A Stratified Gradient Sampling Method for Co-Identification of Cycle Communities

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1 Motivation

In topological data analysis (TDA), matching topological signals is an active area of reseach [6, 8, 10]. At its core, matching the signals involves registering them to a topological template. Stratified Gradient Sampling (SGS) is a recently introduced procedure for registering topological objects to a common template [8]. The SGS method works by learning a *filter* function on the template such that it can faithfully recover all topological objects registered to it. After computing a topological template, the task of matching topological objects reduces to matching their topological features in the shared template space.
In the space of topological signal matching, an equally important concept is the "similarity" of signals within a given topological object or to a more general setting, across groups of topological objects. In this work, our interest is in the *cycle* structure of topological objects and the signals defined on them. By constructing cycle communities, we study the similarities of cycles within and across groups of topological objects. To this end, we extend the SGS procedure for learning a single filter function to learning a collection of filter functions simultaneously. We show that the collection of filter functions are optimal *cycle barycenter* functions, each of which can faithfully reconstruct a set of cycles. The set of cycles each filter function can reconstruct will be termed the cycle communities, where these communities are non-overlapping.

2 Preliminary on Topology

We provide a brief introduction to some topological concepts necessary for formulating our cycle community identification problem.

Graphs as Simplicial Complexes A k-simplex $\sigma_k = (v_0, \cdots, v_k)$ is a k-dimensional polytope of nodes $v_0, \cdots, v_k$. A simplicial complex K is a finite set of simplices such that for any $\sigma_k^i, \sigma_k^j \in K$, $\sigma_k^i \cap \sigma_k^j$ is a face of both simplices; and a face of any $\sigma_k^i \in K$ is also a simplex in K [5]. A 0-skeleton is a simplicial complex consisting of only nodes, whiles a 1-skeleton consists of nodes and edges. A k-chain is a finite sum of simplices. For two successive chain groups $\mathcal{K}_k$ and $\mathcal{K}_{k-1}$, the boundary operator $\partial_k : \mathcal{K}_k \longrightarrow \mathcal{K}_{k-1}$ for each σ_k is given by

$$\partial_k(\sigma_k) = \sum_{i=0}^{k} (-1)^i (v_0, \cdots, \widehat{v_i}, \cdots, v_k), \tag{1}$$

where $(v_0, \cdots, \widehat{v_i}, \cdots, v_k)$ gives the k-1 faces of σ_k obtained by deleting node $\widehat{v_i}$. Figure 1 provides an illustration of this chain mapping.
For the purposes of computation, the matrix representation $\mathbb{B}_k = (\mathbb{B}_k^{ij})$ of ∂_k is often defined as follows

$$\mathbb{B}_k^{ij} = \begin{cases} 1, & \text{if } \sigma_{k-1}^i \subset \sigma_k^j \text{ and } \sigma_{k-1}^i \sim \sigma_k^j \\ -1, & \text{if } \sigma_{k-1}^i \subset \sigma_k^j \text{ and } \sigma_{k-1}^i \nsim \sigma_k^j \\ 0, & \text{if } \sigma_{k-1}^i \not\subset \sigma_k^j \end{cases}, \tag{2}$$

where $\sim$ and $\nsim$ denote similar and dissimilar orientations respectively. Two important components of the boundary map (1) are its kernel $ker(\partial_k)$ and image $img(\partial_{k+1})$, which are subspaces of $\mathcal{K}_k$. The elements of $ker(\partial_k)$ and $img(\partial_{k+1})$ are known as *k-cycles* and *k-boundaries* respectively [7]. Graphs are 1D simplicial complexes. For graphs, $img(\partial_2) = \emptyset$ and the first homology module $\mathcal{H}_1 = \ker(\partial_1)$, whose elements are 1-cycles. For the remainder of this work, we will simply refer to the 1-cycles as cycles.

2.1 Filter Functions and Persistent Homology

The common approach to studying the persistence of homology generators is to construct a filtration on the set of 0-simplices (nodes). We adopt a slightly different approach in this work and define the filtration along the 1-simplices. By adopting this approach, we assume the homology generators are dependent on the connection relation (correlation, distance, among others) between any two points in the topological space. To properly develop the theory, we also restrict our exposition to one-dimensional simplicial complex. This stems from the fact that 1-cycles/loops can be fully identified from the one-dimensional simplicial complex. We start with the full simplex which we assume is a graph, and sequentially threshold.

