A Simplical Complex-Based Kernel Estimation Method for Cracking Higher-Order Graph Structures in Cell Complex Topology

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Abstract

The primary goal of the article is to examine the data s shape and crack higher-order graph structures in cell complex topology. Further simplical complex-based kernel estimation methods are explored and discussed.

Keywords: Simplicial complex; Euler characteristic; Simplicial homology; Cell complex topology

1 introduction

Topological data analysis (TDA) is an approach to applied mathematics dataset analysis using topological concepts. Extracting information from noisy, high dimensional, incomplete datasets is generally difficult. TDA offers a broad framework for analyzing such data that reduces dimensionality and is noise resistant while remaining insensitive to the specific metric selected. Further more, because of its topological properties, which enable it to adjust to new mathematical instruments, it carries over the essential idea of functionality from modern mathematics. The foundation of TDA is the notion that pertinent in formation can be found in the shape of data sets. Real high-dimensional data usually has pertinent low-dimensional features and is sparse. Giving a detailed description of this fact is one of TDA s tasks. For instance, a closed circle is formed in state space by the trajectory of a basic predator-prey system controlled by the Lotka Volterra equations [1] [1] Munkres, J. Elements of Algebraic Topology. Addison Wesley Publishing Company. (1984).

TDA offers instruments to identify and measure this kind of repetitive action [2]duction. American Mathematical Society.. Assigning topological invariants to data is the concept behind Topological Data Analysis (TDA). On the other hand, data is usually presented as a discrete sample with a very boring topology.

To match shapes of geometric objects from which the data are collected topologically, we have to convert the data into continuous objects.

Consider the discrete collection of data points shown in the following graphic. The data undoubtedly has a ”circular structure,” and our pattern-seeking brains have little issue deducing this information. Topology in and of itself does not quantify this circularity; rather, an annulus develops when each point is thickened to a

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predetermined degree. This object is topological and has a distinct ”circular structure.” Many data analysis algorithms, like the ones in TDA, need you to set different parameters. Selecting the appropriate collection of parameters for a data set might be challenging if one lacks prior domain knowledge [3][3] Bertrand, J. (1858). Note sur la théorie des polyèdres réguliers, Comptes. Persistent homology’s primary insight is to utilize the data collected from all parameter values by encoding this massive amount of data into a clear and simple format. When the data is a homology group, TDA has a mathematical interpretation. Generally speaking, it is assumed that characteristics that hold across a large range of parameters are ”true” features. It is thought that features that endure for a limited range of parameters are noise, while it is not quite obvious why this is the case theoretically [4]via U. Paci c, Stockton, CA..

To investigate the resulting continuous spaces on a computer, they must first be discretized, and simplicial complexes are usually used for this purpose. The Cech and Vietoris-Rips complexes are two specific constructions of simplicial complexes covered in this section.

To investigate the resulting continuous spaces on a computer, they must first be discretized, and simplicial complexes are usually used for this purpose.

Definition 1.1. If the point $p_i \in \mathbb{R}^d$, then $\{p_i\}_{i=0}^{n}$ is geometrically independent [1] Company. (1984). if $\forall a_i \in \mathbb{R}$, the following conditions hold:

(i) $\sum_{i=0}^{n} a_i = 0$

(ii) $\sum_{i=0}^{n} a_i p_i = 0$

(i) and (ii) imply that $a_1 = a_2 = ... = a_n$.

Remark 1.2. Any singleton is geometrically independent.

The $n-$simplex spanned by $a_1, a_2, ..., a_n$ is the convex hull of these points.

Definition 1.3. (i) If the set $\{p_i\}_{i=0}^{n}$ is geometrically independent, then $x = \sum_{i=0}^{n} a_i p_i$ is called $n-$simplex spanned by the points [1] Company. (1984). such that $\sum_{i=0}^{n} a_i = 1 \; \forall a_i > 0$, $i = 0, 1, ..., n$.

(ii) The point $x = \sum_{i=0}^{n} a_i p_i$ is convex combination of $p_1, p_2, ..., p_n$,and the scalers $a_1, a_2, ..., a_n$ are barycentric coordinates.

