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Relatore Prof. F. Vaccarino

Graphlet Counting for Topological Data Analysis

Candidate: Marco Guerra

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1 Introduction

Abstract

The field of Topological Data Analysis is a recent approach to the task of extracting information from especially troublesome datasets. The rationale of applying topological methods lies in the essentiality of the concept of topological shape, which only accounts for the effective structure of data and is blind to the dimensionality and particular metric, features that in some cases convey more noise than information. The main tool to have been employed in this endeavor is persistent homology, a concept in algebraic topology which extends the homological group representation of a space X to a discrete filtration of subspaces of X. In particular, we assume to have a chain of gradually more refined simplicial complexes over a given set of data points, with the corresponding inclusion maps between them: homology provides a computable method to count the *holes*, while persistence is applied to analyze their evolution as connectivity grows [12].
In the present work we introduce a minimality constraint and focus on computing the shortest possible basis of the first homology group H_1 of a weighted simplicial complex. The task is proved to be an NP-hard problem for H_k with $k > 1$ [7], but the k=1 case is subject of recent research. Taking the lead from the recent work of Dey [6], which borrows ideas from previous studies ([8],[9]) to improve computational complexity, I have implemented a polynomial-time algorithm for the shortest homology basis of a simplicial complex over $\mathbb{Z}_2$ coefficients and extended it to compute persistence over a family of its refinements. The final objective is to experiment with existing datasets of neuroscientific measurements, in the light of the framework proposed by [14], where a new topological object called *homological scaffold* is introduced to evaluate brain neuron activity correlations at a mesoscopic level, interpreting holes as inhomogeneities in the network structure. The algorithm has been tested on real-world examples concerning neural activity of a model organism, the nematode worm *C. Elegans*. The foreseeable developments include incorporating the method in the pipeline of the scaffold computation, as an effort to shed light on challenging questions in neuroscience.

Motivation

It is a well-established fact that the modern era of data calls for increasingly refined approaches to obtain knowledge out of the unprecedented amount of information at our disposal. Machine-gathered data is cheap and abundant, but its processing has from the beginning had to pay the price of its sheer size; besides the obvious expenses of dealing with a higher-than-ever volume of records, along with the Big Data come new challenges that are tied to the very structure (or lack thereof) of the information management process:

for example, information is not always reliable, invariably noisy, often unstructured and intractably high-dimensional, and sometimes it is even hard to compute a metric on data points. Classic approaches to the problem broadly involve some kind of dimensionality reduction, and various methods both deterministic and stochastic have been proposed to project data on smaller-dimensional subspaces. Their focus is on finding an efficient and sensible way of doing so while maintaining a sufficient sense of distance and the most possible amount of variance. Another recent approach which has gained momentum in the last decade tackles the problem in a novel and somehow radical way: geometric relations in a datasets can approximately be represented as closeness relations through manifold sampling techniques. Consequently, a purely topological method can arise, concerned solely with the continuous shape of data, which is blind altogether to the dimension of the feature space; as such it avoids the curse of dimensionality while at the same time providing robustness against noise, outliers and lack of structure.

Acknowledgments

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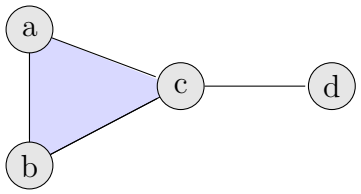
2 Background

2.1 Simplicial Complexes

The essential topological tool we shall utilize to encode relationships between objects is a generalization of the concept of graph. A graph is usually described by a pair of sets, one of vertices and one of edges: which is, a group of objects and some binary relations between them. In general we need to describe higher-order relations between more than two entities, such as triplets and so on. This can be formally encoded by the following definition:

Definition 2.2. *Simplicial Complex*
Let S be a non-empty discrete set. An abstract simplicial complex *is a collection X of finite subsets of S, closed under restriction.*

In words a simplicial complex X is a subset of the power set of S, with the additional property that every element of X must be made up of *other* elements of X. These elements are called *simplices*, more precisely a k-simplex is an element of X of cardinality $k+1$. The subsets of a simplex are called *faces*, and are of course simplices themselves by definition.
If we consider the elements of S to be geometrical points (which is not necessarily the case), we therefore see that a 0-simplex is a single point. A 1-simplex is an (undirected) edge between two points, whose 0-faces are the points. A 2-simplex is a triangle, whose faces are the 3 edges and the 3 points. A 3-simplex is a tetrahedron, subdivided in 4 triangular 2-faces, 6 linear 1-faces and 4 0-simplices, the points.



$$X = \{\{a\}, \{b\}, \{c\}, \{d\}, \{a, b\}, \{c, d\}, \{a, c\}, \{b, c\}, \{a, b, c\}\}$$

Figure 1: An example of a simplicial complex and its graphical representation.

In this frame of reference, we see that a graph is a simplicial complex

containing at most 1-simplices, i.e. $G = (V, E)$ where $V \subset X$ contains the 0-simplices and $E \subset X$ the 1-simplices.

Example 2.3. Consider an undirected graph, defined in the classic sense as $G = (V, E)$, and say for example $V = \{a, b, c\}$ and $E = \{\{a, b\}, \{a, c\}\}$

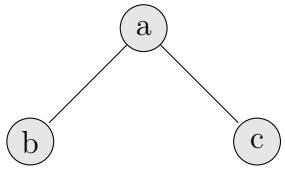


Figure 2: The graph in example 2.3

It is easy to interpret G as a simplicial complex X by defining

$$X := V \cup E = \{\{a, b\}, \{a, c\}, \{a\}, \{b\}, \{c\}\}$$

which clearly follows definition 2.2.

Topology of Simplicial Complexes

In order to discuss the *shape* of an object, it is necessary to at least provide it with a topology. We therefore set forth to construct a suitable open set structure. Let us begin by defining the standard k-simplex

Definition 2.4. *We call the* standard k-simplex *the subset of* $\mathbb{R}^n$

$$\Delta^k \ := \ \{ \ x \in [0, +\infty)^{k+1} \ : \ \sum_{i=0}^{k} x_i = 1 \ \}$$

Therefore, the standard 0-simplex is the point $1 \in \mathbb{R}$, the 1-simplex is a line segment connecting points $(0, 1)$ and $(1, 0)$ in $\mathbb{R}^2$, and so on. One sees that the $(k-1)$-faces of Δ^k are k+1 copies of Δ^{k-1}, and in general faces of Δ^k are standard j-simplices, with $j < k$. The construction of a topological structure for a generic value of k is performed inductively via a procedure of *attaching maps*, which connect faces along the boundary of a higher-dimensional simplex. Define the *k-skeleton* of a complex X as the quotient

$$X^{(k)} \ := \ \left(X^{(k-1)} \bigcup \coprod_{\sigma \ : \ \dim\sigma = k} \Delta^k \right) \Big/ \sim \qquad (2.4.1)$$

where:

- $X^{(0)} = S$
- $\coprod$ represents disjoint union.
- $\sim$ is an equivalence relation that identifies the faces of a standard simplex with the corresponding subsets in the lower dimensional j-skeleton.

The full union $X := \bigcup_{k=0}^{\infty} X^{(k)}$ defines the simplicial complex as a topological space (note the same symbol denotes the actual set-theoretic object as well). The natural choice is to give this space the *weak topology*: a set $U \in X$ is open iff all of its projections onto the subspaces $X^{(k)}$ are continuous, i.e. iff $U \cap X^{(k)}$ is open $\forall k$.
For completeness, notice that other structure can arise through the recursive relation (2.4.1) modifying its base component from the standard simplex to, for example, the k-cube $[0,1]^k$, or modifying the attaching mechanism from the simple identification between borders of a simplex and one-step-smaller simplices, to a very general continuous map between the two. In the first case, the reasonably tame cubical complexes appear, whereas the second case gives rise to some of the most flexible (and complicated) topological spaces, known as *CW complexes*.

2.5 Complexes with a Metric

The set-theoretic notion of simplicial complex is especially suitable for topological applications, because it only relies onto inclusion. In most real-world application, however, topology is only obtained as a byproduct of the metric, as most phenomena are measured in some kind of metric space. It is therefore only natural that there exist ways to construct a simplicial complex from data points that lie in $\mathbb{R}^n$, defining relations on the basis of *distance*. Let us first provide some useful constructions, and later show how these relate to the concept of metric.

Definition 2.6. *Flag, or Clique Complex: We define a* flag complex *or* clique complex *as the maximal simplicial complex having any given graph as its 1-skeleton.*

In practise, a clique complex introduces some sort of constraint on the presence of high-dimensional simplices: requiring it to be *maximal*, every time the underlying graph contains three edges in the form of a triangle, the corresponding 2-simplex *must* belong to the complex. By the same token, every four triangles that form a tetrahedron must be "filled", and so on: a clique complex is said to *fill a frame*.

Definition 2.7. *Nerve of a covering: Let $\mathcal{U} = \{U_\alpha\}$ be a family of subsets of a topological space. The* nerve *of $\mathcal{U}$ is a simplicial complex such that its k-simplices are the non-empty intersections of $k+1$ elements of $\mathcal{U}$.*

The 0-skeleton of this complex is made up of the subsets, its 1-skeleton are the pairs of subsets that intersect on nonempty sets, etc. Notice that this is indeed a well-defined simplicial complex, because if a family of sets has nonempty intersection, all its sub-families do as well.
Notice that a clique complex is remarkably efficient in terms of the input one needs to define it: once the 0- and 1- skeletons are provided, the full complex can be determined uniquely. Conversely, a nerve complex, which lacks the maximality condition, must be explicitly specified in full, with a noticeable increase in complexity.
Let us now see two important classes of simplicial complexes, defined from a *point cloud*, i.e. a set of points in a normed vector space and therefore intrinsically metric, that implement the aforementioned schemes.

Definition 2.8. *Vietoris-Rips Complex: Let $Q \subset \mathbb{R}^n$ be a* discrete *subset, whose elements we regard as data points, and let $\epsilon > 0$. $VR_\epsilon(Q)$ is the simplicial complex over the discrete set Q whose simplices are all the finite collections of points of Q whose pairwise distance is less than or equal to ϵ.*

In words, the Vietoris-Rips complex of radius ϵ is built by computing the pairwise distance of points and generating the 1-skeleton accordingly. Then, higher-dimensional simplices are simply built by grouping together sets of points such that all relative distances are within the ϵ threshold. This amounts to computing only $n(n-1)/2$ distances (keep in mind that, for high-dimensional spaces, computing a distance is not inexpensive).
We can easily see that VR_ϵ is the metric counterpart of a clique complex: if three edges exist and form a triangle, the corresponding 2-simplex satisfies the definition and hence belongs to the complex. This is equivalent to imposing the maximality condition, and therefore the Vietoris-Rips complex is built solely on the basis of the 1-skeleton. Hence it is clique.
Let $S : \mathrm{VR} \to \mathbb{R}^n$ be the projection map which sends singletons in VR to the corresponding points in $\mathbb{R}^n$, and sends any k-simplex into its corresponding convex hull. We define the *shadow* Sh of the complex as the image of projection S. It is easy to see that, tweaking ϵ and the cardinality of Q, it is possible to obtain simplices in VR of dimension (potentially much) higher than n: this is a clear limitation if one intends to employ the VR complex to approximate an unknown geometric structure, usually a differentiable manifold, of which the point cloud is supposedly a sample. Indeed we can make this statement formal by observing that, given the suitable algebraic and topological structures, VR and Sh cannot be homeomorphic due to the difference in their dimensions ([23]). A well-known effort to overcome this flaw is given by a different kind of metric realization of a simplicial complex.

Definition 2.9. *Čech Complex: Let $Q \subset \mathbb{R}^n$ be a* discrete *subset as above, we define $C_\epsilon(Q)$ as a simplicial complex whose k-simplices are sets of $k+1$ points of Q such that the intersection of ϵ-balls centered in those points is not empty.*

The difference with VR lies in the fact that one does just check *pairwise* distances, but requires a $k+1$-fold intersection to be nonempty in order to introduce a k-simplex. This more stringent condition obviously implies $\check{\mathrm{C}}_\epsilon(Q) \subseteq \mathrm{VR}_\epsilon(Q)$, thus maximality is not satisfied in general and $\check{\mathrm{C}}_\epsilon$ is not clique. Moreover, checking for all $k+1$-fold intersections, where

$k = 1, ..., |Q| - 1$ is vastly more expensive than simply computing the 1-skeleton, and requires more memory to store.
On the other hand the *nerve lemma* ensures that a such complex comes with a useful property:

Property 2.10. *$\breve{C}_\epsilon(Q)$ is homotopic to the ϵ-hull around Q.*

This is due to the fact that $\breve{\mathrm{C}}_\epsilon$ is a particular case of a nerve complex: in particular, a nerve complex with the subsets U_α being the ϵ-balls centered in points of Q. Therefore, the Čech complex is topologically superior in its ability to mimic the structure of the data points that it comes from.

2.11 The Free Group and the Fundamental Group

The Free Group

In order to give a proper theoretical grounding to the concept of homology to follow, let us briefly introduce the concept of *free group*. Given a set of groups $G = \{G_\alpha\}$, consider the set of words (strings of objects) $g_1 g_2 ... g_m$ with finite m, such that all g_i's belong to some group in G, they are not its identity, and no two adjacent letters belong to the same group. Such a word is called *reduced*. It is clearly always possible to obtain a reduced word from any string of g_i's, by applying group operations and canceling out the identities, repeating if necessary. Since m is finite this procedure terminates until a reduced word (potentially the empty string) is obtained. It is not too simple to verify that

Property 2.12. *There exists only one reduced form of any word.*

An important consequence of this fact is the following lemma

Property 2.13. $\big(x \sim y$ *iff* x, y *have the same reduced form* $\big)$ *is an equivalence relation*

So now we can consider the set of finite-length words, modulo the equivalence relation induced by reduction.
Let us add to the set of words an operation: given two words, they can be concatenated. Then the empty word functions as the identity element. Concatenation also has another important characteristic:

Property 2.14. *String concatenation and reduction commute.*

I.e., it is the same to reduce two words and then concatenate them, or to first join them and then reduce the resulting string. Therefore, the concatenation operation can be lifted to the quotient set (modulo reduction), yielding a well-defined operation on equivalence classes of words. The class of the empty word still functions as the identity element, and it is easy to produce the general construction of the inverse: given any (reduced) word $g := g_1 ... g_m$, due to the group structure of the G_α's one can form the word $h := g_m^{-1} ... g_1^{-1}$ (which is still reduced). It clearly holds that $gh = hg = 0$, where 0 identifies the identity of the quotient set, i.e. the equivalence class of the empty word.
In order to conclude that this algebraic object is indeed a group, one finally

needs to prove that concatenation is also associative. To prove it directly would be rather complicated and tedious: instead, one can build a map from the quotient set to a known associative group, and show that this map is also a homomorphism. Then we have indirectly proven associativity, and can conclude the final result

Property 2.15. *The set of words modulo reduction, equipped with the concatenation operation, is a group, and is called the* Free Group.

Sometimes, one can specify a nonempty set S to work as an alphabet, and build a set of symbols $W = S \cup S^{-1}$ made up of letters of S and their inverses S^{-1}, instead of giving groups G_α explicitly. In that case, we say that F is the *Free Group* on S.

Example 2.16. Consider the simple alphabet $S := \{1\}$. Let us, in this case, denote its inverse by -1. The free group $F(S)$ is, up to isomorphism and some ingenuity, the group of integers equipped with the sum $(\mathbb{Z}, +)$. Indeed, elements of $F(\{1\})$ are reduced strings of 1's and -1's, which is to say they are either empty or entirely made of either 1's or -1's. Consider the function on $F(\{1\})$ which computes the sum of the elements of the reduced representative of a word class. It holds that (indicating concatenation as $\circ$)

$$s : \ (F(\{1\}), \circ) \to (\mathbb{Z}, +)$$

is a group homomorphism, as

$$s(h \circ g) = s(h) + s(g)$$

Furthermore, $\forall z \in \mathbb{Z}$ there exists exactly one reduced word g such that $s(g) = z$, and therefore s is an isomorphism.
On the other hand, it is rather involved to give a description of the free group on two generators.

Knowledge of the free group will prove handy in the construction of simplicial homology, as a source of the algebraic structure of the k-chains that is the core of the subject.