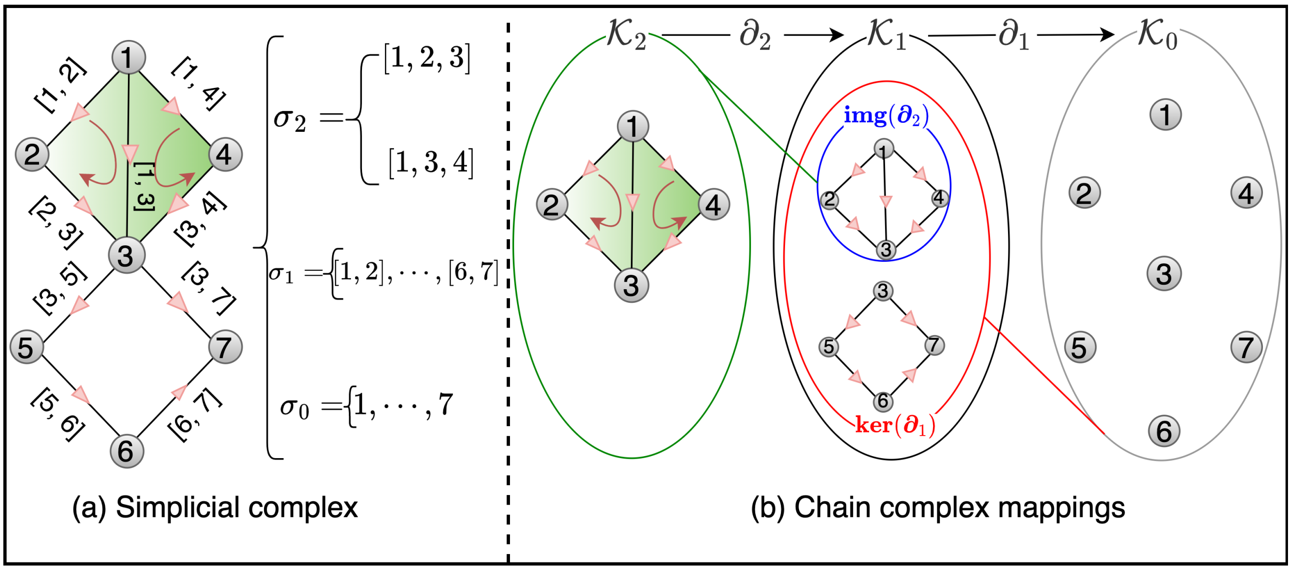

Fig. 1: (a) A 2-dimensional simplicial complex. (b) A chain complex mapping with boundary operators that map higher dimensional simplices to lower dimensional simplices.

Filtration A *filtration* defined on a simplicial complex K is a map $F : K \to \mathbb{R}^{|\mathcal{K}_1|}$. This map induces an inclusion relation of the simplicial complex K such that $K_{\epsilon_r} \subseteq K_{\epsilon_k}$ whenever $F(\epsilon_k) \geq F(\epsilon_r)$ where ϵ_k and ϵ_r are some indexes defined on the k-th and r-th 1-simplices respectively. F will be termed a *filter* function. For example, if the topological space under consideration is a graph, $F(\epsilon_k)$ could be the edge weight associated with that edge (1-simplex). The Figure 2 illustrates an example filtration over a one-dimensional simplicial complex with four nodes (0-simplices) and five edges (1-simplicies). For example, $w_{24} < w_{34} < w_{13} < w_{23} < w_{12}$ are ordered thresholds (edge weights). As we sequentially move along these thresholds, more 1-simplices are disconnected, increasing the number of connected components (β_0), and decreasing the number of 1-cycles (β_1). This increase in β_0 and decrease in β_1 is monotonic. To see the inclusion relation with the filter function F, observe that $F(\epsilon_5) = w_{24}$, and $F(\epsilon_4) = w_{34}$ which implies that $F(\epsilon_5) > F(\epsilon_4)$. Further observe that $K_{\epsilon_4} \subset K_{\epsilon_5}$ since K_{ϵ_4} includes all the 1-simplices in K_{ϵ_5} except that joining point 3 and 4. The filtration allows us to track the birth of connected components (0-cycles) and the death of 1-cycles over the span of the filtration values. The persistence of a connected component or 1-cycle that appears at filtration value b_i and disappears at filtration value d_i is represented by the interval $[b_i, d_i]$. The length of this interval characterizes the persistence (life-span) of the 0-cycles or 1-cycles. This characterization is formalized through the concept of persistent homology and is discussed in the next section.