(iii) The points $p_1, p_2, ..., p_n$ are vertices if they span a simplex σ.

(iv) n represents the dimension of the simplex σ.

(v) Simplex σ is regular, if all its sides possesses the same length.

(vi) Regular simplex is a standard $n-$simplex (denoted by Δ^n) spanned by the unit vectors’ endpoints along the coordinate axes in $\mathbb{R}^{n+1}$.

(vii) If the face $\tau \subset \sigma$ is spanned by the subset of the vertices that are defining σ, then τ is a face of σ.

Each point is $0-$simplex, while $2-$different points create $1-$simplex (line), $3-$non-collinear points form $2-$simplex (triangle), $4-$non-coplanar points form $3-$simplex (tetrahedron), and so on. These observations are immediately apparent without further explanation.

Topological spaces whose combinatorial qualities dictate their properties are obtained by gluing simplices along faces.

Definition 1.4. (i) The simplicial complex C, in $\mathbb{R}^d$, is a finite collection of simplices in $\mathbb{R}^d$ where:

(a) Each face of the simplex of C belonges to C.

(b) The intersection of any two simplices of C forms a face of each.

(c) The dimension of the simplicial complex C (denoted by $dim(C)$) is the maximum dimension of its simplices.

(ii) $|C|$ denotes the union of all simplices in C, with the subspace topology τ_C. (C, τ_C) is the underlying space of C.

(iii) The finite collection A of finite non-empty sets is called the abstract simplicial complex. If $\beta \in A$, then every nonempty subset of β is an abstract simplicial complex of β.

(iv) Simplices are elements of A and the dimension of $\beta \in A$ is $dim(\beta) = |\beta| - 1 = \max\limits_{\beta \in A}(\dim(\beta))$.

(v) $K \subset A$ is a subcomplex of A if K is an abstract simplicial complex.

(vi) The set v_B of vertices of B is the union of the one-point elements of B.

(vii) If A and B are two simplical complexes, then they are isomorphic if $\exists f$ a bijective correspondence: $f : A \to B \; \forall \{a_1, a_2, ..., a_n\} \in A$ iff $\{f(a_1), f(a_2), ..., f(a_n)\} \in B$.

Definition 1.5. If C defines an abstract simplicial complex A by identifying each C with its vertices, then A is its vertex scheme.

Example 1.6. $1-$ simplex connecting $\alpha_\circ$ and α_1 has vertex scheme $\{\{\alpha_\circ\}, \{\alpha_1\}, \{\alpha_\circ, \alpha_1\}\}$.

2 Examples from real life utilizing simplicial complexes

In intense laser-plasma physics, numerical simulation: [5]drodynamic calculations. created the particle-in-cell (PIC) approach, a numerical simulation that tracks particles using n-body techniques. Plasma behavior is significantly shaped by particle-particle (PP) interactions.

The dynamics of proteins in biochemistry and structural biology: Protein structure networks are used to model proteins, which are made up of amino acids joined by covalent peptide bonds. Greene [6] Genomics, 11, 469 478., whose composition is directly related to the way the protein Mannige functions [6] Genomics, 11, 469 478.. In particular, ”protein sectors” model higher-order interactions between amino acid groups. Simplices work well for simulating the intricate relationships among the sectors. These two instances are explained in greater detail in the supplementary material (SM).

Definition 2.1. If A is the vertex scheme of C, then C is a geometric realization of A.

Example 2.2. It is possible to geometrically materialize every abstract simplicial complex on $d + 1$ vertices as a subcomplex of any d-simplex in $\mathbb{R}^d$.

Definition 2.3. If K is a finite subset of $\mathbb{R}^d$,then K is generally positioned if any subset of no more than $d + 1$ points is independent of geometry.

Example 2.4. The majority of point sets are generally positioned, and the points that cannot be moved arbitrarily slightly to become in general perturbation.

Lemma 2.5. *Abstract simplicial complex* K *with* $\dim K = d$ *in* $\mathbb{R}^{2d+1}$ *has a geometric realization .*

Proof. Under the function $f : V_K \to \mathbb{R}^{2d+1}$, let $f(V_K)$ be in the general position.

