embedded in $\mathbb{R}^N$.
  1. **Strong Witness Scoring**

$$\mathfrak{M}^{W^s}(G') = \inf_{x \in \mathbb{R}^N} \{ \sup_{y \in V(G')} d(x,y) - \inf_{z \in V(G)} d(x,z) \}.$$

  2. Similarly, there are **Vietoris-Rips Strong witness scoring**, **Weak witness scoring**, **Vietoris-Rips weak witness scoring** by translating Carlsson's setting for witness complexes into scoring.

Can we get anything new by looking scoring? Quick example 1

Let G be a graph located in $\mathbb{R}^m$. (e.g. graph data on $3D$ objects, data on protein structure.) Take VR-scoring on G. In stead of **complete graph on vertices of** G, we take **clique complex** $\mathrm{Clique}(G)$.

- $\Longrightarrow$ persistent homology converges to $H_*(\mathrm{Clqiue}(G))$.
- **Comparison.** *VR* persistent homology on point cloud data $V(G)$ converges to trivial homology.

- **Why is** $\mathrm{Clique}(G)$ **good?** Let $X = |K|$ be a polyhedron with K simplicial complex. Take G=1-skeleton of bary-centric subdivision of K. Then $|\mathrm{Clique}(G)| \cong |X|$.

Anything new? Quick example 2

Let us consider **pull-back scoring from a non-injective function from the vertex set to a Euclidean space**.

Let $p\colon E \to B$ be a fibration or fibre bundle with E, B polyhedra. Take triangulations on E and B to make p simplicial up to homotopy. Take graphs $G(E)$ and $G(B)$ as 1-skeletons of the bary-centric subdivisions of simplicial models for E and B.

Take scoring scheme on $G(E)$ as the **pull-back** of

$$V(G(E)) \xrightarrow{\text{proj}} V(G(B)) \xhookrightarrow{\text{embedding}} \mathbb{R}^m$$

Consider clique complexes $\mathrm{Clique}(G(E))$ and $\mathrm{Clique}(G(B)) \Longrightarrow$ **persistent Leray-Serre spectral sequence**.

The idea is a mathematization of a practical method

Guo-Wei Wei, *Persistent homology analysis of biomolecular data*, **SIAM News 50 (10)**, December 1, 2017:

> However, persistent homology neglects chemical and biological information ... and is thus **not as competitive as** geometry or physics-based representation in quantitative predictions. **Element-specific persistent homology**, or multi-component persistent homology built on colored biomolecular network, has been introduced... This approach enciphers biological properties—such as hydrogen bonds, van der Waals interactions, hydrophilicity, and hydrophobicity—into topological invariants, rendering a **potentially revolutionary representation** for biomolecules.

Element-specific=subnetworks only having C or O or "C and O"...

The mathematical question

Let G be a working graph. Let $\mathcal{H}$ be a family of finite subgraphs.

Question. What is a natural way to define homology of $\mathcal{H}$?

Rationality of Question: Abstract simplicial complex is a family of (finite) subsets that is closed under subset-operation. There is a well-established **simplicial homology theory**.

New Situation:

1) $\mathcal{H}$ is a family of finite subgraphs, rather than a family of finite sets; and
2) **no hypothesis** that $\mathcal{H}$ is closed under subgraph-operation.

High-dimensional structures

Clique complex (also named as **flag complex**) and **independence complex** (the clique complex of the complementary graph) are widely used notions in mathematics and practical applications.

The *clique complex* of a simple graph G is the abstract simplicial complex $\mathrm{Clique}(G)$ whose simplices consist of all cliques of G.

Let $G = (V, E)$ be a multi-graph. Then the set of cliques $\mathrm{Clique}(G)$ is **no longer** a simplicial complex in general[1]. The correct notion for describing the topological structure of the set $\mathrm{Clique}(G)$ is Δ**-set** (also called **semi-simplicial set**).

[1] let G be a graph with two vertices v and w and two edges e_1 and e_2 joining with them. Then $\mathrm{Clique}(G) = \{ve_1w, ve_2w, v, w\}$, which is not a simplicial complex.

Neighborhood complex—introduced by Lovász

Neighborhood complex $\mathcal{N}(G)$ of a graph G is a simplicial complex whose vertices are the vertices of G and whose simplices are those subsets of the vertex set $V(G)$ which have a **common neighbor**—landmark work on topological combinatorics of L. Lovász's solution to Kneser conjecture:[2].

- If we split the n-subsets of a $(2n+k)$-element set into $k+1$ classes, one of the classes will contain two disjoint n-subsets

The topology on the geometric realization of $\mathcal{N}(G)$ can be quite different from that of $\mathrm{Clique}(G)$ in general[3]. Namely, one could have different higher dimensional structures.