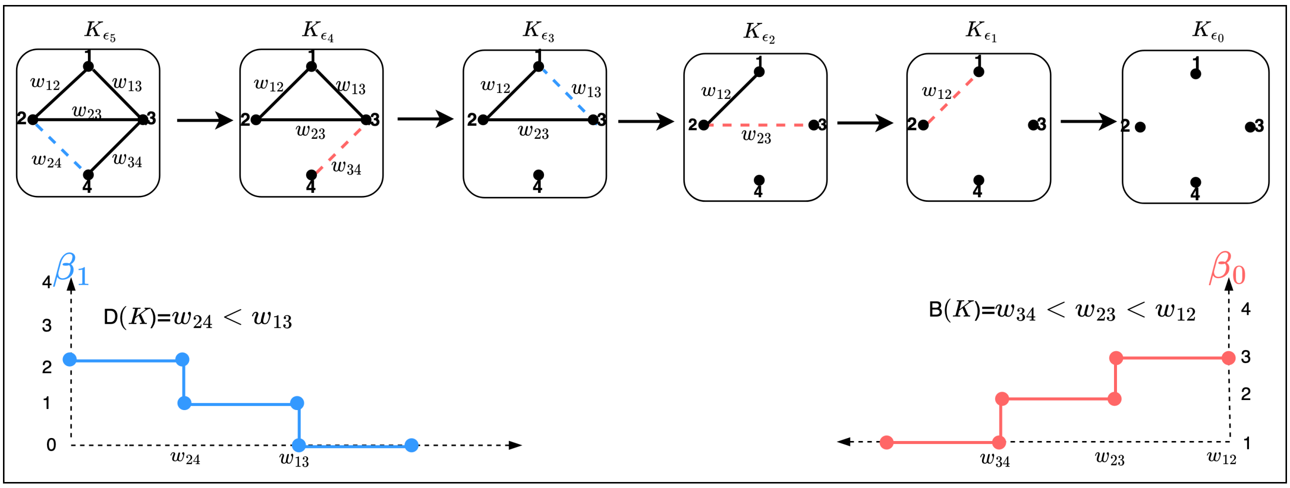

Fig. 2: An illustration of the filtration on a 1-dimensional simplicial complex. A dashed red or blue line indicates an edge that has been deleted. From top-left, the full simplicial complex which is sequentially thresholded to the point set(top-right). Bottom-left, the non-increasing count of the number of 1-cycles/loops. Bottom-right, the non-decreasing count of the number of connected components.

Persistent Homology The *Persistent Homology* (PH) is a framework for tracking the topological changes of K induced by the *filter function* F over the span of the filtration [4, 5]. More specifically, it tracks the filtration value b_i at which a cycle appears and the filtration value d_i at which the cycle disappears. A finite collection of $[b_i, d_i]$ can be summarized in the form of a *barcode* (Figure 2 bottom). For our filtration framework adopted, when a connected component is born, it never dies, hence it's lifespan is $[b_i, \infty)$. Similarly, all the 1-cycles are born when the graph is first formed and it's lifespan is represented as $(-\infty, d_i]$. For practical considerations, it is sufficient to replace the infinite values with the minimum and maximum filtration values, and it is the approach that will be adopted in this work. During the filtration, when an edge is deleted, a 0-cycle is formed or a 1-cycle dies. Both events can not occur at the same time [11]. The persistence of a cycle that appears at filtration value b_i and disappears at filtration value d_i is given by the interval $[b_i, d_i]$. A finite collection of $[b_i, d_i]$ can be summarized in the form of a *barcode*. Ignoring $\pm\infty$, the collection of birth values $B(\mathcal{X})$ and death values $D(\mathcal{X})$ can be represented as the 0D and 1D *barcode*:

$$B(K) = b_1 < b_2 < \cdots < b_p, \quad D(K) = d_1 < d_2 < \cdots < d_q. \tag{3}$$

The point $(b_i, d_i) \in \mathbb{R}^2$ is referred to as the *persistence interval*, and its length measures the persistence of a given cycle. Longer persistence indicates topological signal whiles shorter persistence might represent topological noise.