Each simplex $\alpha \in K$ has at most $d+1$ vertices and is denoted by σ_α.

Hence, the vertices of α correspond to a geometrically independent set (say $f(\alpha)$) under f.

If α and β are two simplices: $|\alpha \cup \beta| \leq 2(d+1)$, then $f(\alpha) \cup f(\beta)$ forms a geometrically independent set.

Hence, $\exists x \in \sigma_\alpha \cap \sigma_\beta$ that can be represented as a convex combination of the vertices $f(\alpha) \cup f(\beta)$, and then the barycentric coordinates of x are non-zero only for $\gamma_i \in f(\alpha \cap \beta)$. ☐

Definition 2.6. X is triangulable if $\exists C$ a simplicial complex whose underlying space is homeomorphic to X.

Remark 2.7. (i) Each homeomorphism $f : |C| \to X$ is a triangulation.

(ii) Each closed surface and $3-$dimensional manifolds can be triangulated.

(iii) The $4-$dimensional manifolds need not admit a triangulation.

Definition 2.8. The Cech complex of $\wp = \{p_\circ, p_1, ..., p_n\}$ at scale r (the closed ball's radius with its center at p) is the simplicial complex:

$Cech_r(\wp) = \{\sigma \subset \wp : \underset{p\in\sigma}{\cap} B(p,r) \neq \varphi\}$ where $B(p,r) = \{a \in X^d : \|x-a\| \leq r\}$

Theorem 2.9. *(Hellys Theorem): [2]duction. American Mathematical Society. If* F *denotes a finite collection of the* $\mathbb{R}^d$ *convex closed sets, and* $\cap V_\alpha \neq \varphi$ *where* V_α *is a* $d+1$ *set* $\forall \alpha$*, then there is a non-empty intersection throughout the entire collection.*

Remark 2.10. (i) Let $\wp \subset \mathbb{R}^3$, then for determining $Cech_r(\wp)$, computing each quadruple intersection will be sufficient.

(ii) $\sigma \in Cech_r(\wp)$ iff the elements of σ belong to $B(a,r)$ $\forall a \in \sigma$.

Definition 2.11. (i) The smallest enclosing ball that contains the set of points $\sigma \in \wp$ is a minimal enclosing ball [2]duction. American Mathematical Society.. This ball can be evaluated with the miniball algorithm.

(ii) The diameter of the subset $\sigma \in \wp$ is $diam(\sigma) = \max\limits_{p_i, pj \in \sigma} \|p_i - p_j\|$

Definition 2.12. Vietoris-Rips complex of $\wp$ at scale r is a simplicial complex $VR_r(\wp) = \{\sigma \subset \wp : diam(\sigma) \leq r\}$

Remark 2.13. $Cech_r(\wp) \subset VR_r(\wp)$

Theorem 2.14. *(Jungs Theorem). [7] ISBN 0-521-79540-0. If* $\wp$ *is a finite set of points in* $\mathbb{R}$, *then the closed ball of radius* $r \leq \delta.diam(\wp)$ *contains* $\wp$ *such that* $\delta = \sqrt{\overline{2(+1)}}$

Proof. By induction, the result is true for $= 1$.

Now, for > 1, it suffices to consider that the points of $\wp$ are independent geometrically and $|\wp| =+1$.

Typically, if the points of $\wp$ are not independent geometrically or $|\wp| <+1$, then $\wp$ could be embedded in $\mathbb{R}^{-1}$ isometrically.

Hence, the inductive hypothesis gives the result.

For $|\wp| >+1$, then Jung's theorem is the equivalence of $\underset{p\in\wp}{\cap} B_{\delta.diam(\wp)} \neq \varphi$.

From Hellys theorem [3], it suffices to show that $\underset{A\in\wp}{\cap} A \neq \varphi$, where A contains $+1$ points.