[2] Lovász, L. *Kneser's conjecture, chromatic number, and homotopy*, J. Combin. Theory Ser. A **25** (1978), no. **3**, 319-324.

[3] For instance, let G be a graph with three vertices a, b, c and two edges given by ab and bc. Then $\mathcal{N}(G) = \{\{a,c\},\{a\},\{b\},\{c\}\}$, which is not connected, and $\mathrm{Clique}(G) = \{\{a,b\},\{b,c\},\{a\},\{b\},\{c\}\}$ which is connected.

High-dimensional structures—Other complexes

- **Hom complexes**, a generalization of neighborhood complex introduced by Lovász[4].
- **Graph complex:** abstract simplicial complex on the edge set.— Jacob Jonsson, book in 2008[5][6].
- **Path complexes**—first introduced by **Shing-Tung Yau** and his collaborators[7], which was a mathematization of the work motivated from physical applications.
  - Recently introduced **magnitude homology** (of graphs) is related to path homology.
- **Tournaplexes**—in Ran Levi's talk.

[4] recent work: Eric, Babson and Dmitry N. Kozlov, *Proof of the Lovász conjecture*, Ann. of Math. (2) 165 (2007), no. 3, 965-1007.

[5] Jonsson, Jakob *Simplicial complexes of graphs. Lecture Notes in Mathematics*, **1928**. Springer-Verlag, Berlin, 2008. xiv+378 pp. ISBN: 978-3-540-75858-7.

[6] **Kontsevich**'s graph complex is a different notion.

[7] A. Grigor'yan, Y. Lin, Y. Muranov, and S.-T. Yau, Homologies of path complexes and digraphs, Math arXiv: 1207.2834v4, 2013.

Two types of topology on $\mathcal{H}$

For creating topology, we regard a subgraph in $\mathcal{H}$ as a **simplex** in certain dimension. It requires a **face-operation** so that we can "**glue**" together.

Face-operation 1. Vertex-deletion: clique complex, neighborhood complex, path complexes.

Face-operation 2. Edge-deletion: graph complex.

Edge-deletion Topology—Need homology of hypergraphs

Let G be a working graph. Let $\mathcal{H}$ be a family of finite subgraphs.

Consider $\mathcal{H}$ as a family of finite subsets of the edge set $E(G)$.

Each subgraph is determined by its edge set.

$\mathcal{H}$ is a **hypergraph** under **edge-deletion operation**.

There is a homology theory (as extension of simplicial homology theory) on hypergraphs: [8]

[8] Stephane Bressan, Jingyan Li, Shiquan Ren, Jie Wu, *The Embedded Homology of Hypergraphs and Applications*, Asia J. Math. **23** (2019), no. 3, 479-500.

Vertex-deletion Topology—Need homology of super-hypergraphs

Let G be a working graph. Let $\mathcal{H}$ be a family of finite subgraphs.

Consider $\mathcal{H}$ as a family of finite subsets of the vertex set $V(G)$.

Each subgraph **may not be** determined by its vertex set.

Example. Let G be a multi-graph with vertices a and b and two edges f_1, f_2 between a and b. Then af_1b and af_2b are two subgraphs having the same vertices.

If we want to explore topology of subgraphs, the notion of hypergraph is insufficient.

We need a new notion. We call it **super-hypergraph**.

Δ-set

A Δ**-set** means a sequence of sets $X = \{X_n\}_{n\geq 0}$ with *faces* $d_i : X_n \to X_{n-1}$, $0 \leq i \leq n$, such that

$$d_i d_j = d_j d_{i+1}$$

for $i \geq j$, which is called the Δ*-identity*.

The notion of Δ-set is a generalization of (abstract) simplicial complex by ruling out **face-operation**.

Simplicial homology can be defined using the notion of Δ-set.

Super-hypergraph

A **super-hypergraph** is a pair $(\mathcal{H}, X)$, where X is a Δ-set and $\mathcal{H}$ is a graded subset of X.

We call $\mathcal{H}$ a **super-hypergraph born from** X, and X is called **a parental Δ-set** of $\mathcal{H}$.

Example. Let G be a multi-graph with vertices a and b and two edges f_1, f_2 between a and b. Let $\mathcal{H} = \{af_1b, af_2b\}$ be two simple subgraphs. Then $\mathcal{H}$ can be viewed as a super-hypergraph with two 1-simplex with sharing the same missing vertices.

Algebraic Lemmas

Let G_* be a chain complex of groups and let D_* be a graded subgroup of G_*. Here we do not assume that G_n is commutative. Define

- $\sup_*^{G_*}(D_*)$ is the intersection of subcomplexes C_* of G_* with property that $D_n \leq C_n$ for $n \in \mathbb{Z}$.
- $\inf_*^{G_*}(D_*)$ is the product of subcomplexes E_* of G_* with property that $E_n \leq D_n$ for $n \in \mathbb{Z}$.