3 Method

The approach to our cycle community construction is to develop a topological optimization process through cycle registration. The cycle registration involves building optimization over PH within cycle generating strata. For this, we adopt the stratified gradient sampling approach introduced in [8]. We define a persistence map and prove that it is Lipschitz continuous. We state some differentiability results and present the convergence analysis. Finally, we present an algorithm for the cycle community construction.

3.1 Stratified Gradient Sampling

The concept of stratified sampling is ubiquitous in machine learning. It mostly used to create a test set in a small-sample machine learning problem. Gradeint sampling is a methodology to extend the steepest descent method of minimizing smooth functions to nonsmooth and potentially nonconvex functions. The main idea is to compute an approximate differential of nonsmooth functions by sampling gradients. When this gradient sampling is restricted to strata of a given space, it is term the stratified gradient sampling. We introduce some of the key concepts used in developing this stratified gradient sampling methodology.

Smooth Stratifiable Functions In topology, stratification involves the partitioning of a topological space. Recall that our main topological objects, graphs (one-dimensional simplicial complexes) are topological spaces. The goal here is to achieve some sense of smoothness for functions defined on the various strata. More formally, consider the stratification of the topological space $K = \{K_n\}_{n \in N}$. Let f be a function from K to the real line, and f_n a restriction of f to the stratum K_n. Then $f : K \to \mathbb{R}$ is deemed a smooth stratifiable function if f_n is twice continuously differentiable in a neighborhood of K_n. Other formal definitions of stratifiable functions exists, in particular, a popular one is the Whitney stratification which requires $\{K_n\}_{n \in N}$ to be Whitney [1]. The smoothness of f restricted to each stratum guarantees that we have a unique limit of the gradient $\nabla f_n(\sigma_l \in K_n)$ given by $\nabla K_n f(\sigma)$ as long as σ_l (a sequence of subsets of K) converges to $\sigma \in K_n$. Given these limit guarantees, we present a gradient descent algorithm for smooth stratifiable functions.

Gradient Descent on Smooth Stratifiable Functions The direction of steepest descent for a function f with non-zero differential at a point say σ is often denoted as $-\nabla f(\sigma)$. This can be obtained via the minimization

$$\arg\min_{||\mathbf{u}||_2 \leq 1} \nabla f(\sigma)^\top \mathbf{u} = -\frac{\nabla f(\sigma)}{||\nabla f(\sigma)||_2}. \tag{4}$$

Notice the slight abuse of notation here, as f is not necessarily the smooth stratifiable function defined in the previous section. We will make this distinction in further expositions below. The assumption on f is that it is smooth and convex. When the differentiability condition $\nabla f(\sigma) \neq 0$ is not satisfied, $-\nabla f(\sigma)$ is no longer the direction of steepest descent, and only small decreases are recorded along this direction. To provide a workaround to this, the gradient sampling solve (approximately) a min max optimization problem and obtaining the direction of descent. More formally, for a δ-subdifferential of f (where f i snow taken to be a smooth stratifiable function) at σ given by $\bar{\partial}_\delta f(\sigma)$, the descent direction is obtained by solving the min max problem

$$\min_{||\mathbf{u}||_2 \leq 1} \max_{g \in \bar{\partial}_\delta f(\sigma)} g^\top \mathbf{u}. \tag{5}$$

Observe that $\bar{\partial}_\delta$ is a convex set, hence the descent direction will be a projection of the origin on this set. In particular, we have that $\langle g(\sigma, \delta), g(\sigma, \delta) - g \rangle \leq 0$ where the descent direction is obtained from (5) and have the explicit form

$$g(\sigma, \delta) = \arg\min\{||g||_2^2, g \in \bar{\partial}_\delta f(\sigma)\}. \tag{6}$$

The following proposition summarizes the descent property of the direction $g(\sigma, \delta)$ of the smooth stratifiable function f.