Suppose $\wp$ has a minimal enclosing ball of radius r and center a that is contained in σ and spanned by $\wp$,in that case, the orthogonal projection of a onto this plane (the affine (-1)-dimensional that is spanned by points belonging to $\wp - p$) is strictly closer to the points of $\wp$.

The center a can be written as $\overset{+1}{\underset{i=1}{t_i}}\, p_i$ where $\overset{+1}{\underset{i=1}{t_i}} = 0\ \forall t_i \geq 0$.

Now, without loss of generality, let $z = 0$, fixing $j \in [1,+1]$ to get$_{i=1,i\neq j}^{+1} t_i||p_i - p_j||^2 - 2p_j \overset{+1}{\underset{i=1}{t_i}} = r^2 - 0 + r^2$

Taking sum over $j \in [1,+1]$ to get $\overset{+1}{\underset{j=1}{}}\ \overset{+1}{\underset{i\neq j}{t_i}}\, ||p_i - p_j||^2 = \overset{+1}{\underset{j=1}{}}\ \overset{+1}{\underset{i\neq j}{t_i}}\, (diam(\wp))^2 =(diam(\wp))^2$.

So, $r \leq \sqrt{\overline{2(+1)}}(diam(\wp))$. ☐

Determining whether 2 simplicial complexes are homomorphic, or homotopy equivalent, is a problem, making the distinction between topological spaces a notoriously difficult problem. This basically indicates that there isn't an algorithm that accepts two simplicial complexes as input and returns true only iff they are homeomorphic.

Even if it is assumed that the simplicial complexes are triangulations of $4-$dimensional manifolds, then this remains true. Therefore, it is frequently more effective to demonstrate that two spaces appear different when viewed through the prism of a tool that is insensitive to homeomorphism in order to demonstrate that they are not homeomorphic. One such method is algebraic topology, which associates topological spaces with algebraic invariants like homology and homotopy groups. The Euler class in mathematics is a characteristic class of oriented, real vector bundles, more precisely in algebraic topology. It gauges how "twisted" the vector bundle is, just like other characteristic classes. It generalizes the traditional idea of Euler characteristic to the case of the tangent bundle of a smooth manifold. For this reason, it bears Leonhard Euler's name.

Definition 2.15. (i) Euler characteristic, or Euler number or Euler–Poincaré characteristic, is a topological invariant that characterizes the structure or shape of a topological space independent of its bend. It is beneficial in polyhedral combinatorics and algebraic topology. χ is a common way to indicate it.

(ii) If $C = \{C_i : C_i$ is an $i-$simplices$\}$, then the Euler characteristic of C is the integer $\chi(C) = \underset{0\leq i}{}(-1)^i C_i$

This integer is defined for the surfaces of polyhedra, based on the formula $\chi = V - E + F \ldots\ldots$ (1)

where V, E, and F are the numbers of vertices, edges , and faces respectively in the polyhedron is stated by [4]via U. Paci c, Stockton, CA. and known as Euler's polyhedron formula. This corresponds to the sphere's Euler characteristic where $\chi = 2$, and applies to spherical polyhedra identically.

Example 2.16. Formula (1) on all Platonic polyhedra is given by the table below Platonic polyhedral

For the regular polyhedra, the modified form of Euler's formula is derived by Cayley [3] rendus des séances de l Académie des Sciences, 46: 79 82, 117..

$d_uV - E + d_fF = 2D \ldots\ldots$ (2)

Where D is the density, d_u is the vertex figure density and d_f represents the face density.

Formula (2) holds for all convex polyhedra, and non-convex $Kepler - Poinsotpolyhedron$ [3] rendus des séances de l Académie des Sciences, 46: 79 82, 117..

Remark 2.17. (i) In the convex $polyhedra$, the densities are all 1.

(ii) All projective polyhedra (like projective plane) possess Euler characteristic 1.

(iii) The surfaces of toroidal polyhedral (like torus) possess Euler characteristic 0.

For the connected plane graphs, Euler's characteristic can be defined by formula [1] Company. (1984). exactly like polyhedral surfaces, where F represents the number of graph's faces, including the exterior face. For the connected graph G, its Euler characteristic is 2.