The Fundamental Group Let (X, x_0) be a pointed topological space. We call a *loop* a closed continuous curve $\gamma \ : \ I \to X$ such that $\gamma(0) = \gamma(1) = x_0$. Consider *homotopy equivalence*: if there exists a continuous map of maps

$f : I \times I \to X$ (continuous in both arguments) such that for two loops γ, γ' it holds that $f(I,0) = \gamma$ and $f(I,1) = \gamma'$, then the loops are said to be homotopical. Homotopy is clearly an equivalence relation on the set of loops with base x_0, and we shall at some point perform its quotient. First, though, we can bring more algebraic structure into play.
Consider any two loops γ, γ'. Define the *concatenation* $\gamma \circ \gamma' : I \to X = \gamma(2t)\mathbb{I}_{[0,\frac{1}{2})} + \gamma'(2t-1)\mathbb{I}_{[\frac{1}{2},1]}$. The resulting curve is still a loop with base x_0, obtained by following the two paths in succession at double speed.
Next, consider a constant curve $e(t) = x_0$. The products $e \circ \gamma$ and $\gamma \circ e$ are both strictly speaking different curves than γ. Nevertheless, there exists a change of parameter, i.e. a bijection φ of I onto I, such that $\gamma = (e \circ \gamma)(\varphi)$ and $\gamma = (e \circ \gamma)(\varphi^{-1})$. In other words, $e \circ \gamma$ and $\gamma \circ e$ are both homotopical to γ.
By the same argument, the two products of loops $(f \circ g) \circ h$ and $f \circ (g \circ h)$ only differ by a change of parameter, and are thus homotopical too.
It is slightly more elaborate to prove that for any loop $\gamma(t)$, the loop $\gamma(1-t)$ is an inverse modulo homotopy. It suffices to produce such homotopy explicitly: consider $\forall t \in [0,1]$ the path $\gamma_t(s) = \gamma(s)\mathbb{I}_{s\in[0,1-t]} + \gamma(1-t)\mathbb{I}_{s\in[1-t,1]}$. Then defining η_t as the inverse path of γ_t, a direct calculation shows that $\gamma_t \circ \eta_t$ is a homotopy of loops connecting smoothly $\gamma(s) \circ \gamma(1-s)$ to the constant path e, and its inverse $(\gamma_t \circ \eta_t)(1-s)$ connects smoothly $\gamma(1-s) \circ \gamma(s)$ to e. Hence we have explicitly built an inverse modulo homotopy.
It remains to prove that concatenation of loops preserves the homotopy class: indeed if f_t and g_t are homotopies connecting f_0 to f_1 and g_0 to g_1 respectively, then the concatenation of the two $f_t \circ g_t$ (as functions of s) connects $f_0 \circ g_0$ to $f_1 \circ g_1$. So denoting by $[f]$ the homotopy class of f, it holds that $[f] \circ [g] = [f \circ g]$ and therefore the operation lifts properly to the quotient set. By now we can safely call the concatenation of loops a product, as it is evident that it represent a group operation modulo homotopy:

Definition 2.17. *The quotient set of loops with basepoint x_0 modulo homotopy equivalence is a group with respect to the concatenation operation, and is denoted $\pi_1(X, x_0)$. We call it the* Fundamental Group of X *at basepoint x_0.*

We may add as a final remark that the dependency on the choice of basepoint x_0 is not as relevant as it may appear: if the space X is path-connected, one can prove that there exists an isomorphism between $\pi_1(X, x_0)$

and $\pi_1(X, x_1)$, $\forall x_0, x_1 \in X$. Therefore, for path-connected spaces the fundamental group is unique up to isomorphism, and is sometimes denoted as simply $\pi_1 X$.

$\pi_1 X$ in action

While the construction of $\pi_1(X)$ is relatively straightforward, it is not so simple to get a sense of its meaning. In particular, one may wonder under what circumstance a topological space has a non-trivial fundamental group: this means proving that a homotopy between two paths *does not exist*, or equivalently that it is necessary to break continuity to deform one path into another.

Clearly, the constant loop belongs to the fundamental group of any space: therefore, if X is path-connected $\pi_1 X$ is trivial if and only if every loop can be smoothly deformed to the constant loop. Intuitively, this means that a space cannot have *holes*. It is easy to accept that for a space with a hole, loops that wind around the hole and loops that do not cannot be homotopical: in some specific sense, every hole in X adds a generator of group π_1. It is therefore not surprising that the fundamental group of the circle is, up to isomorpism, the group of the integers $\mathbb{Z}$: its loops are, up to homotopy, parametrizations of the unit circumference, travelled clockwise or counterclockwise, at multiple speeds $k \in \mathbb{Z}$. Its unit element is the constant loop at the (arbitrary) basepoint x_0, which clearly cannot be smoothly deformed into a path that winds around the circle. On the other hand, the fundamental group of the 2-ball is the trivial one, as any closed path is homotopic to the constant one.

It is useful to consider the fundamental group of some complexes (intended as topological spaces), and more importantly understand the dependency of π_1 from the complex structure. Since it is built onto maps from low-dimensional spaces into X, namely loops $I \to X$ and homotopies of them $I \times I \to X$, it is not surprising that π_1 of a complex depends only on its low-dimensional structure. In fact, when X is a CW complex, $\pi_1(X)$ only depends on its 2-skeleton. This is useful on the one hand for simplicity of understanding, but constitutes a serious limitation in the ability to tell higher-dimensional structures apart: for example, on the n-sphere it happens that

$$\pi_1(S^n) = \pi_1(S^m)\ \forall m, n \geq 2$$

The fundamental group is essentially blind to high-dimensional features. A workaround to this is given by a higher-dimensional equivalent of the funda-

mental group: index 1 in π_1 indicates that the quotient is performed with respect to loops and homotopies of loops. One can compute it with respect to a more complex map equivalence, given by surfaces and their homotopies $I^2 \to X$ and $I^2 \times I \to X$, yielding $\pi_2(X)$, and in general the *n-th homotopy group* $\pi_n(X)$ computed through maps $I^n \to X$ and their homotopies $I^n \times I \to X$ (where I^n denotes the n-cube). In this case, the above problem is solved: when X is a CW complex, $\pi_n(X)$ only depends on the n+1 skeleton of X and it holds

$$\pi_i(S^n) = 0 \ \ \forall i < n \ , \ \pi_n(S^n) \simeq \mathbb{Z}$$

This solution is hindered by a practical reason: computing higher-order homotopy groups is extremely complicated, even for such simple cases as the sphere. In general $\pi_i(S^n)$ for $i > n$ displays a surprisingly complex behaviour, and at present much remains unknown of these objects. This provides the main motivation for the development of the alternative concept of homology. We shall see in the following that, again, the homology group, denoted by $H_n(X)$, only depends on the n+1-skeleton when X is a CW complex. Furthermore

$$\forall \ 1 \leq i \leq n \ H_i(S^n) \simeq \pi_i(S^n) \ \text{ but } H_i(S^n) = 0 \ \forall i > n$$

2.18 Simplicial Homology

We now come to the fundamental concept that underpins most of Topological Data Analysis. The first introduction of homology-like concepts dates back to the definition of Euler characteristic, the genus of a surface, and Poincaré's studies of the topological properties of manifolds in dynamical systems. The modern concept of homology has been given a remarkably theoretical framing, essentially rooted in category theory, which provides a common ground for a number of different theories. All these variants, however, share the essential property that homology is a method to associate an algebraic object, sometimes a structure of algebraic objects, to other mathematical entities, and most notably topological spaces.
For the sake of the present work, we shall limit ourselves to introducing a homology theory that is especially tailored to apply to simplicial complexes, hence named *simplicial homology*. Consider a simplicial complex X, and suppose it is given an *orientation*. An orientation of a k-simplex is an equivalence class of orderings of the vertices modulo even permutations. Hence, given an ordering on the set of vertices, one can fix an orientation for every k-simplex in X, up to parity. Therefore, there exist only two orientations for each simplex.

Chain Complex

Consider an oriented simplicial complex, and the formal sum

$$\sum_i c_i \sigma_i \ , \quad c_i \in \mathbb{Z} \tag{2.18.1}$$

i.e. the space of linear combination of k-simplices with integer coefficients. The inverse of a simplex is intended as the simplex with the opposite orientation. The intuition behind this result is as follows: concatenating the same path in two opposite directions amounts to the identity element, that is not moving at all.

Definition 2.19. K-Chain *We call the* k^{th} chain group C_k of X *the free Abelian group on the set of its oriented* k*-simplices.*

As per the insight given above, we can build "strings" of k-simplices and cancel out occurrences with different orientation. Keeping in mind that the group is Abelian, we can reorder words so as to build consecutive "paths". Taking linear combinations of simplices as in (2.18.1) with coefficients in

the ring of the integers yields a module structure. We will show in the following that it is of paramount importance for computational reasons for this structure to be, instead, a vector space. Consider, this time, the linear combinations of the form (2.18.1) with coefficients in the finite field $\mathbb{Z}_2$. The field structure, namely the existence of the multiplicative inverse, entails that the k-chain with $\mathbb{Z}_2$ coefficients is a vector space, and as such can be given a basis from a linearly independent set of vectors.

Boundary Operator

Consider, again, the k-chain with integer coefficients. Let us define a *boundary operator* ∂_k as follows

Definition 2.20.

$$\partial_k : \ C_k \to C_{k-1}$$

$$\partial_k : \sigma = [v_0, ..., v_k] \in C_k \longmapsto \sum_{i=0}^{k} (-1)^i \ [v_0, ..., \hat{v_i}, .., v_k]$$

where $\hat{v_i}$ denotes that the i-th component has been removed.

It is easy to see that ∂_k is a group homomorphism between C_k and C_{k-1}. To understand why it is called boundary operator, let us first notice that it associates to elements of dimension k elements of the previous dimension, obtained by removing one vertex at a time. As such, its image is a linear combination of *faces* of σ. Its action on low-dimensional simplices is illuminating:

Example 2.21. Consider simplices $\{a, b\}$ and $\{a, b, c\}$, oriented according to alphabetical order. The boundary of an edge is

$$\partial_1 (\{a, b\}) = +\{b\} - \{a\}$$

The boundary of a triangle, instead, is

$$\partial_2 (\{a, b, c\}) = +\{b, c\} - \{a, c\} + \{a, b\}$$

That is, edges ab and edge bc forward, and edge ac backwards, yielding the closed sequence $a \to b \to c \to a$

It is worth noting that

$$\partial_1\partial_2\left(\{a,b,c\}\right) = \partial_1\{b,c\} - \partial_1\{a,c\} + \partial_1\{a,b\} =$$

$$= \{c\} - \{b\} - \{c\} + \{a\} + \{b\} - \{a\} = 0$$

This is true in general

Property 2.22. *The boundary operator is nihilpotent*

$$\partial_k\partial_{k+1} = 0 \quad \forall k \tag{2.22.1}$$

This lemma has a rather deep meaning: the image of the boundary operator on a k-simplex is a closed *cycle* of $(k-1)$-simplices. These closed cycles are, in particular, *borders* of higher-dimensional simplices. Borders themselves form a subgroup of C_{k-1}

$$B_k := \text{Im } \partial_{k+1} \subseteq C_k$$

Another statement of property (2.22.1) is

Property 2.23.

$$\text{Im } \partial_{k+1} \subseteq \ker \partial_k$$

But what is $\ker \partial_k$? As we have just seen, the kernel certainly contains the borders of all the $(k+1)$-simplices in X. But not all closed concatenations of k-simplices come from borders of $k+1$-simplices. Indeed, one can concatenate three edges that form a triangle, even if the corresponding triangular 2-simplex does not belong to X. In general, $\ker \partial_k$ is the subgroup of C_k formed of all possible closed *cycles* of k-simplices, be they borders or not.

$$Z_k := \ker \partial_k \subseteq C_k$$

Hence we have a group inclusion

$$B_k \subseteq Z_k \subseteq C_k$$

Remark Notice that the exact same line of reasoning works if we consider k-chains with coefficients in $\mathbb{Z}_2$, if we take care to redefine the border operator as

Definition 2.24.

$$\partial_k : \ C_k \to C_{k-1}$$

$$\partial_k : \sigma = [v_0, ..., v_k] \in C_k \longmapsto \sum_{i=0}^{k} [v_0, ..., \hat{v_i}, .., v_k]$$

Indeed, in $\mathbb{Z}_2$ sum and subtraction coincide, $+\sigma = -\sigma$ and $2\sigma = 0$, so only simplices that are taken odd times are not zero.
We can now proceed to the main definition of the section

Definition 2.25. k-th Homology Group
We call the k^{th} Homology Group H_k *the quotient*

$$H_k := \frac{\ker \partial_k}{\text{Im } \partial_{k+1}} = \frac{Z_k}{B_k}$$

The concept of homology classes is the following: we identify with the null element every cycle that is a border of a higher-dimensional simplex, or that can be built as a linear combination of borders of simplices. Therefore, the only non-zero elements (more precisely, the only non-trivial homology classes) are represented by those cycles which *do not* come from borders. Two cycles are homologous (i.e. they belong to the same class in H_1, i.e. they are equal modulo borders) if they differ by a sum of null cycles, namely in dimension 1 if they differ by a triangulated path.

Graded modules, vector spaces and basis of H_1

As we have introduced above, the k-chains groups, equipped with a linear combination with coefficients in an Abelian unitary ring (usually $\mathbb{Z}$), form a module structure. It is well-known that, if the ring is also a field, the module is in fact a vector space. So it holds that the group H_1 with finite field $\mathbb{Z}_2$ coefficient, quotient of two vector spaces, is itself a vector space; conversely, as a quotient of two modules, it is a module.
The structure of these algebraic objects can be made clearer by employing a known result.

Definition 2.26. *Graded Ring*
We call a graded ring R *a ring for which there exists a direct sum decomposition into groups* R_i

$$R = \bigoplus_i R_i$$

which respects multiplication, i.e.

$$R_h R_k \subseteq R_{h+k}$$

The typical example of a graded ring is the ring of polynomials, where the grading is given by the *degree*. Specifically, over $R[x]$ it holds that $R[x] = \oplus_n R\ x^n$, namely each polynomial over R can be expressed as a sum of homogeneous terms on degree n for $n \in \mathbb{N}$.
The concept extends naturally to a module

Definition 2.27. *Graded Module*
We call a graded module M *a module over a graded ring* R *such that*

$$M = \bigoplus_i M_i$$

as well and multiplication follows

$$R_h M_k \subseteq M_{h+k}$$

Let us state the standard structure theorem for graded modules over a principal ideal domain.

Property 2.28. *Structure Theorem*
Let M *be a graded module over a principal ideal domain* A

$$M \simeq \left(\bigoplus_{i=1}^{n} \Sigma^{\alpha_i}\ A \right) \oplus \left(\bigoplus_{j=1}^{m} \Sigma^{\gamma_j} \frac{A}{\gamma_j A} \right)$$

The first term represents the *free part*, which is a vector space and is made of the generators of M that can yield and infinite number of elements. The second term is called the *torsional part*, and represents generators that can only generate a finite number of elements. Notice that, if the module is itself a vector space as in the case of the coefficient set being a field, the second term vanishes and the decomposition becomes simply a direct sum of orthogonal one-dimensional vector spaces, with as many entries as the dimension of M.

Definition 2.29. *Betti numbers*
We call the k^{th} Betti number β_k *the rank of the free part of* H_k.

Notice that, if H_k is torsion-free, specifically if it is taken with coefficients in a field, β_k is simply the vector space dimension of H_k.

2.30 Persistent Homology

Filtration of Simplicial Complexes

Let X be a simplicial complex. We say Y is a subcomplex of X if it is a subset of X which is still a simplicial complex.

Definition 2.31. *Filtration*
Given a simplicial complex X, a filtration *of a complex is a family $\mathcal{X}$ of subcomplexes*

$$0 = X^0 \subseteq X^1 \subseteq ... \subseteq X^m = X$$

From a metric point of view, one can build a filtration of complexes from a point cloud by applying a scheme such as Vietoris-Rips repeatedly onto the same data points, while increasing the threshold parameter ϵ. This yields a nested family of simplicial complexes with growing connectivity, which entails a growing number of cycles as well as a growing number of borders.

Property 2.32. *Let $\{\epsilon_i, 1 \leq i \leq m, \epsilon_i > 0\}$ be an* increasing *sequence of positive real numbers, $Q \subset \mathbb{R}^n$ a discrete set. The sequence*

$$\{\ VR_{\epsilon_i}(Q)\ \}_{i=1}^{m}$$

is a filtration of simplicial complexes.