Proposition 1 *Let $\mathbb{B}(\sigma, \delta_0)$ be a ball such that the gradients of the function restrictions f_n to it have a Lipschitz constant L. The function restriction f_n is with respect to the base function f which is assumed to be stratifiably smooth. Then for any $0 < \alpha < 2L$, and a non-stationary point δ, the following two conditions holds:*

(i) If we choose δ small enough, we have the upper bound $\delta \leq \frac{1}{\alpha}||g(\sigma, \delta)||_2$.
(ii) Given the upper bound in (i), it follows that $f(\sigma - \gamma g(\sigma, \delta)) \leq f(\sigma) - \gamma||g(\sigma, \delta)||_2^2$ for all $\gamma \leq \frac{\delta}{||g(\sigma,\delta)||_2}$.

This proposition is a derivative of the Lebourg Mean value Theorem, and the proof also follows directly from this theorem [3]. For a given δ-neighborhood the convex set $\bar{\partial}_\delta f(\sigma)$ will consists of infinitely many gradients, hence we will work with the assumption that, the gradient information in $\bar{\partial}_\delta f(x)$ are δ-close to σ. We now present a computational heuristic for the stratified gradient sampling in Algorithm 2. In the algorithm, we will make the assumption that the iterates are points of differentiability with respect to f otherwise a small perturbation can be added to make it a point of differentiability. The α in Proposition1 controls the rate of descent. A couple

Algorithm 1 A Stratified Gradient Sampling Algorithm for f

Require: Stratifiably smooth function f, initial iterate σ_0, initial sampling radius δ, a constraint on the exploration radius C_0, descent rate α, step size decay η, termination tolerance $(\delta_{opt}, \nu_{opt}) \in [0, \infty) \times [0, \infty)$.
Ensure: $0 < \alpha \leq 2L$, $\delta > 0$, $0 < \eta < 1$.

for $k \in \mathbb{N}$ **do**
  $C_{k+1} \leftarrow C_k$
  $\delta_{k+1} \leftarrow \delta$
  $\gamma_{k+1} \leftarrow \gamma_k$
  while $f(\sigma_k - \gamma_k g(\sigma_k, \delta_k)) > f(\sigma_k) - \gamma||g(\sigma_k, \delta_k)||_2^2$ and $\delta_k > C_{k+1}||g(\sigma_k, \delta_k)||_2$ **do**
    Independently sample $\{\sigma_k^1, \cdots, \sigma_l^m\}$ from $\mathbb{B}(\sigma_k, \delta_k) = \{\sigma : ||\sigma - \sigma_k||_2 \leq \delta_k\}$
    $\mathcal{G}_k \leftarrow conv\{\nabla f(\sigma_k), \nabla f(\sigma_k^1), \cdots, \nabla f(\sigma_k^m)\}$ ▷ This will eventually converge to the δ_k-subgradients $\bar{\partial}_{\delta_k} f(\sigma_k)$.
    $g(\sigma_k, \delta_k) \leftarrow \arg\min\{||g||_2^2, \quad g \in \mathcal{G}_k\}$
    if $||g(\sigma_k, \delta_k)|| \leq \nu_{opt}$ and $\delta_k \leq \delta_{opt}$ **then** terminate
    end if
    $\gamma_k \leftarrow \frac{\delta_k}{||g(\sigma_k, \delta_k)||_2}$
    $\delta_k \leftarrow \eta\delta_k$ ▷ Reduction in sampling radius
  end while
  $\sigma_{k+1} \leftarrow \sigma_k - \gamma_k g(\delta_k, sogma_k)$ ▷ It might be necessary to perturb σ_{k+1} such that $\nabla f(\sigma_{k+1}) \neq 0$
  if $||g(\sigma_k, \delta_k)|| \leq \nu_{opt}$ and $\delta_k \leq \delta_{opt}$ **then** terminate
  end if
end for

of remarks about Algorithm 2. The $conv(.)$ is just the convex hull of the gradients from the remote strata. This algorithm is also quite similar to the gradient sampling algorithm presented in [2]. A more elaborate set of algorithms that accomplishes a similar sampling scheme can be found in Algorithm 2 - Algorithm 6 of the recent paper [8]. The development in this section lays both the theoretical and practical foundations for optimizing persistence maps which falls in the class of nonsmooth and nonconvex functions but can be made stratifiably smooth. The optimization over these persistence maps is required for our cycle community construction and will presented in the next section.