A stereographic projection [5]drodynamic calculations. is a perspective projection of the sphere onto a plane that is perpendicular to the diameter through a specific point on the sphere (referred to as the pole or center of projection).

A linked graph maps to a polygonal decomposition of the sphere with Euler characteristic 2, and the plane maps to the $2-$sphere via stereographic projection.

3 CW Complex (Cell Complex Topology)

An important type of topological space in algebraic topology is a CW complex [7] ISBN 0-521-79540-0., also known as a cellular complex or cell complex. Whitehead [14]ics,2(1):108 introduced it in order to satisfy the requirements of homotopy theory. Compared to simplicial complexes, this class of spaces is broader and has some better categorical properties, but it still has a combinatorial nature that makes computation possible (usually with a much smaller complex). The letters C and W represent "closure-finite" and "weak" topology, respectively.

Remark 3.1. The polyhedral surfaces are finite $CW-$complexes in two dimensions. (They are called two-dimensional finite simplicial complexes when one uses only triangle faces.) Broadly speaking, the Euler characteristic of any finite CW-complex is given by

$\chi = k_\circ + k_1 + k_3 \ldots\ldots(3)$

where k_n represents the complex's dimension n number of cells.

For the simplicial complex, Euler characteristic is the alternating sum given by formula (3) where k_n represents the complex's n-simplexes number.

Definition 3.2. Let C be an arbitrary field and S a finite set. The vector space $F(S)$, with elements provided by the formal linear combinations $a_i + b_i \in C$, where each $a_i \in C$ and $s_i \in S$, is what we define as the free $C-$vector space generated by S [8][8] Greub, W. (1975). Linear Algebra, Springer-Verlag, Fourth edition.. In this case, addition is defined in an obvious component-wise manner:

$$\underset{s_i \in S}{} a_i s_i + b_i s_i = \underset{s_i \in S}{} (a_i + b_i) s_i \ldots\ldots (4)$$

Resulting $C - vector\ space$ possesses a canonical vector space basis that are given by the elements in S.

Example 3.3. If $C = \mathbb{Z}_3$ and $S = \{x, y\}$, then $F(S)$ is $9-$dimensional vector space. Its elements are $\{0, x, y, 2x, 2y, 2x + y, x + 2y, x + y, 2x + 2y\}$

Definition 3.4. (i) The rank of the n^{th} singular $homology$ group can be defined as the n^{th} Betti number β_n [9] England: Cambridge University Press, 1998. for any topological space. Then, the alternating sum can be used to define the Euler characteristic for the simplical complex C as

$$\chi = \beta_\circ - \beta_1 + \beta_2 - \beta_3 \ldots\ldots\ldots (5)$$

$$\overset{\infty}{\underset{i=0}{=}} (-1)^n C_i \overset{\infty}{\underset{i=0}{=}} (-1)^n b_i \ldots\ldots (6)$$

(ii) If an edge path-connects any two vertices in the simplicial complex C, then C is path-connected.

If all of the Betti numbers are finite and remain zero after a specific index $n_\circ$, then this quantity is well-defined. Although this definition is different from the one for simplicial complexes provided in the previous paragraph, a homology calculation shows that the two definitions will produce the same value for χ.

Lemma 3.5. *A simplicial complex C is path-connected iff* $|C|$ *,in the topological sense, is* $path - connected$.

Proof. Suppose that $|C|$ is $path-connected$. Let $C_\circ$ represent the simplicial complex made up of all simplices having the feature that every vertex in $C_\circ$ can be connected to p through an edge-path.

Fix a vertex p in $C_\circ$.

The subcomplex of K made up of all simplices that do not belong to $C_\circ$ is designated as C_1.

So, $C_\circ$ and C_1 are disjoint and $C_\circ \cup C_1 = C$.

Now, $|C_\circ|$ and $|C_1|$ are closed subsets of $|C|$.

Hence, $|C_1|$ is an empty set. □

Theorem 3.6. $\beta_\circ(C)$ *is the number of paths connecting components of* $|C|$.

Theorem 3.7. *A genus g surface's Euler characteristic is* $2 - 2g$.