Persistence

Given a filtration of complexes X^i, the associated groups and operators are denoted as ∂_k^i, Z_k^i, B_k^i, C_k^i and H_k^i. In this case, intuitively, beside having a "vertical" mapping between decreasing-dimension chains of k-simplices, we also have a "horizontal" inclusion between more and more refined complexes.

Definition 2.33. *We call the* p-persistent k^{th} homology group of X^i *the group*

$$H_k^{i,p} \ = \ \frac{Z_k^i}{B_k^{i+p} \cap Z_k^i}$$

In this case, intuitively, we quotient with respect to borders that remain such in the more refined complexes p steps ahead of i. Hence the name *persistence*.
We define the *persistent Betti numbers* $\beta_k^{i,p}$ as the rank of the free subgroup of $H_k^{i,p}$. Again, if this is a vector space one can simply consider the rank of

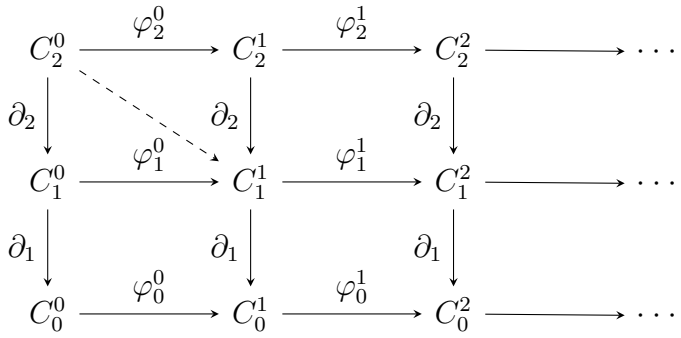


Figure 3: Persistence diagram of C_k^i chains.

the whole group. Obviously, since $B_k^i \subseteq Z_k^i$, if we set $p = 0$ we recover the usual homology group

$$H_k^{i,0}(\mathcal{X}) = H_k(X^i)$$

In our setting, the structure of persistence is represented by the diagram in Figure 3, where we move horizontally through inclusion maps φ_k^i, and vertically via the border operator ∂_k. It is a known, but important, result, that every square in the diagram of Figure 3 commutes, i.e. it is the same to compute $\varphi_{k-1}^i \circ \partial_k$ or $\partial_k \circ \varphi_k^i$ ([4]).

3 Shortest Homology Basis

The Problem

Having given an overview of what homology is, we now proceed to stating the problem we wish to address ([6]). Assuming we place ourselves in the context of H_1 homology with $\mathbb{Z}_2$ coefficients, we know that all groups Z_1, B_1, C_1 and H_1 are finite-dimensional vector spaces, and therefore can be given a basis. We denote by $Z := \dim Z_1$ the dimension of the cycle group, $B := \dim B_1$ the dimension of the borders, and $g := \dim H_1$ is the first Betti number of a fixed simplicial complex X.
Notice that, for any simplicial complex X, there exists a bijection between the set of its k-simplices X_k and its group of k-chains. So if we call $n_k = |X_k|$ the number of k-simplices in X, then C_k is isomorphic to $(\mathbb{Z}_2)^{n_k}$, the vector space of column vectors such that the j^{th} entry is 1 if the j^{th} simplex belongs to the chain, and zero otherwise. Naturally a basis of C_k is the canonical basis of $(\mathbb{Z}_2)^{n_k}$, where each *one-hot* vector identifies a k-simplex.
Since Z_1 is a vector space of dimension Z, there exist set(s)

$$\{c_1, ..., c_Z\} \ , \ c_i \in Z_1$$

which form a basis of Z_1. We call such a set a *cycle basis*.
Recalling the definition of homology, we call $[c]$ the homology class of cycle c. It is formed by all cycles in Z_1 which differ the one from the other by elements of B_1. In the light of what stated above, there must exist

$$\{[c_1], ..., [c_g]\} \ , \ [c_i] \in H_1$$

which form a basis of H_1. We call such a set a *homology basis*.
Assume now there exists a function that assigns a non-negative *weight* to each cycle c

$$\mu : Z_1 \longrightarrow [0, +\infty)$$

One way to build a such function, and the one that will be employed in the applications, is to think of the 0- and 1-skeleton of X as a *weighted graph* with non negative weights, (V, E). Weights can be thought of as lengths. Then a 1-cycle can be represented as a vector of $\mathbb{Z}_2^{|E|}$, which is a basis of Z_1 as stated above. The function that assigns to each cycle the sum of the weights of the edges that belong to it is our weighting function for the following analysis.
We can now state our problem: given a simplicial complex X, find a set of

cycles $\{c_1, ..., c_g\}$ such that

$$\{c_1, ..., c_g\} = \text{argmin} \sum_{i=1}^{g} \mu(c_i)$$

subject to $\{[c_1], ..., [c_g]\}$ being a *homology basis* of $H_1(X)$.
In words, we aim at finding cycles of the shortest possible length, which generate the whole homology group.

3.1 Prior Work

In this section we examine known results from past works which turn out useful in our analysis. Let us begin by stating that the choice to restrict ourselves to the group H_1 is somehow unavoidable, as the problem of computing a minimal homology basis for dimension higher than one is proven to be NP-hard (Chen and Freedman, [7]).

Property 3.2. *[7], Corollary 6.1*
For homology of dimension 2 or higher, the minimal homology basis is NP-hard to approximate within any constant factor.

The meaning of this statement is two-fold: on the one hand, for $k > 1$ computing exactly a minimal basis of H_k is NP-hard (we recall that a problem Q is NP-hard if any problem in NP can be reduced to Q in polynomial time, hence the intuition that Q is at least as hard as any problem in NP), and even a polynomial-time algorithm that computes an approximate solution which differs from the exact one by a constant multiplicative factor does not exist. The class of problems with polynomial-time, constant factor approximation is usually called APX. Then an alternative statement of the above theorem is that computing a minimal homology basis in dimension 2 or higher does not belong to APX.
As a consequence, we can shift our focus onto simplicial complexes of dimension at most two, so as to distinguish 1-cycles which are borders of triangles from those which are not. It therefore appears only natural to examine graph theory results, as our base structure is essentially a decorated graph, possessing some cycles which are declared to be *null*, namely those coming from borders of the 2-skeleton, and other which effectively contribute with a non-trivial generator to the homology group.
The first algorithm to find a minimal cycle basis (MCB) of a weighted graph dates back to 1987, with the work of Horton [18], who provided a $O(m^3n)$ running-time procedure for a graph with m nodes and n edges. His approach involved generating a superset of cycles guaranteed to contain a MCB, by computing for every possible pair of source node and edge a cycle generated by shortest path, and then reducing the obtained set by Gaussian elimination.
More recently, de Pina in [8] improved this result by applying a different approach, which yields a $O(m^3 + mn^2 \log n)$ complexity. In his case, a spanning tree T is computed over graph G, and the set of edges in $G \setminus T$ is employed

to represent each cycle. Then the MCB is obtained by representing cycles as vectors of $\{0,1\}^Z$, maintaining a basis of the orthogonal subspace to the set of MCB, and at each step computing the shortest cycle which is linearly independent of the previous ones by enforcing a non-zero scalar product with the orthogonal basis.
Both these algorithms were later improved by applying *fast matrix multiplication*, the most recent incarnation of which is described in [20], [21], which computes the product of two $n \times n$ matrices in $O(n^\omega)$ steps with $\omega < 2.376$. Yet more recently, Mehlhorn et al. ([9]) found a further improvement of de Pina's scheme by imposing a relaxed version of the maintenance of a basis of the orthogonal complement while the cycle basis is extended. Their method presents a recursive approach which extends both the cycles and the support vectors at the same time while maintaining relative orthogonality. It results in a time complexity of $O(m^2 n + mn^2 \log n)$.
The computation of the MCB had yet to be lifted to the context of simplicial homology, where one has to deal with the added complexity of having to generate a basis of a smaller space than Z_1, as a consequence of different cycles being identified by the border equivalence. On the other hand, if exploited correctly, the smaller dimension can represent a computational advantage. The recent work of Dey et al. ([5], [6]) moves in this direction, combining the recursive approach of [9] with a cohomological technique called *simplex annotation* [10] which allows for efficient computation of the homology basis.

3.3 Cohomology and Simplex Annotation. Homology Basis.

As we mentioned above, the problem we face has a different character than those addressed in the previous section in that we not only search for a *cycle basis*, but require the minimal set to form a *homology basis*, hence taking into account the border equivalence. Notice that in general it is not straightforward to obtain a solution of our problem from a solution of MCB, since the quotient alters the structure of the vector space, modifying linear dependence between cycles. In particular, our solution is in general not a subset of the MCB.
A different approach to the problem is proposed in [10] and relies on a concept arising from cohomology theory, called *simplex annotation*. Let us define, for the homology group $H_k(X)$ of simplicial complex X, with rank g

Definition 3.4. *Simplex Annotation [10]*
An annotation *for a k-simplex is a function from the k-skeleton into 0-1 vectors of length g*

$$a : X_k \longrightarrow (\mathbb{Z}_2)^g$$

such that any two k-cycles c_1 and c_2 are homologous if and only if

$$\sum_{\sigma \in c_1} a(\sigma) \;=\; \sum_{\sigma inc_2} a(\sigma)$$

The above sum is referred to as the annotation of the cycle c_i.

Restricting ourselves to the one-dimensional case, we can compute the annotation of the edges in X_1 so that two cycles are homologous iff their annotation vectors coincide. As such, given any cycle, its annotation provides a coordinate representation of its homology class in a given basis. Different annotating function refer to different choices of a basis on $H_1(X)$.
Regarding the existence of such a function, it is worth noting what follows ([10]): if we denote by $\{\phi^j\}_{j=1}^g$ the *cocycles* whose equivalence classes are generators of the *cohomology group* $H^1(X)$, then an annotation can be obtained by assigning

$$a : \; \sigma \longmapsto (\phi^1(\sigma), ..., \phi^g(\sigma))$$

The procedure to obtain this coordinate representation of cycles is roughly as follows ([10]):

- First, a basis of the cycles group is obtained.
- Then, the cycle basis is reduced to obtain a homology basis. This step naturally requires knowledge of the border structure, which shall be expressed as a matrix representation of the border operator ∂_2 in the given basis.
- Finally, every cycle in Z_1 can be assigned to its homology class, which has a natural vector representation in the computed basis.

Step one relies on the computation of a spanning tree of graph $G = (X_0, X_1)$, which we call T. Consider the difference between the edges of G and those of the spanning tree. These are called *sentinel edges*. The cycle obtained in the spanning tree T by adding each sentinel edge is called a *sentinel cycle*.

Property 3.5. *[10] The set of sentinel cycles is known to form a basis of* Z_1.

Hence we can express any cycle in Z_1 as a linear superposition of sentinel cycles, each identified by its sentinel edge. Recalling we deal with $\mathbb{Z}_2$ coefficients, any $z \in Z_1$ coincides with the sum of the sentinel cycles for every sentinel edge that belongs to z (notice that, for z to be a cycle, at least one of its edges must be a sentinel).
For step two, we need as mentioned a description of the border structure. Recall that the border operator ∂_2 is a group homomorphism between C_2 and C_1 that associates 2-simplices (triangles) to their border 1-cycle. As such, given the vector description of 1-cycles induced by the pair *spanning tree - sentinel edges*, operator ∂_2 can be cast in matrix form by writing side by side the vectors describing the boundary cycles, for each 2-simplex in X. The resulting matrix has as many rows as the dimension of Z_1, and as many columns as the cardinality of X_2.
To its right, we add all column vectors of the cycles of Z_1, as represented in the sentinel basis (let us call this submatrix S). Recall that all said vectors have $\mathbb{Z}_2$ elements. We obtain a matrix of the form

$$[\partial_2 \mid S]$$

The next step allows us to obtain a suitable homology basis: we compute the so-called *earliest basis* of the above matrix, i.e. we proceed by columns, from left to right, eliminating any column that can be expressed as a linear

combination of those that precede it. The resulting matrix has full rank, and is of the form

$$[B \mid H]$$

where submatrix B of columns which derived from ∂_2 is a basis of the border group $B_1 := \operatorname{Im} \partial_2$ and submatrix H is a basis of H_1. In particular the number of columns of the two submatrices give us $\dim B_1$ and g, respectively. Finally, we have to express each sentinel cycle in the basis of $[B \mid H]$. This notoriously amounts to solving a linear system, in our case in $\mathbb{Z}_2$. If we solve for $\tilde{z}$

$$[B \mid H]\, \tilde{z} = z$$

where z is the vector representation of a cycle in the sentinel basis, its last g entries form the annotation of cycle z, i.e. the homology representation z_h without the cyclic components deriving from borders.
If we consider the full matrix of cycles Z, one can globally solve system

$$[B \mid H]\, \tilde{Z} = Z$$

The last g rows of $\tilde{Z}$ form the annotation vectors of the sentinel cycles. Then each sentinel edge can be given the annotation of the sentinel cycle it generates. All other edges are given annotation $0 \in (\mathbb{Z}_2)^g$.

3.6 Methodology

In the light of the results mentioned in the previous sections, we now set forth to tackle the optimization part of our problem: i.e., finding a *minimal* basis. In the recent work of Dey [6], the approach of Mehlhorn [9], which itself improved on de Pina's [8], was combined with the annotation technique [10] to yield a $O(n^3)$ worst-case complexity in the cardinality of the complex. The method proceeds as follows: first, a candidate set of cycles is generated by the shortest path tree method. For each node p, we compute the SPT rooted in p and keep track of the *non-tree edges*. Each non-tree edge identifies a cycle with respect to vertex p. The union of all cycles for all vertices $p \in X_0$, which we call G, is guaranteed to contain a shortest homology basis ([5], [6], [19]).
Next, we move on to the annotation of edges to obtain a homology basis. As described above, we must generate a basis of cycles by means of a spanning tree and its sentinel edges. Notice that the SPT computed at the previous step can be employed for the case, taking care to consider a root node for each connected component of X, hence speeding the computation. Given our vector representation of cycles in the sentinel edge basis, we can form the matrix representation of the border operator ∂_2 by placing side by side the vectors describing borders, for each 2-simplex in X. Next to it, we can place our cycle basis, and operate the left-to-right reduction, as described above ([10]). From this step, we obtain the Betti number of X, and solving the following linear system, a basis of $H_1(X)$ and the annotation vectors.
Finally, we proceed to produce the j-th minimal basis vector of H_1 for $j = 1, ..., g$ as follows:

1. Initialize a basis of $(\mathbb{Z}_2)^g$, for example with the canonical basis. We call these *support vectors* S_i.

2. At step j, generate the set of cycles, subset of G, whose annotation has $\mathbb{Z}_2$-scalar product equal to 1 with S_j. These are cycles which are not orthogonal to S_j. Of these, pick the shortest one in length, c_j. Add this vector to the minimal basis.

3. Update the support vectors $S_{j+1}, ..., S_g$ so as to guarantee that they still form a basis of $\mathrm{Span}\{c_1, ..., c_j\}^{\perp}$, and that c_j and S_{j+1} are orthogonal.

Repeat steps 2 and 3 for $j = 1, ..., g$. Then

Property 3.7. *[6],[5]*
The resulting set of cycles $\{c_1, ..., c_g\}$ *is the minimal homology basis of* $H_1(X)$.

Node Labeling

The computation of the the subset of cycles which are non-orthogonal requires to compute a possibly large number of scalar products. There exists a technique called *node labelling* to expedite the task at its best possible performance ([6]). It is in essence an application of linearity of both scalar product and annotation: for each support vector S_i and calling m the cardinality of X_0, one can build a $m \times m$ matrix of *labels* of nodes such that the entry (h, k) is the $\mathbb{Z}_2$ sum of scalar products of S_i with the annotation of the edges that connect h to k, in the shortest path tree rooted in h. Hence, one can follow the SPT from the root to the leaves, computing a scalar product for every new edge that one encounters and summing it to the label of its parent node. Therefore, all it takes to check orthogonality with respect to S_i of a cycle described by a pair $(p, (v, w))$ (where p is the root node and (v, w) are the extremes of a sentinel edge) is to sum the labels of index (p, v) and (p, w) with the scalar product between S_i and the annotation of edge (v, w).

3.8 Implementation

We now give a brief description of the Python 3 code we have implemented for the algorithm described above.