We briefly denote $\sup_*(D_*)$ for $\sup_*^{G_*}(D_*)$ and $\inf_*(D_*)$ for $\inf_*^{G_*}(D_*)$ if the embedding of $D_* \subseteq G_*$ is clear.

Algebraic Lemmas

Proposition. Let G_* be a chain complex of groups and let D_* be a graded subgroup of G_*.

1. The inclusion
$$\inf_*(D_*) \longrightarrow \sup_*(D_*)$$
induces an injective mapping on homology.

2. Suppose that $\partial^{G_*}_{n+1}(D_{n+1})$ is contained in the normalizer of D_n for each n. Then the inclusion
$$\inf_*(D_*) \longrightarrow \sup_*(D_*)$$
induces an isomorphism on homology. In particular, if D_n is normal in G_n for $n \in \mathbb{Z}$, then the inclusion $\inf_*(D_*) \longrightarrow \sup_*(D_*)$ induces an isomorphism on homology.

Embedded Homology of Super-hypergraphs

Let $(\mathcal{H}, X)$ be a super-hypergraph. Let A be an abelian group. The **embedded homology** $H_*^{\mathrm{emb},X}(\mathcal{H}; A)$ **with coefficients in** A of $(\mathcal{H}, X)$ is defined by the homology of the chain complex of $\inf_*$ and $\sup_*$ of the graded subgroup $\mathbb{Z}(\mathcal{H}) \otimes A$ in the chain complex $C_*(X; A)$.

Note. The **gap complex** $\sup_*(\mathbb{Z}(\mathcal{H}) \otimes A)/\inf_*(\mathbb{Z}(\mathcal{H}) \otimes A)$ is contractible. If there are some additional information, one may get further information on the gap complex. For instance, if there is a group G-action, then one may look at homology $H_*((\sup_*/\inf_*) \otimes_{\mathbb{Z}(G)} M)$ for G-modules M.

Remark

Embedded Homology of a hypergraph/super-hypergraph **may not be equal to** homology of a simplicial complex in general.

Let $\mathcal{H}$ be the boundary of a 2-simplex with **removing all three vertices**. Let X be the boundary of the 2-simplex. Then $H_1(X) = \mathbb{Z}$, $H_0(X) = \mathbb{Z}$, and $H_1(\mathcal{H}) = \mathbb{Z}$, $H_0(\mathcal{H}) = 0$.

No nonempty space whose unreduced 0-th homology is 0.

hypergraphs/superhypergraphs seem **geometry-like** objects.

Geometric gap complex: Let $\Delta\mathcal{H}$ be the minimal Δ-subset of X containing $\mathcal{H}$, and let $\delta\mathcal{H}$ be the maximal Δ-subset of X contained in $\mathcal{H}$. The inclusion $\delta\mathcal{H} \to \Delta\mathcal{H}$ may not be homotopy equivalent.

Mayer-Vietoris Sequence

Let $(\mathcal{H}, X)$ be a super-hypergraph and let A and B be Δ-subsets of X such that $A \cup B = X$. Let $\mathcal{H}^A = \mathcal{H} \cap A$, $\mathcal{H}^B = \mathcal{H} \cap B$ and $\mathcal{H}^{A \cap B} = \mathcal{H} \cap A \cap B$. Let G be an abelian group, and let $(\mathcal{H}, Y)$ be a super-hypergraph. Denote by $\sup_*^Y(\mathcal{H})$ and $\inf_*^Y(\mathcal{H})$ for $\sup_*^{C_*(Y;G)}(\mathcal{H})$ and $\inf_*^{C_*(Y;G)}(\mathcal{H})$, respectively.

Theorem. With the notation above, there is a commutative diagram

Mayer-Vietoris Sequence

$$
\begin{array}{ccccc}
 & & & & \sup_*^X(\mathcal{H}) \\
 & & & & \| \\
\sup_*^A(\mathcal{H}^A) \cap \sup_*^B(\mathcal{H}^B) & \hookrightarrow & \sup_*^A(\mathcal{H}^A) \oplus \sup_*^B(\mathcal{H}^B) & \xrightarrow{j_A - j_B} & \sup_*^A(\mathcal{H}^A) + \sup_*^B(\mathcal{H}^B) \\
\uparrow & & \uparrow \simeq & & \uparrow \\
\inf_*^A(\mathcal{H}^A) \cap \inf_*^B(\mathcal{H}^B) & \hookrightarrow & \inf_*^A(\mathcal{H}^A) \oplus \inf_*^B(\mathcal{H}^B) & \xrightarrow{j_A| - j_B|} & \inf_*^{A)}(\mathcal{H}^A) + \inf_*^B(\mathcal{H}^B), \\
\| & & & & \\
\inf_*^{A \cap B}(\mathcal{H}^{A \cap B}) & & & &
\end{array}
$$

where the middle two rows are short exact sequence of chain complexes, the maps j_A and j_B are canonical inclusions and the upper arrows are inclusions.