If two closed, oriented surfaces have this property in common, they are homeomorphic.For manifolds of any dimension, this is obviously not possible.

For competent workers in each other field, or more broadly, in any Abelian group, homology is well-defined. The Betti numbers for simple complexes in $\mathbb{R}^3$ are independent of the coefficients selected. The Betti numbers, however, may vary depending on the underlying field in higher dimensions.

4 Simplicial Homology

Vector spaces are the method used nowadays to define the Betti numbers. By using vector spaces instead of just integers, we can move homological data along continuous maps. The development of persistent homology and the demonstration of invariance under topological invariance depend on this characteristic, known as functoriality. The sequence of $homology$ groups of a simplicial complex is known as simplicial homology in algebraic topology. It gives formal form to the concept of the number of holes in a complex of a given dimension. In the case of dimension 0, this generalizes the some of connected components.

The study of topological spaces whose constituents are $n-$simplices, the $n-$dimensional equivalents of triangles, gave rise to simplicial homology. This consists of a tetrahedron ($3-$simplex), a triangle ($2-$simplex), a line segment ($1-$simplex), and a point ($0-$simplex).

An orientation of a simplex is a crucial idea in the definition of simplicial homology. An ordering of the vertices, denoted as $(v_\circ,v_1,\ldots,v_n)$ determines the orientation of an $n-$simplex by definition. Two orderings define the same orientation iff they differ by an even permutation. As a result, there are precisely two orientations for any simplex, and an orientation can be changed to the other orientation by simply rearranging its vertices. Selecting the orientation of a $1-$simplex, for instance, corresponds to selecting one of the two available directions, while selecting the orientation of a $2-$simplex corresponds to selecting the meaning of ”counterclockwise”.

A formal linear combination of the $n-$cells in a cell complex is called an $n-$chain in algebraic topology. $n-$chains in simplicial complexes (or cubical complexes) are combinations of $n-$simplices (or $n-$cubes), however they are not always related. Homology uses chains; equivalence classes of chains make up a homology group’s members.

Definition 4.1. If S and T are two simplicial complexes, then:

(i) The simplicial $n-$chain is $\overset{N}{\underset{n=1}{}} c_n\sigma_n \; \forall c_n \in \mathbb{R}$ and σ_n is an oriented $n-$simplex.

(ii) A simplicial function f connecting S and $T\prime s$ vertex sets is a function that makes every simplex in S, when seen as a set of vertices, have an image in T.

Remark 4.2. All oriented simplexes are equivalent to the negative of their oppositely oriented simplex.

C_n is the notation for the group of $n-$chains on S. This is a free abelian group whose basis is the set of $n-$simplices in S, in a one-to-one relationship. Each simplex has an orientation that must be selected in order to expressly specify a basis. Choosing an ordering for all the vertices and assigning the orientation of each simplex to the induced ordering of its vertices is a common method for doing this.

A related theory more suited to theory than computation is singular homology. Singular homology is defined for all topological spaces and is independent of triangulation; for spaces that are triangulable, it agrees with simplicial homology. However, simplicial homology has gained importance for usage in real-world scenarios like image analysis, medical imaging, and data analysis in general since it can be computed automatically and effectively for a simplicial complex. Cellular homology is an additional related theory [10] WSEAS Transactions on Mathematics, 19: 606-609..

Finding a topological feature among a set of points such as measurements or dark pixels in a bit map is a common scenario in many computer applications. Since homology is easily computed from combinatorial data, such a simplicial complex, it can be used as a qualitative tool to look for such a trait. The data points must first be triangulated, which entails substituting a simplicial complex approximation for the data [11] Protein Structure, Function and Evolution, Proteomes, 2: 128 153..

Analysis of homology at various resolutions is required for the computation of persistent homology [12] 511 533., which registers homology classes (holes) that continue when the resolution is altered. These characteristics can be used to identify cluster structures in complex data, malignancies in X-rays, and molecular structures. Generally, simplicial homology is essential to topological data analysis, a data mining technique [13] Basel. ISBN 978-3-0346-0188-7..

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