Geometry

For testing applications, point clouds were usually random-sampled. Then the 1-skeleton and its consequent clique simplicial complex were generated by computing pairwise distances. In real-world applications, data is usually given as weighted adjacency matrices, in the form of lists of triplets (node, node, weight). This gives the 1-skeleton in a precomputed manner, and one is left with the task of identifying triangles to tile in order to generate the ∂_2 operator matrix (2.8).

```
def getTriangles(A):
    '''
    returns set of triangles in a graph given its adjacency
       matrix
    '''
    n = len(A)
    tri = []
    for vertex in range(n):
        vList = np.nonzero(A[vertex,vertex:])
        vList = [x for x in vList[1]]
        vList = [i + vertex for i in vList] #list of vertices
            adjacent to vertex
        for i in range(len(vList)-1):
            for j in range(i+1,len(vList)):
                if A[vList[i],vList[j]] > 0:
                    tri.append([vertex,vList[i],vList[j]])
    return tri

def getD2(A, edgesList):
    '''
    returns 2-boundary matrix of the clique complex, given
       the adjacency matrix of the graph
    '''
    triangles = getTriangles(A)
   # print(triangles)

    d2 = []
    n = len(edgesList)
    #print(n)
```

```
    for row in triangles:
        newTriangle = [0 for i in range(n)]
        newTriangle[edgesList.index( (row[0],row[1] ) )] = 1
        newTriangle[edgesList.index((row[0],row[2]) )] = 1
        newTriangle[edgesList.index( (row[1],row[2]) )] = 1
        d2.append(newTriangle)
    d2 = np.array(d2)

    return d2

def points2adj(P, epsilon):
    '''
    given a set of points and a threshold returns the weight
       and adjacency matrix of the corresponding graph
    points is a list where each element is the coordinates of
        the point
    '''

    def dist(p1,p2):
        '''
        euclidean distance
        p1 and p2 need to be list of the same length
        '''
        return math.sqrt(sum([(p1[i]-p2[i])**2 for i in range
           (len(p1))]))

    n = len(P)
    W=np.zeros((n,n))
    for i in range(n):
        for j in range(i,n):
            W[i,j]= dist(P[i],P[j])
    W = W + W.T #weight matrix
    W[W >= epsilon] = 0

    A = (W >0).astype(int)
    return W , A

    def getEL(A):
        edgesList = []
        for i in range(len(A)):
            for j in range(i,len(A)):
                if A[i,j] > 0:
                    edgesList.append([i,j])
        return edgesList
```

Listing 1: Code for the generation of the simplicial structure

In the applications, as is standard procedure in topological data analysis, we have built filtrations of simplicial complexes to analyze how the homological structure changes at different length scales. This requires computing subsets of the *full* complex X, by restricting its 1-skeleton to those edges having length smaller than a given threshold ϵ, and tiling the 2-skeleton accordingly via the definition of clique complex (2.6, 2.32).

```
def filterMatrix(W,epsilon):
    Wb = np.matrix(W)
    Wb[Wb >= epsilon] = 0
    return Wb
```

Listing 2: Code for the filtration of the 1-skeleton

Shortest Path Tree

The following describes the computation of the shortest path tree. Its generation is necessary to obtain a candidate set of cycles among which to find the optimal ones ([6], Proposition 3.1).

```
def computeShortestPath(self, withDistances=False):
        (self.dist, self.pred) = csgraph.shortest_path(self.
            Weights.tocsr(),directed=False,return_predecessors
            =True)

        # Aggiungiamo il calcolo dei successori. Struttura di
            lista^3
        for source in range(self.NVert): # per ogni sorgente
            link = self.pred[source,:] # predecessori
            forward = [ [] for i in range(self.NVert) ] #
                lista di liste vuote lunga NVert
            for (foll, prev) in enumerate(link):
                if (prev != -9999): # se è connesso e non è
                    source
                    forward[prev].append(foll)
            self.Followers.append(forward)
def shortestPathTree(self, source, withD=False, justEdges=
    False):
        # ...
```

```
        if (type(source) is not int or source<0 or source>=
            self.NVert ):
            raise Exception('Indice del vertice non valido!')

        if withD:
            if (self.dist is None or self.pred is None):
                _ = self.computeShortestPath(withD)
        else:
            if self.pred is None:
                _ = self.computeShortestPath(withD)

        link = np.array(self.pred[source,:])

        data = []
        rows = []
        col = []
        # ...
        if withD:
            data = np.array(data, dtype=float)
        else:
            data = np.array(data, dtype=int)
        rows = np.array(rows)
        col = np.array(col)
        SPT = scipy.sparse.coo_matrix( (data,(rows,col)),
            shape=(self.NVert,self.NVert))

        rw,cl,_ = scipy.sparse.find(self.Weights)

        edgeSPT = list( zip(list(rows),list(col)))
        edgeW = list(zip( list(rw),list(cl)))

        # Affinchè il metodo funzioni, è necessario che il
            nodo source non abbia -9999 per distinguerlo da
            quelli davvero disconnessi
        link[source] = source # creiamo un "finto" self-loop
        edgeW = [ x for x in edgeW if link[x[0]] != -9999 ]

        NTE = list(set(edgeW) - set(edgeSPT)) # differenza
            insiemistica tra i set di edges

        NTE = [ x for x in NTE if (x[0]<x[1]) ]

        if justEdges:
            return NTE
        else:
```

```
            return (SPT, NTE)
```

Listing 3: Code for the computation of the SPT

Basis of cycles

This piece of code computes a basis of the group of cycles from the sentinel edge description ([10], Proposition 2)

```
def getCycleBase(self):

        if (self.Sentinel is None):
            _ = self.spanningTree()

        SC = [] # lista di sentinel cycles
        for e in self.Sentinel:
            SC.append( self.closeCycle(e) )

        return SC
```

Listing 4: Code for the generation of a cycle basis

Annotation

The following piece of code computes the annotation matrix of sentinel edges ([10])

```
def getAnnotation(self,d2,Z):
        def low(col):

                l=-1;
                for i in range(len(col)):
                    if col[i]>0:
                        l=i
                return l
        lowSet = {}; #dictionary with low indexes and
           relative rows
        if len(d2) == 0: # controlla se d2 è vuoto!
            dimB1 = 0
            i = 0
        else:
            i=0;
            while i != len(d2):
                    lowRowi=low(d2[i])
```

```
                while lowRowi in lowSet.keys():
                    d2[i]=(d2[i]+d2[lowSet[lowRowi]])%2
                    lowRowi=low(d2[i])
                if lowRowi > -1 :
                    lowSet[lowRowi]=i
                    i=i+1
                else:
                    d2=np.delete(d2,(i),axis=0)
        dimB1=i # dimensione dello spazio dei bordi
    if (dimB1 != 0):
        Z=np.concatenate((d2,Z),axis=0)
    else:
        pass

    totRow=len(Z)
    reductionMatrix=np.identity(totRow,dtype=int)
    Id=np.identity(totRow,dtype=int)
    elementsToDelete=[]

    while i != totRow:
        lowRowi=low(Z[i])
        while lowRowi in lowSet.keys():
            Z[i]=(Z[i]+Z[lowSet[lowRowi]])%2
            reductionMatrix[i]=(reductionMatrix[i]+Id[
                lowSet[lowRowi]])%2
            lowRowi=low(Z[i])

        if lowRowi > -1:
            lowSet[lowRowi]=i
            i=i+1
        else:
            elementsToDelete.append(i)
            i=i+1
    reductionMatrix=np.delete(reductionMatrix,
        elementsToDelete,axis=1);
    reductionMatrix=np.delete(reductionMatrix,range(dimB1
        ),axis=1);
    A=np.delete(reductionMatrix,range(dimB1),axis=0);

    self.dimB1 = dimB1
    self.dimZ1 = np.shape(A)[0]
    self.dimH1 = np.shape(A)[1]
    self.Ann = np.matrix(A).transpose()

    self.AnnDict = {}
```

```
        for i,e in enumerate(self.Sentinel):
            ann = self.Ann[:,i]
            self.AnnDict[e] = ann

        return (self.Ann, self.dimB1, self.dimZ1, self.dimH1)
```

Listing 5: Code to compute the annotation

Labeling

The following piece of code computes the labels of nodes with respect to support vector Sup ([6], Base case).

```
def innerProd(self,S,C):
        if (len(S) != len(C)):
            raise ValueError("Dimensioni non compatibili!")

        return np.dot( np.array(S).transpose() , np.array(C)
           ) % 2

def computeLabels(self, Sup):
        if (self.Ann is None):
            raise ValueError("Non è stata calcolata l'
               annotazione degli edges!")
        for p in range(self.NVert):
            forward = self.Followers[p]
            self.Labels[p,p] = 0
            driver = [] # lista di push/pop DI TUPLE (
               PREVIOUS,FOLLOWER)
            add = [ (p,x) for x in forward[p] ]
            driver.extend( add )
            while ( len(driver) != 0):
                (prev,foll) = driver.pop(0)
                lab = self.Labels[p,prev]
                edge = (prev, foll) if prev<foll else (foll,
                   prev)
                try:
                    ann = self.AnnDict[edge]
                except KeyError:
                    self.Labels[p,foll] = lab
                else:
                    self.Labels[p,foll] = (lab + self.
                       innerProd(Sup,ann))%2
                add = [ (foll, x) for x in forward[foll] ]
                driver.extend(add)
```

Listing 6: Code to compute the labeling with respect to support vector Sup

Shortest New Cycle

The following piece of code finds the shortest cycle that is non-orthogonal to support vector Sup ([6], Claim 3.1).

```
def findShortestNonOrtho(self, Sup, allDraws=False):
        _ = self.computeLabels(Sup)

        def checkOrt(s, e):
            try:
                ann = self.AnnDict[e]
            except KeyError:
                lab = 0
            else:
                lab = self.innerProd(Sup , ann) # calcola il
                    prodotto
            return (self.Labels[s,e[0]] + self.Labels[s,e[1]]
                + lab ) %2
        candidates = []
        candidates = [ x for x in self.NTE if checkOrt(x[0],x
            [1]) == 1 ]
        candidates = [ self.closeCycle(x[1], force=x[0]) for
            x in candidates ]
        def lenCycle(C):
            return np.dot( self.WEdges , C)

        candidates = list(zip( candidates, map(lenCycle,
            candidates) ))
        if allDraws:
            shortest = candidates[0][1]
            minList = []
            for x in candidates:
                if x[1] < shortest:
                    minList = [x]
                    shortest = x[1]
                elif x[1] == shortest:
                    minList.append(x)
                else:
                    pass
            return minList
        else:
```

```
            min_len = lambda x,y : x if x[1] <= y[1] else y
            minCycle = functools.reduce( min_len , candidates
                )
            return minCycle
```

Listing 7: Code to find the new shortest basis vector with respect to support vector Sup

Update of support vectors

The following piece of code updates the basis of the orthogonal complement of the first basis vectors ([6], Theorem 3.1)

```
def updateSup(self, newC, index):
        self.SHB.append( newC ) # aggiungi il nuovo ciclo
        sup_i = self.Support[index] # support vector del
            nuovo ciclo
        AnnNewC = self.cycleAnnotation(newC)
        for j in range(index+1,self.dimH1):
            sup_j = self.Support[j]
            self.Support[j] = (sup_j + sup_i * self.innerProd
                ( AnnNewC , sup_j )) % 2
```

Listing 8: Code to update the support vectors.

4 Results and Applications

In this section we run the algorithm we have implemented. A series of test will be shown, after which we move on to some actual data analysis on a real-world dataset.

4.1 Testing

Erdős-Rényi

We begin by testing the code on some random-generated Erdős-Rényi graph, through the python library *networkx*.

```
import numpy as np
import scipy
import networkx as nx
import matplotlib.pyplot as plt
%matplotlib inline

def getRandomGraph(nVert,p):
    G = nx.erdos_renyi_graph(nVert,p)
    flag = nx.is_connected(G)

    A = nx.adjacency_matrix(G).todense()
    return (G,A,flag)

(G,A,f) = getRandomGraph(10,0.15)
nx.draw(G)
```

Listing 9: Networkx Example.

Plotting the output we obtain as in figure 4 :

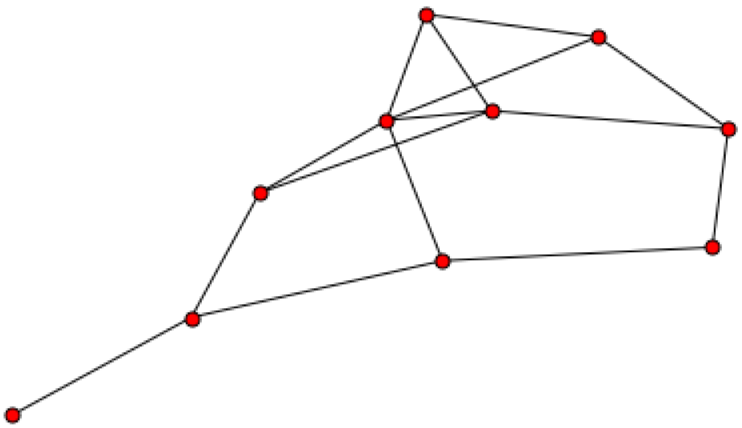


Figure 4: The input graph. Erdős-Rényi random model with 10 nodes and $p = 0.15$.

In this case, the borders are chosen randomly among cycles. Hence the simplicial complex this graph belongs to is not clique. Indeed, we highlight in blue an arbitrary choice of cycles to form borders (Figure 5).

```
NBorders = 2
NBorders = min(NBorders, len(cycles))
indexes = random.sample(xrange(len(cycles)) , NBorders)
# ...
d2 = []
for i in indexes:
    d2.append( cycles[i] )
# ...
nx.draw(Gn, pos=Gn_pos, edge_color=OrderedColorB, node_size
   =50)
```

Listing 10: Choice of borders.

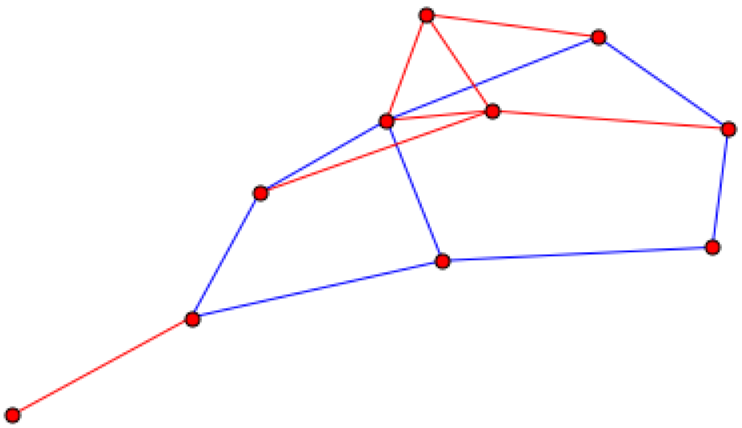


Figure 5: The (arbitrary) borders highlighted in blue. Notice this complex is, therefore, not clique.

Let us run the algorithm on matrix A representing this graph. Highlighted in yellow, the algorithm evidences that all the remaining cycles do belong to the shortest homology basis (Figure 6). On the one hand this confirms the correctness of the output for what concerns homology; on the other, this example is clearly too small to suffice to demonstrate the algorithm is able to identify the *shortest* possible basis.

```
(An, B1, Z1, H1) = G.getAnnotation(d2,cycles)

for i in xrange(H1):
    (mincycle, length) = G.findShortestNonOrtho( G.Support[i]
        )
    G.updateSup(mincycle, i)
    print np.matrix(G.Support).transpose()

nx.draw(Gn, pos=Gn_pos, edge_color=OrderedColorH, node_size
   =50)
```

Listing 11: Shortest Homology Basis

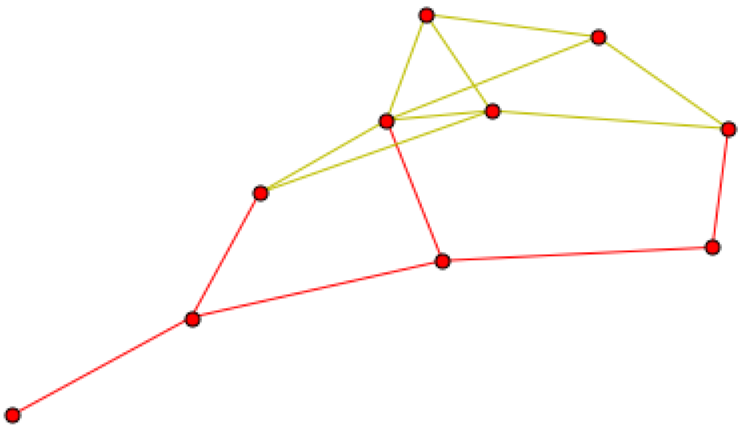


Figure 6: The minimal homology basis, in yellow.