Super Persistent Homology

Let G be a directed or undirected multi-graph with a **scoring scheme** $\mathfrak{M}$.

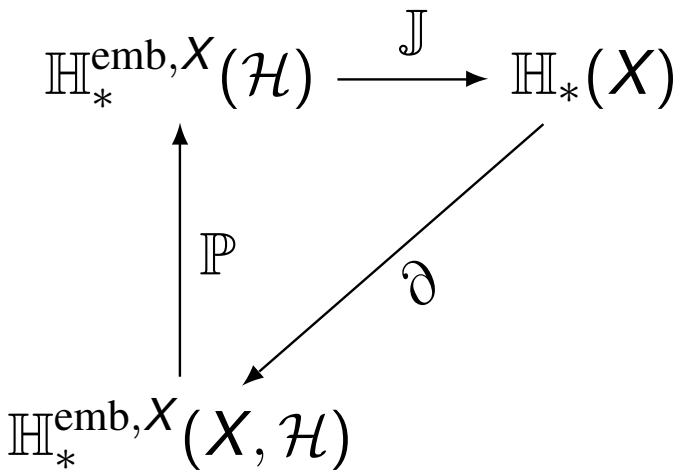
Let $(\mathcal{H}, X)$ be a super-hypergraph dominated by G, i.e X is a collection of finte subgraphs with face operation defined in certain way. Then there is a **filtration** $(\mathcal{H}^t, X^t)$, $t \in \mathbb{R}$, defined by

$$\mathcal{H}^t = \{G' \in \mathcal{H} \mid \mathfrak{M}(G') \leq t\} \text{ and } X^t = \{G' \in X \mid \mathfrak{M}(G') \leq t\},$$

The *associated persistent homology* of this filtration is called **super-persistent homology** of $(\mathcal{H}, X)$ under scoring scheme $\mathfrak{M}$.

Persistence modules of super-persistent homology

Let $(\mathcal{H}, X)$ be a super-hypergraph dominated by a directed/undirected (multi-)graph G with a scoring scheme. There is an exact triangle of graded persistence modules



with ∂ of degree -1.

Structure Theorem

Let $(\mathcal{H}, X)$ be a super-hypergraph dominated by a directed/undirected (multi-)graph G with a scoring scheme. Suppose that X is of finite type. Then the graded persistence modules $\mathbb{H}_*(X)$, $\mathbb{H}_*^{\mathrm{emb},X}(\mathcal{H})$ and $\mathbb{H}_*^{\mathrm{emb},X}(X,\mathcal{H})$ admit unique direct sum decompositions in terms of graded **interval persistence modules** up to the order of factors in the category of graded persistence modules.

Proof follows from a theorem of Crawley-Beovey derived from the classical Gabriel Theorem in representation theory.

Interval persistence module $\mathbb{F}^J$: J is an interval, $\dim(\mathbb{F}_t^J) = 1$ if $t \in J$, and 0 otherwise. The map $\mathbb{F}_t^J \to \mathbb{F}_s^J$, $t \leq s$, is defined in the canonical way.

What does Structure Theorem tell?

Let $\mathbb{M}$ and $\mathbb{N}$ be persistence modules that admit unique (up to order of factors) decompositions in terms of interval persistence modules. Let $\phi\colon \mathbb{M} \to \mathbb{N}$ be a morphism of persistence modules. Let $\mathbb{F}^{I_\alpha}$ be a factor of $\mathbb{M}$, and let $\mathbb{F}^{J_\beta}$ be a factor of $\mathbb{N}$. Then the composite

$$\mathbb{F}^{I_\alpha} \hookrightarrow \mathbb{M} \xrightarrow{\phi} \mathbb{N} \xrightarrow{\text{proj.}} \mathbb{F}^{J_\beta}$$

is either isomorphic or zero. Hence we have a **correlation matrix** M for ϕ with $m_{\alpha\beta} = 1$ if ϕ is an isomorphism and 0 if ϕ is zero.

$\Longrightarrow$ super-persistent homology gives (1) **three multi-layered barcodes**, and (2) **three multi-layered correlation matrices**.

Scoring Scheme and sequence of cochains

Any scoring scheme $\mathfrak{M}$ **restricted to** $\mathcal{H}$ gives a sequence of cochains $\mathfrak{M}^n = \mathfrak{M}| : \mathcal{H}_n \to \mathbb{R}$.

Conversely, any sequence of cochains extends to a scoring scheme on G.

The relationships and product structures on chains and cochains might help for studying the **adjustment or learning** on scoring schemes.

Also **geometry** might help for studying the **adjustment or learning** on scoring schemes.

Thank You for Your Attention!