Random Point Sampling

As a second testing step, we proceed to generate a random point cloud in the $\mathbb{R}^2$ plane. Then, we compute pairwise distances between points to generate the 1-skeleton, and tile the cliques accordingly (2.8) .

```
def sampleCircle(x0,y0,r,n, noise):
    P = []
    for i in range(n):
        theta = random()*2*pi
        R = r+noise*random()
        xp = x0 + R*cos(theta)
        yp = y0 + R*sin(theta)
        P.append([xp,yp])
    return P

P = sampleCircle(10,1,8,90,3)
P +=sampleCircle(-10,1,8,90,3)
P +=sampleCircle(0,10,8,90,3)

# ...
```

```
G = SimplexGraph(nVert,W)
cycles = G.getCycleBase()
(An, B1, Z1, H1) = G.getAnnotation(d2,cycles)
sup = np.eye( H1, dtype = int )
Sup = []
for i in range(H1):
    Sup.append( sup[:,i] )

G.Support = Sup
for i in range(H1):
    (mincycle, length) = G.findShortestNonOrtho( G.Support[i]
        )
    G.updateSup(mincycle, i)

SHB = np.matrix(G.SHB).transpose()
```

Listing 12: Shortest Homology Basis of a random sampling of nodes.

This larger example exhibits the desired behaviour: the algorithm identifies *hole-like features* in the dataset, and is able to localize them tightly, yielding the shortest possible cycle as a generator for each class.
Output:

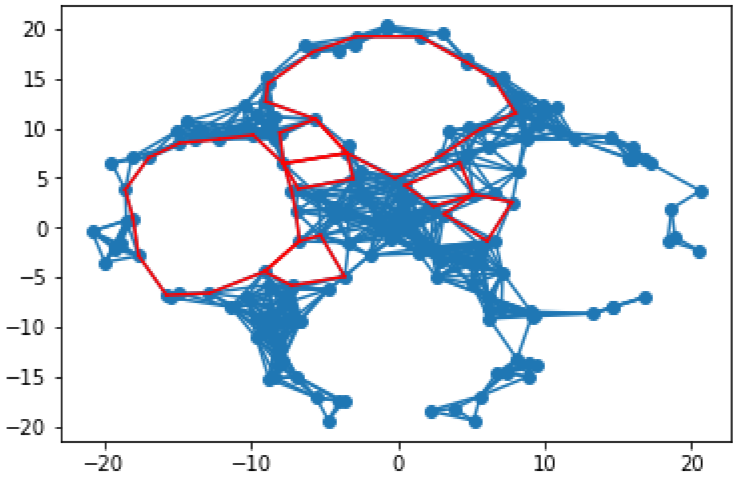


Figure 7: Example of SHB on a random sampling of 180 nodes.

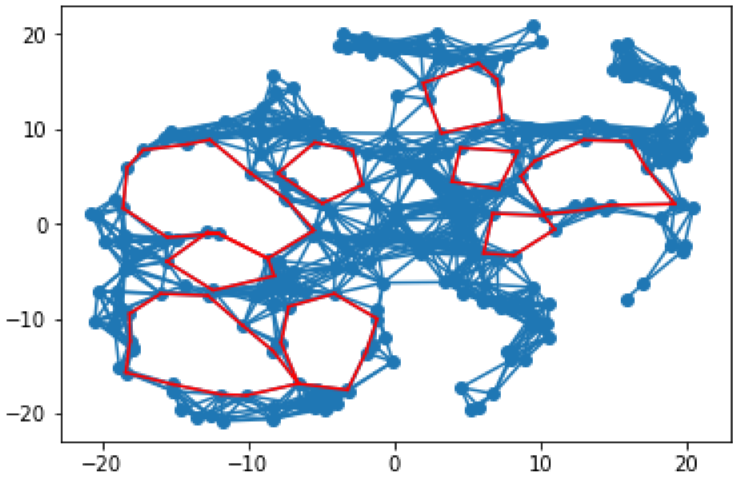


Figure 8: Example of SHB on a random sampling of 270 nodes.

Filtration of Random Samplings

Let us now move to a typical application in Topological Data Analysis: i.e., let us repeat the previous analysis on a *filtration* of simplicial complexes VR_ϵ built from the same set of nodes, increasing the threshold that defines the 1-skeleton, and consequently the cycles (2.32).

```
def filterMatrix(W,epsilon):
    Wb = np.matrix(W)
    Wb[Wb >= epsilon] = 0
    return Wb

# ...

P = sampleCircle(10,1,8,45,3)
P +=sampleCircle(-10,1,8,45,3)
P +=sampleCircle(0,10,8,45,3)

# ...

def filtration_pipeline(W,epsList):
    nVert = len(W)
    SHB = []
    Ws = []
```

```
    maximal = SimplexGraph.getEdgeList(W)
    for eps in epsList:
        Wstep = filterMatrix(W,eps)
        Ws.append(Wstep)
        G = SimplexGraph(nVert,Wstep, maximal)
        cycles = G.getCycleBase()
        d2 = getD2( Wstep , maximal[0] )
        (An, B1, Z1, H1) = G.getAnnotation(d2,cycles)
        sup = np.eye( H1, dtype = int )
        Sup = []
        for i in range(H1):
            Sup.append( sup[:,i] )
        G.Support = Sup
        for i in range(H1):
            (mincycle, length) = G.findShortestNonOrtho( G.
               Support[i] )
            G.updateSup(mincycle, i)

        SHB.append(np.matrix(G.SHB).transpose() )

    return SHB, Ws, maximal

epsList = [3.0,4.0,5.0,6.0]
SHB,Ws,maximal = filtration_pipeline(W,epsList)
```

Listing 13: Shortest Homology Basis for a filtered complex.

Step 0:

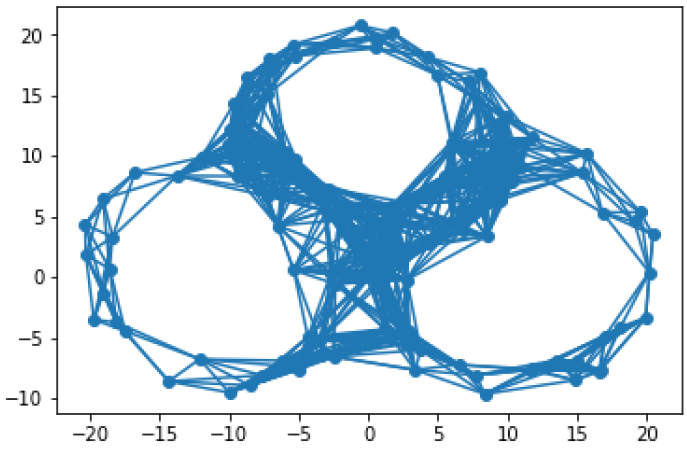


Figure 9: The maximal simplicial complex, unfiltered.

Step 1, $\epsilon = 3.0$:

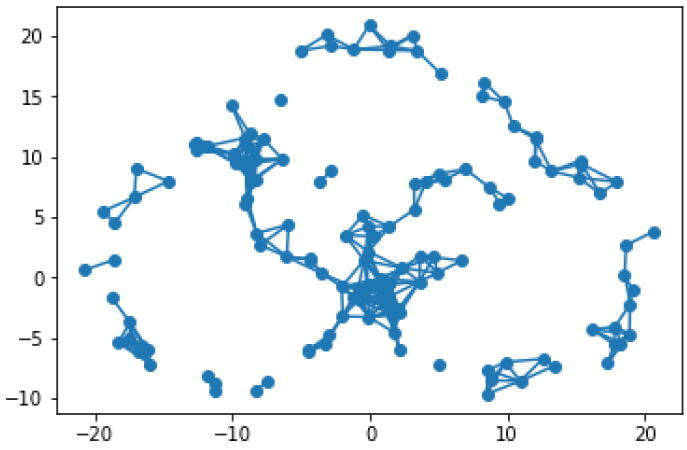


Figure 10: The filtered complex with threshold $\epsilon = 3.0$. We notice that the only cycles are the cliques, which are borders. Hence the homology group is trivial and has no representatives.

Step 2, $\epsilon = 4.0$:

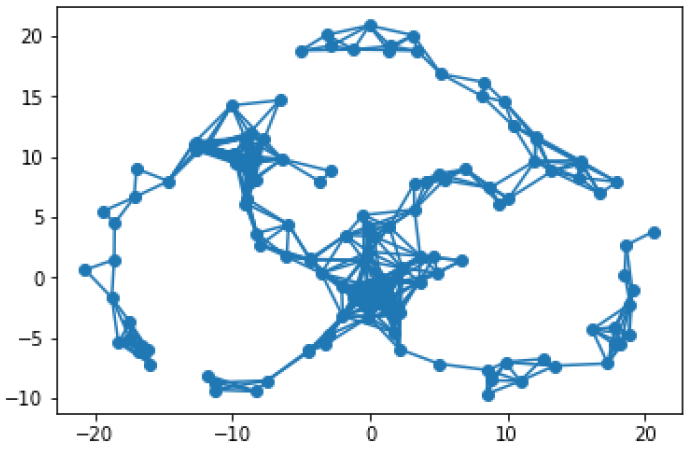


Figure 11: The filtered complex with threshold $\epsilon = 4.0$. Longer edges begin to appear, but they are as yet unable to close *macroscopic* cycles; the only cycles are still cliques, and the homology group is still trivial.

Step 3, $\epsilon = 5.0$:

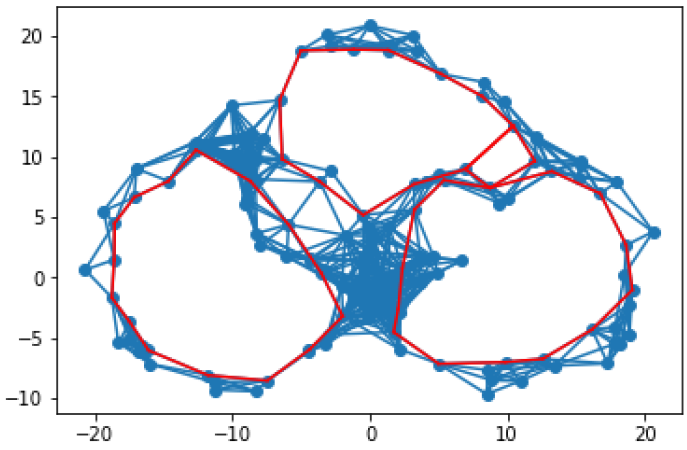


Figure 12: The filtered complex with threshold $\epsilon = 5.0$. At last, "big" cycles are closed and contribute to H_1 with non-trivial generators. We may notice that the homology basis is indeed localized, i.e. the cycles are the *shortest* possible.

Step 4, $\epsilon = 6.0$:

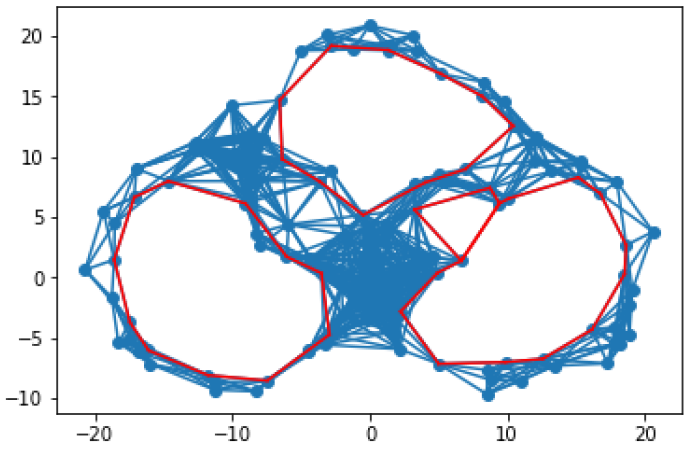


Figure 13: The filtered complex with threshold $\epsilon = 6.0$. At this step we may notice that increasing the connectivity can alter the structure in complex ways. Specifically, in this case the Betti number has remained unaltered, but the homology classes are clearly different. The smaller cycle at the previous step has been *tiled out*, while a new cycle was born due to the appearance of a new edge splitting the large bottom-right hole.

.

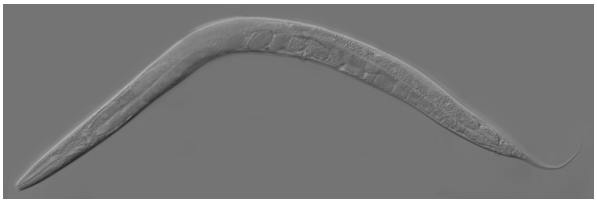


Figure 14: An adult specimen of *C. Elegans*. Courtesy of Penn State.

4.2 C. Elegans

Finally, we have applied the algorithm to a real dataset. The data in our possession concerns time-averages of correlations between neuron firings in the nematode worm *Caenorhabditis elegans*. This organism was the first multicellular, albeit small, species whose genome was entirely sequenced, and it features another interesting peculiarity: every single individual in this species has the exact same nervous system, composed of 306 neurons. It therefore represents the model organism for the study of *connectomes*, i.e. the detailed mapping of connections between single neurons.

Dataset

The dataset consists of an edgelist describing the intensity of correlation between pairs of neurons, intended as graph nodes. In principle, this could yield a complete graph K_{306}. In practice, this is not the case as several correlation pairs are virtually zero, nonetheless the connectivity remains remarkably high. As a consequence, it is practically impossible to give an understandable graphical representation of the dataset; some subsets extracted from the whole aggregate are shown in Figures 15 and 16.
In order to perform a persistence analysis, it is useful to distinguish between the different values of the edge weights. As evinced in Figure 17, there exist 31 different weights for the total 2148 edges, hence to perform a single step persistence analysis we shall need to run 31 instances of the shortest homology basis finder. One must notice, however, that the edge weights represent *correlations* between neurons. Therefore, in order for our analysis to be meaningful (i.e. represent "distances") we need, as a preliminary step, to invert the value of weights.

```
216 217 1.0
216 152 4.0
```

```
216 155 2.0
216 198 4.0
216 157 1.0
216 195 2.0
216 264 5.0
216 265 3.0
216 193 5.0
216 133 2.0
216 234 1.0
216 117 1.0
216 179 1.0
216 82 2.0
216 174 2.0
```

Listing 14: An excerpt from the edge-list description of the dataset.

```
data = np.loadtxt("celegans_weighted_undirected.edges")
v1 = data[:,0]
v1 = np.array(v1, dtype=int)
v2 = data[:,1]
v2 = np.array(v2,dtype=int)
weights = data[:,2]
wmax = max(weights)
weights = [ float(wmax)/x for x in weights ]
weights = np.array(weights, dtype=float)
FullEpsList = list(set(weights))
print( "Min: ", min(weights), "Max: ", max(weights), "Total:
    ", len(weights), "Different: ", len(set(weights)))
plt.hist(weights, range(int(min(weights)), int(max(weights)))
    )
>
Numero vertici: 306
Min:  1.0 Max:  70.0 Total:  2148 Different:  31
```

Listing 15: An overview of the input dataset.

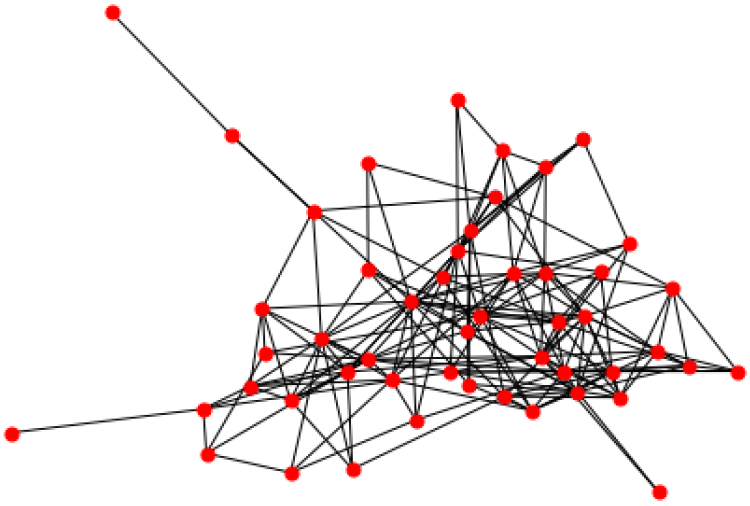


Figure 15: A subset of the input dataset.

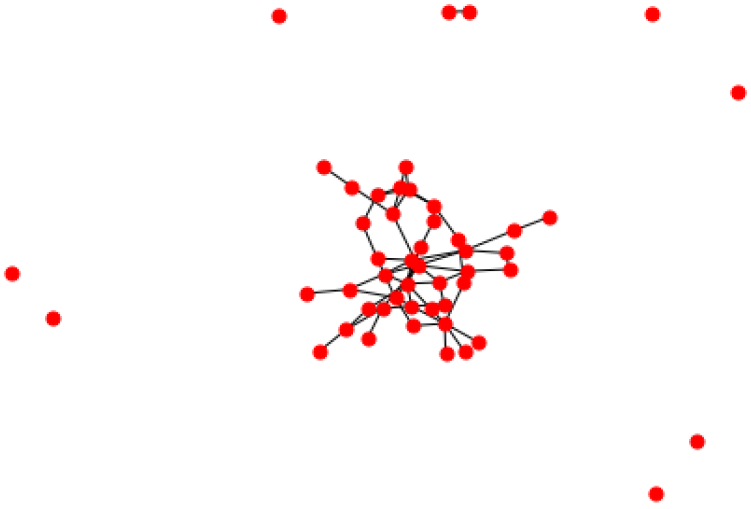


Figure 16: A subset of the input dataset.

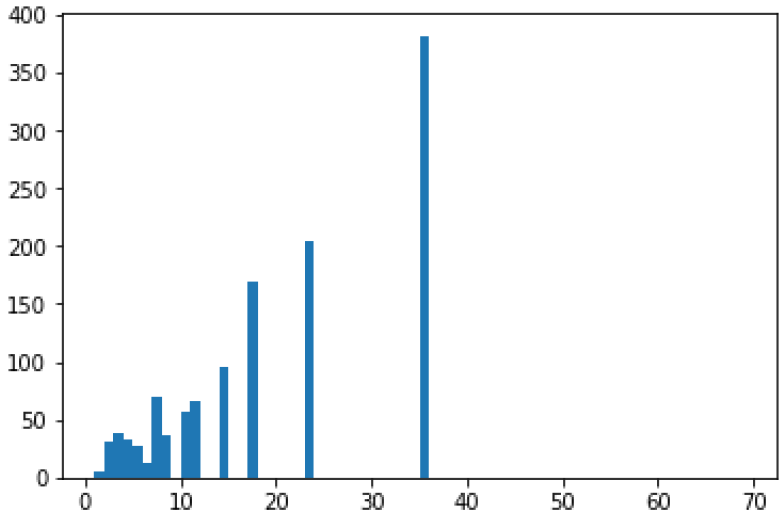


Figure 17: The histogram distribution of *distance* values. One can see there exist 31 different values for the 2148 edges.

Analysis

We now have a graph of 306 nodes and 2148 positively-weighted edges, plus a set of 31 threshold values to generate a single step filtration. Our objective is to analyze the behaviour of the homology group as the threshold increases. This example requires quite some computational effort in order to obtain a result. This is why a multithreaded approach was chosen: in order to reduce the total time requirement, different steps of the filtration were assigned to different cores of an off-the-shelf workstation. This introduces some complexity for what concerns coordinating the instances and some memory overhead to keep the outputs comparable, as is visible in the slightly more elaborate code in the listings below, but at the same time provides a substantial speed-up. The whole analysis ran for an approximate four and a half hours.

```
def parallel_pipeline(eps):
    W = GlobalOptions['Matrix']
    nVert = len(W)
    SHB = []
    Ws = []
```

```
    res = {}
    maximal = SimplexGraph.getEdgeList(W)
    stats = []
    Wstep = filterMatrix(W,eps)
    Ws.append(Wstep)

    G = SimplexGraph(nVert,Wstep, maximal)
    cycles = G.getCycleBase()
    stats.append( 'NVert = ' + str(G.NVert) + ' NEdges = ' +
       str(G.NEdges) )
    stats.append( 'Filtration Eps = ' + str(eps) )
    stats.append( 'Keep all Draws = ' + str(GlobalOptions['
       Draws']) )
    d2 = getD2( Wstep , maximal[0] )
    (An, B1, Z1, H1) = G.getAnnotation(d2,cycles)
    stats.append( 'H1= '+ str(H1) + ' B1= ' + str(B1) + ' Z1=
        ' + str(Z1) )
    sup = np.eye( H1, dtype = int )
    Sup = []
    for i in range(H1):
        Sup.append( sup[:,i] )
    G.Support = Sup
    G.fixNTE()
    t1 = time.time()
    for i in range(H1):
        if GlobalOptions['Draws']:
            listMin = G.findShortestNonOrtho( G.Support[i] ,
               allDraws=True)
            mincycle = listMin[0][0]
            SHB.append(listMin)
        else:
            (mincycle, length) = G.findShortestNonOrtho( G.
               Support[i], allDraws=False )
        G.updateSup(mincycle, i)

    if GlobalOptions['Draws']:
        res['SHB'] = SHB
    else:
        res['SHB']=np.matrix(G.SHB).transpose()
    res['Draws'] = GlobalOptions['Draws']
    res['Filtration Eps'] = eps
    if GlobalOptions['ReturnMatrix']:
        res['Filtered Matrix'] = Ws
    else:
        res['Filtered Matrix'] = None
```

```
    if GlobalOptions['ReturnMaximal']:
        res['Max'] = maximal
    else:
        res['Max'] = None
    res['stats'] = stats

    return res
```

Listing 16: The parallel pipeline to analyze the filtration.

```
file_stream = open(filename,'wb')
FullThreshList = [ x + 0.05 for x in FullEpsList ]
epsList = FullThreshList
cut = 306
Wn = W[0:cut,0:cut]
GlobalOptions['Matrix'] = Wn

pool = Pool(processes=4)
job = pool.map_async(parallel_pipeline, epsList)
result = job.get()

cPickle.dump(result, file_stream)
file_stream.close()
```

Listing 17: The multithreaded instance of the *C. Elegans* analysis.

As mentioned above, it is hardly useful to give a graphical representation of the resulting homology basis. The reason for this is twofold:

- The size and the sheer connectivity of the graph make it nearly impossible to get any sense of the underlying structure.
- The input data is intrinsically non-geometrical: as said, edge weights represent statistical correlations, and as such do not induce a metric on the graph, in that they do not obey any triangular inequality. Therefore, it is in general impossible to obtain a geometric realization of data points which respect the pairwise distance relations defined by the edge weights. At best one can dispose nodes according to a force-directed layout, giving up on the concept of distance while still obtaining a cluttered result (see Figure 18).

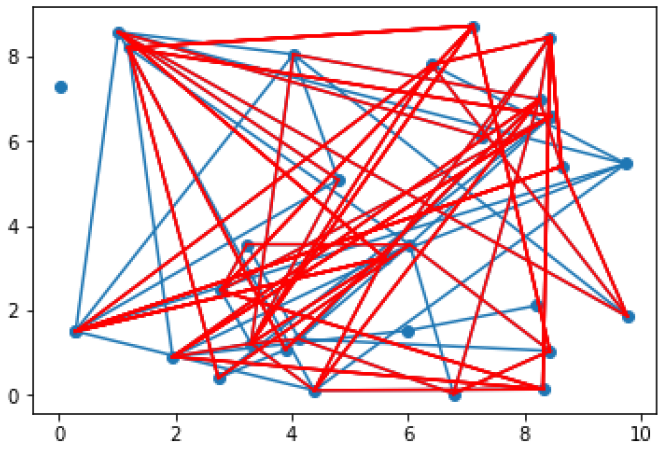


Figure 18: The minimal homology basis (in red) of a small subset of the data.

Saturation of the complex

It could instead be interesting to analyze the relationship between the filtration threshold and the rank of the resulting homology group. As evidenced in Figure 19, a known behaviour occurs: when the scale is very low, few edges exist and therefore very few cycles. Hence the Betti number is zero or small. As soon as the connectivity scale grows, a number of holes appear rapidly and the curve spikes up. Then, when the scale crosses a certain critical value, the number of cycles that become tiled (borders) exceeds the number of cycles that are created, and therefore the rank of H_1 decreases. Obviously, there exists a value $\epsilon_M := \max_e w_e$ where w_e is the weight of edge e such that $\forall \epsilon \geq \epsilon_M$ any clique complex VR_ϵ is entirely tiled, and therefore its homology group is trivial and the Betti number zero. Hence the β/ϵ curve is definitively zero.

```
file_stream = open('CEFullNoDraws.dat','rb')
restore = cPickle.load(file_stream)
file_stream.close()

epsList=[]
HList = []
for i in restore:
    epsList.append( i['Filtration Eps'] )
    if  i['SHB'].shape[0] != 0:
```

```
        HList.append( i['SHB'].shape[1] )
    else:
        HList.append(0)

plt.plot(epsList,HList, '|r')
```

Listing 18: Post-processing of the C. Elegans analysis.

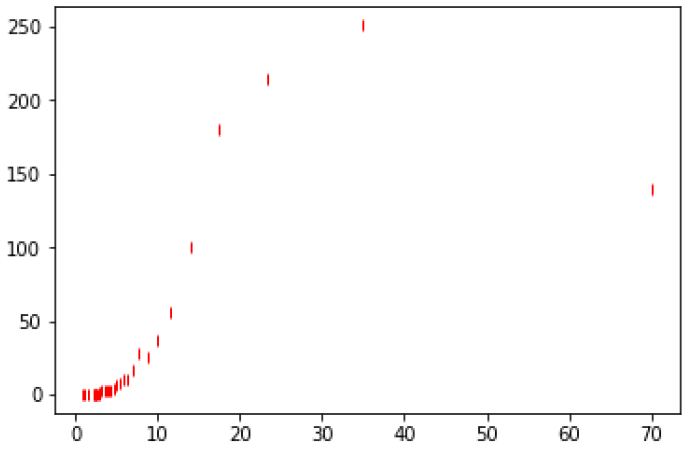


Figure 19: The rank of $H_1(\mathrm{VR}_\epsilon(X_0))$ as a function of the threshold ϵ.

Edge relevance

Let us lastly give a heuristic measure of the *importance* of an edge in the simplicial structure. The graph in Figure 20 is obtained by summing, for each edge from 1 to 2148, how many times it takes part into a shortest homology basis, along the filtration. One can immediately tell that there exists a very small number of edges that are very often part of a minimal cycle, while a large majority is rarely involved in the SHB structure. This gives us some valuable insight as to which links in the graph are the most critical.

```
V = np.zeros((2148,1), dtype=int)
nonNull = [ x for x in restore if x['SHB'].shape[0] != 0 ]
tot = 0

for i in nonNull:
    tot += i['SHB'].shape[1]
    Sum = i['SHB'].sum(axis=1)
    V += Sum

print(tot)
V = Vect/tot
V = np.sort(V, axis=0)
V = np.flip(V, axis=0)
plt.plot(V,'_b')
```

Listing 19: Edge hits distribution.

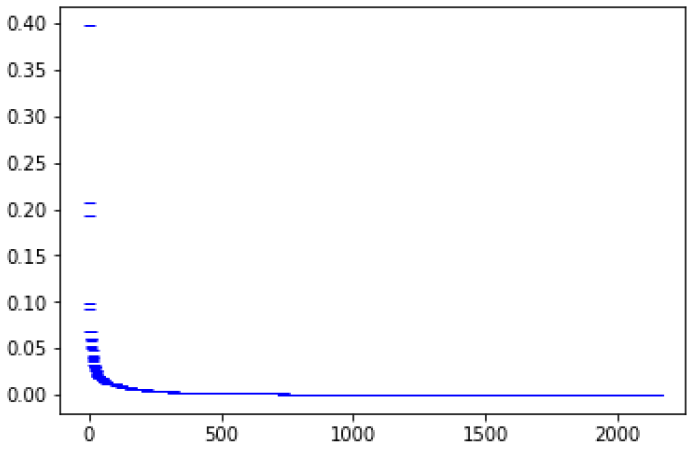


Figure 20: The descending-order normalized plot of how many times each edge from 1 to 2148 is part of a shortest homology basis. In this case, the total number of cycles in the SHB's of the 31 simplicial complexes (sum of the Betti numbers at each filtration step) is 1096.

.

5 Appendix - Code

Repository available at https://github.com/marcoguerra192/PHScaffold ([25])

```
# -*- coding: utf-8 -*-
### TESI: CLASSE per il problema SHORTEST PATH TREE

import numpy as np
from scipy.sparse import csgraph
import scipy.sparse
import functools
#from line_profiler import LineProfiler

class SimplexGraph:
    """ Classe che implementa un grafo come matrice
       di adiacenza pesata, e fornisce metodi per
       ottenere lo shortest path tree
        a partire da un nodo arbitrario, più l'
           elenco dei non-tree edges.
        Input costruttore: Il numero di vertici, o
           il numero di vertici e la matrice dei
           pesi
    """
    def __init__(self, numVertices, weights, maximal
       =None):
        self.NVert = numVertices
        self.Weights = scipy.sparse.coo_matrix(
           weights)
        ## coo_matrix può essere istanziata a
           partire da una matrice densa di tipo np.
           ndarray
        self.Weights = self.Weights.tocsr()
        # al momento ci serve che sia csr per
           accedere ai pesi

        self.dist = None
        self.pred = None
```

```
self.Followers = []
self.Sentinel = None
self.CCC = None
self.CCV = None
self.Origins = None
self.Ann = None
self.dimH1 = None
self.dimB1 = None
self.dimZ1 = None
self.Labels = -1 * np.ones( (self.NVert,self
   .NVert), dtype=int )
self.Support = [] # vettori di supporto
self.SHB = [] # base minima di omologia
self.NTE = None # array di liste di NTE
self.closedCycles = {} # dizionario di cicli
    già chiusi
# la chiave è la terna (source, v1, v2)

# diversifichiamo il caso in cui abbiamo la
   filtrazione dal caso
# singolo step
if (maximal == None):
    rw,cl,_ = scipy.sparse.find(self.Weights
       ) # righe e colonne sparse
    self.Edges = list(zip(list(rw), list(cl)
       )) # lista di coppie di vertici
    self.Edges = [x for x in self.Edges if x
       [0]<x[1]] # scelgo solo quelli da un
       vertice più basso ad uno più alto
    # funziona perchè non ci sono self loops
    def orderEdges( edgeList ):
        """ Funzione che ordina la lista di
           edge secondo qualche criterio.
           Per ora il criterio è prima
           rispetto al primo vertice,
        poi rispetto al secondo.
        """
        return sorted(edgeList, key = lambda
```

```
                t: (t[0],t[1]) )
        self.Edges = orderEdges(self.Edges) #
           ora è una lista ordinata di edges,
           senza ripetizioni!
        # può essere usata per tenere traccia
           dell'ordine degli edges
        self.NEdges = len(self.Edges) # numero
           di edges IN SENSO INDIRETTO
        self.WEdges = [] # lista delle lunghezze
            (pesi) degli edges
        for e in self.Edges:
            self.WEdges.append( self.Weights[e
               [0] , e[1]] )

        self.WEdges = np.array(self.WEdges) #
           trasformo in array
    else: # se ho definito la matrice più fine
       della filtrazione
        # maximal è una tupla = (edgelist,
           weightlist)
        # la edgelist deve già essere ordinata
        self.Edges = maximal[0]
        self.NEdges = len(self.Edges)
        self.WEdges = maximal[1]

def getEdgeList(Weights):
    """ Metodo Statico per ottenere l'edgelist
       da una matrice massimale
        In input solo la matrice dei pesi
    """
    rw,cl,_ = scipy.sparse.find(Weights) # righe
        e colonne sparse
    edgelist = list(zip(list(rw), list(cl))) #
       lista di coppie di vertici
    edgelist = [x for x in edgelist if x[0]<x
       [1]] # scelgo solo quelli da un vertice
       più basso ad uno più alto
    # funziona perchè non ci sono self loops
```

```
        def orderEdges( edgeList ):
            """ Funzione che ordina la lista di edge
                secondo l'ordine lessicografico
            """
            return sorted(edgeList, key = lambda t:
               (t[0],t[1]) )
        edgelist = orderEdges(edgelist) # ora è una
           lista ordinata di edges, senza
           ripetizioni!
        WEdges = [] # lista delle lunghezze (pesi)
           degli edges
        for e in edgelist:
            WEdges.append( Weights[e[0] , e[1]] )
        WEdges = np.array(WEdges) # trasformo in
           array

        return (edgelist,WEdges)

    def getEdgeVector(self): # ordinamento degli
       archi
        return self.Edges

    def getHeatMap(self, edgeList):
        """ Prende in input una lista di coppie di
           vertici (v1, v2), li ordina in modo che
           v1 < v2, e restituisce un vettore 0-1
           lungo             quanto la dimensione
           dello spazio vettoriale delle 1-catene,
           che descrive la 1-catena corrispondente.
            Se l'input contiene un edge inesistente
               o un self-loop, solleva ValueError
        """
        edgeList = [ x if (x[0] < x[1] ) else tuple(
           reversed(x)) for x in edgeList ] # impone
            v1 <= v2
        # e se v1 == v2 ?
        if ( any( [ x[0] == x[1] for x in edgeList ]
            ) ):
```

```
            raise ValueError('La lista contiene un
               self-loop!') # eccezione

        edgeList = list(set(edgeList)) # elimina i
           duplicati

        heatMap = np.zeros(self.NEdges, dtype=int) #
            vettore di zeri

        for val in edgeList:
            try:
                i = self.Edges.index(val)
            except:
                errstr = "L'edge ", val, " non
                   esiste!"
                raise ValueError(errstr)
            heatMap[i] = 1
        return heatMap

    def set_weights_by_coo(self, data, rows, col):
        """ Istanzia la matrice dei pesi nel formato
            sparso attraverso tre array data, rows e
            col"""
        self.Weights = scipy.sparse.coo_matrix((data
           ,(rows,col)), shape=(self.NVert,self.
           NVert))

    def computeShortestPath(self, withDistances=
       False):
        """ Restituisce la matrice dei predecessori
           nello Shortest Path Tree. Ogni riga si
           riferisce ad un nodo
            di origine dello SPT. Se l'argomento
               opzionale è vero ritorna anche la
               matrice delle distanze
        """
        # va convertito in un formato su cui può
           fare i calcoli
```

```
        (self.dist, self.pred) = csgraph.
            shortest_path(self.Weights.tocsr(),
            directed=False,return_predecessors=True)

        # Aggiungiamo il calcolo dei successori.
            Utile da fare una volta invece di n
        # Viene utile una struttura di lista^3
        for source in range(self.NVert): # per ogni
            sorgente
            link = self.pred[source,:] #
                predecessori
            forward = [ [] for i in range(self.NVert
                ) ] # lista di liste vuote lunga
                NVert
            for (foll, prev) in enumerate(link):
                if (prev != -9999): # se è connesso
                    e non è source
                    forward[prev].append(foll)
            self.Followers.append(forward)
        # non c'è nessun bisogno di restituire una
            matrice densa
        # if withDistances:
        #     return (self.pred, self.dist)
        # else:
        #     return self.pred

    def shortestPathTree(self, source, withD=False,
        justEdges=False):
        """ Restituisce la matrice dello shortest
            path tree centrata nel vertice source. Se
            withD è vero
            la matrice è pesata, altrimenti è solo
                0-1. Se source non è un vertice
                valido solleva un'eccezione
            I VERTICI VANNO DA 0 A N-1!!
            Se justEdges == True restituisce solo i
                non tree edges
            Input: L'indice del nodo sorgente,
```

```
        opzionale un bool per le distanze
    Output: La matrice sparsa del grafo SPT
"""
if (type(source) is not int or source<0 or
   source>=self.NVert ): ## da qui in poi
   source è un valore affidabile
    raise Exception('Indice del vertice non
       valido!')

if withD:
    if (self.dist is None or self.pred is
       None):
        _ = self.computeShortestPath(withD)
else:
    if self.pred is None:
        _ = self.computeShortestPath(withD)

# definiamo una matrice sparsa della giusta
   dimensione che andrà in output
# SPT = scipy.sparse.coo_matrix(self.NVert,
   self.NVert) # NO, SPRECA SOLO TEMPO!
# estraiamo dalla matrice dei precedenti la
   riga che ci serve
link = np.array(self.pred[source,:])
# predisponiamo i vettori data, rows e col
   per creare la matrice del SPT
data = []
rows = []
col = [] # man mano faremo append dei dati
   in queste liste
# scorriamo il vettore e creiamo i link
for i in range(len(link)):
    prev = link[i]
    if (prev == -9999): # non appartiene
       alla stessa componente connessa =>
       non ha predecessori
        pass
    else:
```

```
            rows.append(prev)
            col.append(i) # aggiungi un edge dal
                predecessore del nodo i-esimo al
                nodo i-esimo
            rows.append(i) # devo aggiungere
               anche il simmetrico!
            col.append(prev)
            if withD: # se devo aggiungere le
               distanze le cerco in self.dist
                data.append(self.dist[prev,i])
                data.append(self.dist[prev,i]) #
                    aggiungo anche il simmetrico
                    (stessa distanza)
            else: # se no inserisco solo 1 per
               indicare l'edge fra prev e i
                data.append(1)
                data.append(1)

    if withD:
        data = np.array(data, dtype=float)
    else:
        data = np.array(data, dtype=int)
    rows = np.array(rows)
    col = np.array(col)
    SPT = scipy.sparse.coo_matrix( (data,(rows,
       col)), shape=(self.NVert,self.NVert))
    # crea matrice del grafo
    #Per trovare i non-tree edge: trovare gli
       elementi di Weights che NON SONO in SPT
    rw,cl,_ = scipy.sparse.find(self.Weights) #
       restituisce vettori di righe, colonne e
       valori non nulli
    # ignoro il vettore di dati, che non ci
       interessa
    edgeSPT = list( zip(list(rows),list(col))) #
        creo una lista di edge per SPT
    edgeW = list(zip( list(rw),list(cl))) #
       stessa cosa per il grafo originale
```

```
        # MA CONTIENE ANCHE TUTTI GLI EDGES NELLE
           COMPONENTI NON CONNESSE!
        # Affinchè il metodo funzioni, è necessario
           che il nodo source non abbia -9999 per
           distinguerlo da quelli davvero
           disconnessi
        link[source] = source # creiamo un "finto"
           self-loop
        edgeW = [ x for x in edgeW if link[x[0]] !=
           -9999 ]
        # limito a solo gli edge fra nodi che sono
           raggiungibili da source
        NTE = list(set(edgeW) - set(edgeSPT)) #
           differenza insiemistica tra i set di
           edges
        # contiene ancora entrambe le versioni dell'
           edge (v1,v2 e v2,v1). Imponiamo solo
           quella (v1,v2) con v1<v2
        NTE = [ x for x in NTE if (x[0]<x[1]) ]

        if justEdges:
            return NTE
        else:
            return (SPT, NTE)

    def spanningTree(self):
        """ Calcola uno spanning tree a partire
           dalla stessa matrice dei predecesori di
           SPT. Questa volta, oltre a lavorare su
           tutte le componenti
           connesse, restituisce tutti i sentinel
           edges.
        """
        if self.pred is None:
            _ = self.computeShortestPath(True)
        # prepariamo le liste per la matrice del
           grafo
        rows = []
```

```
col = []
data = []
self.CCV = list(np.zeros(self.NVert, dtype=
   int)) # lista indice delle componenti
   connesse
self.CCC = 0 # contatore delle componenti
   connesse
self.Origins = [] # lista lunga come il
   numero di CC. In posizione k contiene l'
   origine della componente connessa k+1-
   esima
# che sarà necessario utilizzare per
   calcolare i sentinel edges!
while (0 in self.CCV): # finchè non ho
   assegnato ogni vertice ad una componente
    self.CCC += 1
    vert = self.CCV.index(0) # trova il
       primo vertice non assegnato ad alcuna
        componente
    # Questo vertice diventerà l'origine
       della CC!! Sarà necessario usare lui
       per calcolare i sentinel edges!
    self.Origins.append(vert) # questa CC
       origina da vert
    self.CCV[vert] = self.CCC # assegna
       questo vertice alla nuova componente
    link = np.array(self.pred[vert,:]) #
       estrai i predecessori connessi a vert
    for i in range(len(link)):
        prev = link[i]
        if (prev == -9999): # se è
           disconnesso fai nulla
            pass
        else:
            self.CCV[i] = self.CCC # se è
               connesso assegna lo stesso
               indice di componente
            rows.append(prev)
```

```
                col.append(i) # aggiungi un edge
                    dal predecessore del nodo i-
                   esimo al nodo i-esimo
                rows.append(i) # devo aggiungere
                    anche il simmetrico!
                col.append(prev)
                data.append(1)
                data.append(1)
        data = np.array(data, dtype=int)
        rows = np.array(rows)
        col = np.array(col)
        ST = scipy.sparse.coo_matrix( (data,(rows,
           col)), shape=(self.NVert,self.NVert))
           # matrice del grafo Spanning Tree
        # per trovare i sentinel edges. Questo
           spanning tree è già generato a partire
           dall'origine di ogni CC!
        rw,cl,_ = scipy.sparse.find(self.Weights) #
           tutti gli edge del grafo originale
        edgeW = list(zip( list(rw),list(cl))) #
           lista edge grafo originale
        edgeST = list( zip(list(rows),list(col))) #
           lista edge spanning tree
        self.Sentinel = list(set(edgeW) - set(edgeST
           )) # differenza insiemistica
        # contiene ancora entrambe le versioni dell'
           edge (v1,v2 e v2,v1). Imponiamo solo
           quella (v1,v2) con v1<v2
        self.Sentinel = [ x for x in self.Sentinel
           if (x[0]<x[1]) ]
        return (ST,self.Sentinel,self.CCV)

    def closeCycle(self, E, force=None):
        """
        Funzione che prende in input un sentinel
           edge E, e sfruttando la matrice
        self.pred e l'ordinamento self.Edges,
           restituisce un vettore dello spazio
```

```
delle 1-catene che descrive il ciclo
   identificato da E nello Shortest Path
   Tree.
Lo SPT è quello radicato nel nodo ORIGINE
   DELLA CC DI E!
Se l'input non è quello atteso, solleva
   ValueError.
SE E NON É UN SENTINEL EDGE NON SO BENE COSA
    SUCCEDA!
Se è definito force, forza il nodo sorgente
   ad essere quello. Utile per
generare il candidate set.
Sfrutta la struttura self.closedCycles per
   verificare se una certa chiusura
è già stata calcolata
"""

if (force is not None): # se è fissata l'
   origine
    key = (force , E[0] , E[1] ) # la chiave
        è (source, v1,v2)
    try: # trova se è già stato calcolato
        cycle = self.closedCycles[ key ]
        return cycle
    except:
        pass

try:
    cycle = self.getHeatMap([E]) # trova l'
       heatmap del sentinel edge. Gestisce l
       'errore se E non è giusto
except Exception as ex:
    raise ex
# ora cycle contiene l'heatmap del solo
   sentinel edge.
# Proviamo a fare un controllino che sia un
   sentinel edge. Se self.Sentinel non
   esiste può comunque far danni
```

```
if ( self.Sentinel is not None and force is
   None): # solo se non è definito force
                                                #
                                                   (
                                                   in

                                                   quel

                                                   caso

                                                   ci

                                                   sta

                                                   che

                                                   non

                                                   siano

                                                   sentinel

                                                   edges
                                                   )

    if (E not in self.Sentinel and tuple(
       reversed(E)) not in self.Sentinel ):
        raise ValueError("E non è un
           sentinel edge!")

# fissiamo i bordi del sentinel edge
v1 = E[0]
v2 = E[1]

if (force is not None):
    if (force<0 or force>= self.NVert):
        raise ValueError("Parametro force
           non valido!")
```

```
            else:
                source = force
        else:
            # troviamo il NODO ORIGINE della CC di E
            source = self.Origins[ self.CCV[ v1 ] -1
                ] # -1 perchè le CC partono da 1 ma
                i vettori da 0. Sarebbe uguale usare
                v2
            key = (source, E[0] , E[1]) # calcoliamo
                la chiave del ciclo da chiudere
        # Calcoliamo i pred, se non è già stato
            fatto
        if (self.pred is None):
            self.pred = self.computeShortestPath(
                False)

        link = self.pred[source,:] # vettore dei
            precedenti rispetto a source
        pr = link[v2]
        if (pr == -9999 and v2 != source ): #
            significa che v2 è irraggiungibile da
            source, ci deve essere stato un errore
            raise ValueError('Critical Error! Source
                e v2 dovrebbero essere per
                costruzione nella stessa CC')
        follow = v2
        while (pr != -9999): # segue all'indietro i
            precedenti verso source (che ha link
            -9999)
            cycle += self.getHeatMap( [ (pr , follow
                ) ] )
            follow = pr
            pr = link[pr]

        # Ora stessa cosa per v1, ma gli edge in
            comune fra i due path vanno eliminati =>
            SOMMA % 2
```

```
        pr = link[v1]
        if (pr == -9999 and source != v1): #
           significa che v1 è irraggiungibile da
           source, sono in due componenti connesse
           diverse
            raise ValueError('Critical Error! Source
                e v1 dovrebbero essere per
               costruzione nella stessa CC')
        follow = v1
        while (pr != -9999): # finchè non torno a
           source
            cycle += self.getHeatMap( [ (pr , follow
               ) ] )
            follow = pr
            pr = link[pr]
        # ora alcuni cicli saranno stati contati 2
           volte. Quelli in comune vanno eliminati!
        cycle = cycle % 2

        # ora cycle contiene la descrizione
           vettoriale del ciclo identificato dal
        # sentinel edge E, rispetto all'ordinamento
           self.Edges

        # aggiorniamo il dizionario dei cicli chiusi
        self.closedCycles[ key ] = cycle

        return cycle

    def getCycleBase(self):
        """ Calcola una base dei cicli a partire dai
            sentinel edges. Per ottenere l'
           annotazione
        """
        # se ancora non l'ha fatto calcola i
           sentinel edges
        if (self.Sentinel is None):
            _ = self.spanningTree()
```

```
        SC = [] # lista di sentinel cycles
        for e in self.Sentinel:
            SC.append( self.closeCycle(e) )

        return SC

    def getAnnotation(self,d2,Z):
        """
        d2: border matrix of the set of faces of the
            simplicial complex, borders are written
           as rows.
        Z: basis of 1-dim-cycles. Each row is a
           cycle obtained from a spanning tree and a
            sentinel edge.
        returns an annotation of sentinel edges. Non
            sentinel edges have annotation equal to
           0.
        """

        def low(col):
                """
            col: 1-dimensional array.
                gets the index of the "lowest"
                   element in col different from 0.
                if col=0 then low = -1
                """
                l=-1;
                for i in range(len(col)):
                    if col[i]>0:
                        l=i
                return l

        lowSet = {}; #dictionary with low indexes
           and relative rows

        if len(d2) == 0: # controlla se d2 è vuoto!
            dimB1 = 0
```

```
    i = 0
else:
    i=0;
    while i != len(d2):
            lowRowi=low(d2[i])
            while lowRowi in lowSet.keys():
                d2[i]=(d2[i]+d2[lowSet[
                   lowRowi]])%2
                lowRowi=low(d2[i])
            if lowRowi > -1 :
                lowSet[lowRowi]=i
                i=i+1
            else:
                d2=np.delete(d2,(i),axis=0)
    dimB1=i # dimensione dello spazio dei
       bordi

if (dimB1 != 0):
    Z=np.concatenate((d2,Z),axis=0)
else:
    pass # lasciamo Z
#we start the reduction from row dimB1
totRow=len(Z)
reductionMatrix=np.identity(totRow,dtype=int
   )
Id=np.identity(totRow,dtype=int)
elementsToDelete=[]

while i != totRow:
    lowRowi=low(Z[i])
    while lowRowi in lowSet.keys():
        Z[i]=(Z[i]+Z[lowSet[lowRowi]])%2
        reductionMatrix[i]=(reductionMatrix[
           i]+Id[lowSet[lowRowi]])%2
        lowRowi=low(Z[i])

    if lowRowi > -1:
        lowSet[lowRowi]=i
```

```
                i=i+1
            else:
                elementsToDelete.append(i)
                i=i+1

        #eliminate coordinates of cycles that are
           borders:
        reductionMatrix=np.delete(reductionMatrix,
           elementsToDelete,axis=1);
        reductionMatrix=np.delete(reductionMatrix,
           range(dimB1),axis=1);
        A=np.delete(reductionMatrix,range(dimB1),
           axis=0);
        """observation: the number of rows of A is
           the dimension of the 1-dim-cycle group;
           the number of columns is the dimension of
               the 1st homology group
        """
        self.dimB1 = dimB1
        self.dimZ1 = np.shape(A)[0]
        self.dimH1 = np.shape(A)[1]
        self.Ann = np.matrix(A).transpose()

        # OTTIMIZZAZIONE!
        # Qui verrebbe bene creare un dizionario di
           coppie edge-annotazione
        # per velocizzare la ricerca negli step
           successivi. Edge nel formato
        # (v1, v2), con v1<v2
        self.AnnDict = {}
        for i,e in enumerate(self.Sentinel):
            ann = self.Ann[:,i]
            self.AnnDict[e] = ann

        return (self.Ann, self.dimB1, self.dimZ1,
           self.dimH1)

    def innerProd(self,S,C):
```

```
        """ Scalar Product over Z2 of support vector
            S and the ANNOTATION of cycle C
        """
        if (len(S) != len(C)):
            raise ValueError("Dimensioni non
               compatibili!")

        return np.dot( np.array(S).transpose() , np.
           array(C) ) % 2

    def computeLabels(self, Sup):
        """ Calcola i labels rispetto al support
           vector S_i Sup
        """
        if (self.Ann is None):
            raise ValueError("Non è stata calcolata
               l'annotazione degli edges!")
        for p in range(self.NVert): # per ogni root
            #link = self.pred[p,:]
            forward = self.Followers[p]
            """ Utilizziamo un metodo tipo push pop:
                ad ogni nodo aggiungiamo la
            lista dei successori in coda, poi pop di
                uno e avanti così """
            self.Labels[p,p] = 0 # il label di
               source è 0
            driver = [] # lista di push/pop DI TUPLE
                (PREVIOUS,FOLLOWER)
            # iniziamo dai sucessori di source
            add = [ (p,x) for x in forward[p] ]
            driver.extend( add )
            while ( len(driver) != 0): # finchè non
               ho esaurito i successori
                (prev,foll) = driver.pop(0) # pop
                   del primo elemento (BREADTH FIRST
                   !)
                lab = self.Labels[p,prev] # leggiamo
                    il label del nodo precedente
```

```
                edge = (prev, foll) if prev<foll
                   else (foll, prev) # scriviamo l'
                   edge
                try: # leggiamo l'annotazione dell'
                   ege
                    ann = self.AnnDict[edge]
                except KeyError:
                    self.Labels[p,foll] = lab # non
                       è un sentinel e quindi non
                       cambia
                else:
                    # calcola il prodotto scalare in
                        Z2 e somma
                    self.Labels[p,foll] = (lab +
                       self.innerProd(Sup,ann))%2
                # Ora aggiungiamo alla lista driver
                   i successori di foll e avanti
                add = [ (foll, x) for x in forward[
                   foll] ]
                driver.extend(add)

        #return self.Labels # inutile restituire una
            struttura pesante

    def fixNTE(self):
        """ Calcola un array di NTE per ogni
           sorgente p, e la salva in self.NTE
        """
        self.NTE = []
        for p in range(self.NVert):
            nte = self.shortestPathTree(p,justEdges=
               True)
            for e in nte:
                self.NTE.append( (p,e) )
        # ora tutti i NTE sono calcolati una volta
           per tutte

    def resetLabels(self):
```

```
        """ Resetta i labels per poterli calcolare
           rispetto al nuovo vettore di supporto
        """
        self.Labels = -1 * np.ones( (self.NVert,self
           .NVert), dtype=int )


    def findShortestNonOrtho(self, Sup, allDraws=
       False):
        """ Funzione che genera una lista di cicli
           non-ortogonali (m = 1) a Sup
            I NTE seguono la convenzione
               lessicografica
            If allDraws ritorna una lista di tutti i
                cicli minimi a parità!
        """
        # bisogna controllare che sia stato generato
            tutto il resto
        # calcolare i labels
        #self.resetLabels() # riporta i labels a -1
           Con i followers non serve più

        _ = self.computeLabels(Sup)

        def checkOrt(s, e):
            """ In input una sorgente dello SPT e un
                edge scritto giusto
            """
            try:
                ann = self.AnnDict[e] # trova l'
                   annotazione dal dizionario
            except KeyError: # se non appartiene ai
               sentinel vale 0
                lab = 0
            else:
                lab = self.innerProd(Sup , ann) #
                   calcola il prodotto
```

```
        return (self.Labels[s,e[0]] + self.
            Labels[s,e[1]] + lab ) %2

    candidates = [] # lista di tuple (origine,
        NTE)

    # selezioniamo solo quelli non ortogonali
    candidates = [ x for x in self.NTE if
        checkOrt(x[0],x[1]) == 1 ]

    # generiamo i vettori dei cicli a partire da
        (source, non-tree edge)
    candidates = [ self.closeCycle(x[1], force=x
        [0]) for x in candidates ]

    # definiamo un metodo per calcolare la
        lunghezza di un ciclo
    def lenCycle(C):
        """ Calcola la lunghezza di un ciclo
            come prodotto scalare tra il
              vettore dei pesi self.WEdges e la
                descrizione del ciclo nella
              base self.Edges
        """
        return np.dot( self.WEdges , C)

    # list of tuples (ciclo, lunghezza)
    candidates = list(zip( candidates, map(
        lenCycle, candidates) ))

    if allDraws: # restituisce tutti i pareggi
        shortest = candidates[0][1]
        minList = []
        for x in candidates:
            if x[1] < shortest:
                minList = [x]
                shortest = x[1]
            elif x[1] == shortest:
```

```
                minList.append(x)
            else:
                pass
        return minList
    else: # trovane solo uno
        min_len = lambda x,y : x if x[1] <= y[1]
            else y
        minCycle = functools.reduce( min_len ,
           candidates )
        return minCycle

def cycleAnnotation(self, C):
    """ Calcola l'annotazione del ciclo C (somma
        delle ann degli edges)
    """
    # seleziona gli edges del ciclo
    C = map( lambda x: bool(x) , C) # rendilo
       bool
    edges = [ e for (e , filt) in zip(self.Edges
       , C) if filt ]
    ann = np.zeros( (self.dimH1,1), dtype = int
       )
    for e in edges:
        try:
            a = self.AnnDict[e]
            ann = (ann + a) % 2
        except KeyError:
            pass # se non è un sentinel fai
               nulla

    return ann

def updateSup(self, newC, index):
    """ Funzione che aggiorna i support vector
       per ogni nuovo ciclo minimo
        della base di omologia. Fa in pratica un
            Grahm-Schmidt in Z2
        Deve calcolare l'annotazione del ciclo.
```

```
            index deve andare da 0 a g-1
        """

        #print("Ciclo della SHB numero (i) = ",
           index)
        self.SHB.append( newC ) # aggiungi il nuovo
           ciclo
        #print( "Il nuovo ciclo è ", newC)
        #index = len(self.SHB) # indice del nuovo
           ciclo
        sup_i = self.Support[index] # support vector
            del nuovo ciclo
        #print( "Il support vector relativo è ",
           sup_i)
        AnnNewC = self.cycleAnnotation(newC) #
           annotazione del nuovo ciclo
        #print( "L'annotazione del nuovo ciclo è ",
           AnnNewC)
        for j in range(index+1,self.dimH1) : # per
           S_j da i+1 a g
            #print( "scorri su (j) = ", j)
            sup_j = self.Support[j]
            #print( "Sup_j = ", sup_j)
            #print( "Prodotto scalare = ", self.
               innerProd( AnnNewC , sup_j ))
            #print( "S_i * <C,S_j> = ", sup_i * self
               .innerProd( AnnNewC , sup_j ))
            #print( "S_j + S_i * <C,S_j> = ", ((
               sup_j + sup_i * self.innerProd(
               AnnNewC , sup_j )) % 2))
            self.Support[j] = (sup_j + sup_i * self.
               innerProd( AnnNewC , sup_j )) % 2 #
               somma ( =sottrae) la proiezione
        #print("Fine ciclo i = ",index)


    def run(self):
        """ Metodo che concatena tutti i passaggi e
```

```
    calcola la base minima di omologia

"""
pass
```

```
import math
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.lines as lines
from math import sin, cos, pi
from random import random
from SPT import SimplexGraph
import scipy.sparse
import time
from multiprocessing import Pool
from datetime import datetime
import _pickle as cPickle

filename = 'CElegansDataDump'
timestamp=str(datetime.now()).replace(" ", "h")
filename += timestamp
filename += '.dat'
print(filename)

def getTriangles(A):
    '''
    returns set of triangles in a graph given its
       adjacency matrix
    '''
    n = len(A)
    tri = []
    for vertex in range(n):
        vList = np.nonzero(A[vertex,vertex:])
        vList = [x for x in vList[1]] #NB: qui c'era
            uno zero che non faceva più funzionare l
           'algoritmo
        vList = [i + vertex for i in vList] #list of
            vertices adjacent to vertex
        for i in range(len(vList)-1):
            for j in range(i+1,len(vList)):
                if A[vList[i],vList[j]] > 0:
                    tri.append([vertex,vList[i],
                       vList[j]])
```

```
    return tri

def getD2(A, edgesList):
    '''
    returns 2-boundary matrix of the clique complex,
        given the adjacency matrix of the graph
    '''
    triangles = getTriangles(A)
   # print(triangles)

    d2 = []
    n = len(edgesList)
    #print(n)
    for row in triangles:
        newTriangle = [0 for i in range(n)]
        newTriangle[edgesList.index( (row[0],row[1]
           ) )] = 1
        newTriangle[edgesList.index((row[0],row[2])
           )] = 1
        newTriangle[edgesList.index( (row[1],row[2])
            )] = 1
        d2.append(newTriangle)
    d2 = np.array(d2)

    return d2


def points2adj(P, epsilon):
    '''
    given a set of points and a threshold returns
       the weight and adjacency matrix of the
       corresponding graph
    points is a list where each element is the
       coordinates of the point
    '''

    def dist(p1,p2):
        '''
```

```
            euclidean distance
            p1 and p2 need to be list of the same length
            '''
            return math.sqrt(sum([(p1[i]-p2[i])**2 for i
                in range(len(p1))]))

    n = len(P)
    W=np.zeros((n,n))
    for i in range(n):
        for j in range(i,n):
            W[i,j]= dist(P[i],P[j])
    W = W + W.T #weight matrix
    W[W >= epsilon] = 0

    A = (W >0).astype(int)
    return W , A

def filterMatrix(W,epsilon):
    Wb = np.matrix(W)
    Wb[Wb >= epsilon] = 0
    return Wb

def plotCycle(ax,cic,edList,P):
    for i in range(len(cic)):
        if cic[i] > 0:
            edge = edList[i]
            p1 = edge[0]
            p2 = edge[1]
            line = lines.Line2D([P[p1][0],P[p2
               ][0]],[P[p1][1],P[p2][1]],color='r')
            #line = lines.Line2D([P[edList[cic[i
               ]][0]][0],P[edList[cic[i]][1]][0]],[P
               [edList[cic[i]][0]][1],P[edList[cic[i
               ]][1]][1]], color='r')
            ax.add_line(line)

def sampleCircle(x0,y0,r,n, noise):
    P = []
```

```
    for i in range(n):
        theta = random()*2*pi
        R = r+noise*random()
        xp = x0 + R*cos(theta)
        yp = y0 + R*sin(theta)
        P.append([xp,yp])
    return P

def getEL(A):
    edgesList = []
    for i in range(len(A)):
        for j in range(i,len(A)):
            if A[i,j] > 0:
                edgesList.append([i,j])
    return edgesList

def plot_examples(SHBi,Wi,maximal, P):
    fig, ax = plt.subplots()

    x = [i[0] for i in P]
    y = [i[1] for i in P]
    ax.scatter(x,y)
    for row in getEL(Wi):
        line = lines.Line2D([P[row[0]][0],P[row
           [1]][0]],[P[row[0]][1],P[row[1]][1]])
        ax.add_line(line)
    for row in SHBi.T:
        row = row.tolist()
        row=row[0]
        plotCycle(ax,row,maximal[0],P)

    plt.show()
    return

def plot_filtration(SHB,Ws,maximal,data):
    for index in range(len(SHB)):
        plot_examples(SHB[index],Ws[index],maximal,P
           )
```

```
    return

def createRandomScatter(N, noise):
    P = []
    for i in range(N):
        x = noise * random()
        y = noise * random()
        P.append([x,y])

    return P

def parallel_pipeline(eps):
    W = GlobalOptions['Matrix']
    nVert = len(W)
    SHB = []
    Ws = []
    res = {}
    maximal = SimplexGraph.getEdgeList(W)
    stats = []
    Wstep = filterMatrix(W,eps)
    Ws.append(Wstep)
    G = SimplexGraph(nVert,Wstep, maximal)
    cycles = G.getCycleBase()
    stats.append( 'NVert = ' + str(G.NVert) + '
       NEdges = ' + str(G.NEdges) )
    stats.append( 'Filtration Eps = ' + str(eps) )
    stats.append( 'Keep all Draws = ' + str(
       GlobalOptions['Draws']) )
    t = time.time()
    d2 = getD2( Wstep , maximal[0] ) # ottiene d2 da
        Wstep ed edgelist
    (An, B1, Z1, H1) = G.getAnnotation(d2,cycles)
    elapsed = time.time()-t
    stats.append( 'H1= '+ str(H1) + ' B1= ' + str(B1
       ) + ' Z1= ' + str(Z1) )
    stats.append( 'Annotazione in sec ' + str(
       elapsed) )
    sup = np.eye( H1, dtype = int )
```

```
Sup = []
for i in range(H1):
    Sup.append( sup[:,i] )
G.Support = Sup
G.fixNTE() # precalcoliamo i non tree edges
t1 = time.time()
for i in range(H1):
    if GlobalOptions['Draws']:
        listMin = G.findShortestNonOrtho( G.
           Support[i] , allDraws=True)
        # scegli il primo per l'update
        mincycle = listMin[0][0]
        SHB.append(listMin)
    else:
        (mincycle, length) = G.
           findShortestNonOrtho( G.Support[i],
           allDraws=False )
    G.updateSup(mincycle, i)
elapsed = time.time() -t1
stats.append( 'Cicli minimi in sec ' + str(
   elapsed) )
if GlobalOptions['Draws']:
    res['SHB'] = SHB
else:
    res['SHB']=np.matrix(G.SHB).transpose()
res['Draws'] = GlobalOptions['Draws']
res['Filtration Eps'] = eps
if GlobalOptions['ReturnMatrix']:
    res['Filtered Matrix'] = Ws
else:
    res['Filtered Matrix'] = None
if GlobalOptions['ReturnMaximal']:
    res['Max'] = maximal
else:
    res['Max'] = None
res['stats'] = stats
return res
```

```
data = np.loadtxt("celegans_weighted_undirected.
   edges")
v1 = data[:,0]
v1 = np.array(v1, dtype=int)
v2 = data[:,1]
v2 = np.array(v2,dtype=int)
weights = data[:,2]
wmax = max(weights)
weights = [ float(wmax)/x for x in weights ]
weights = np.array(weights, dtype=float)
FullEpsList = list(set(weights))
NVert = max(max(v1),max(v2))
print("Numero vertici:",NVert)
print( "Min: ", min(weights), "Max: ", max(weights),
    "Total: ", len(weights), "Different: ", len(set(
   weights)))
plt.hist(weights, range(int(min(weights)), int(max(
   weights))))
print(FullEpsList)
v1 = np.array([x-1 for x in v1])
v2 = np.array([x-1 for x in v2])
# matrice dei pesi
W = scipy.sparse.coo_matrix((weights,(v1,v2)), dtype
   =float)
W = W.todense()
# I dati non sono SIMMETRICI!
W = (W+W.T)

GlobalOptions = {}
GlobalOptions['Matrix'] = W
GlobalOptions['Draws'] = False
GlobalOptions['ReturnMatrix'] = True
GlobalOptions['ReturnMaximal'] = True

file_stream = open(filename,'wb')
FullThreshList = [ x + 0.05 for x in FullEpsList ]
epsList = FullThreshList
cut = 306
```

```
Wn = W[0:cut,0:cut]
GlobalOptions['Matrix'] = Wn

pool = Pool(processes=4)
job = pool.map_async(parallel_pipeline, epsList)
result = job.get()

cPickle.dump(result, file_stream)
file_stream.close()

file_stream = open(filename,'rb')
restore = cPickle.load(file_stream)
file_stream.close()
print(restore[0].keys())
```

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