3.2 Topological Centroid Registration

We introduce the concept of topological centroid registration. The main idea is to find a cycle centroids of one-dimensional simplicial complexes (graphs). Since each cycle is a sub-complex, the process is akin to finding the the topological barycenter of a collection of subcomplexes.

The exposition in this section will be restricted to the one-dimensional simplicial complex K and its first homology group/module $\mathcal{H}_1$. Since $\mathcal{H}_1$ is fully characterized by $D(K)$, the 1D-barcode, any reference to a barcode will be assumed to be $D(K)$. We define a persistence map $PH(.)$ that takes values from K to $D(K)$ through the filter function F. This involves transforming $D(K)$ into a metric space by equipping it with the Wasserstein distance. Let ϕ be a bijective map between two barcodes D_1 and D_2 with the form $\phi : D1 \to D_2$. The p-th Wasserstein distance between two diagrams has the form

$$W_p(D_1, D_2) = \inf_{\phi} \left(\sum_{(b,d)\in D} ||\phi(b,d) - (b,d)||_2^p \right)^{1/p}. \tag{7}$$

We observe that under the filtration approach adopted in this work, this distance admits a simplified form for $p = 2$ summarized in the proposition below.

Proposition 2 *Let D_1 and D_2 be two sets of barcodes defined according to (3). The 2-Wasserstein distance between D_1 and D_2 admits the simplified form*

$$W_2(D_1, D_2) = \inf_{\phi} \left(\sum_{(b,d)\in D} ||\phi(b,d) - (b,d)||_2^2 \right)^{1/2} = \left(\sum_{j=1}^{q} |d^1_{(j)} - d^2_{(j)}|^2 \right)^{1/2}, \tag{8}$$

where $d^1_{(j)}$ and $d^2_{(j)}$ are the j-th ordered values of the death times in D_1 and D_2 respectively.

The proof is a direct consequence of order statistics, since by the assumption of our filtration, all the cycles are formed when the simplex is first created hence have the same birth values. This allows us to simply sort and match the death values. Following from this, we have the map $PH : K \to D(K)$ is Lipschitz continuous, and is a result of the stability results associated with persistence diagrams [5]. In what follows, any discussion of the p-Wasserstein distance will be the context of $p = 2$. It remains to show that the filter functions are stratifiably smooth.

Consider a map from the set of barcodes $D(K)$ to the real line: $U : D(K) \to \mathbb{R}$. The differentiability of U is guaranteed by some results on the differentiability of persistence functions established in [9]. From this it follows that a filter function F can be written as the composition of PH and U, i.e., $F = UoPH$, and it is in fact a stratifiably smooth function from our previous discussions. This now allows us to optimize over this set of filter functions using the stratified gradient sampling method introduced detailed in Algorithm 2. The centroid registration can be summarized as follows.

Let $\mathcal{C}_K \in \mathcal{H}_1$, $k = 1, \cdots, \mathcal{Q}$ be the set of cycles, where $\mathcal{Q}$ is the cardinality of the basis cycles in $\mathcal{H}_1$. Define $\mathbb{F} = \{F_1, \cdots, F_{\mathcal{Q}}\}$ to be the set of filter functions, each corresponding to $\mathcal{C}_k$. Let $\mathcal{C}'_r$, $r = 1, \cdots, \mathcal{P}$ be a set of template cycles such that $\mathcal{P} \ll \mathcal{Q}$. We can learn a set of filter functions $\mathbb{F}' = \{F'_1, \cdots, F'_{\mathcal{P}}\}$ such that

$$\sum_{r=1}^{\mathcal{P}} \sum_{k=1}^{\mathcal{Q}} W_p \left(PH(F'_r, \mathcal{C}'_r), PH(F_k, \mathcal{C}_k^{(r)}) \right) \tag{9}$$

is minimized. $W_p(.,.)$ is the p-th Wasserstein metric between the persistence intervals [12], and $\mathcal{C}_k^{(r))}$ is used to denote that it can faithfully be reconstructed from the filter function F'_r. Since the optimization is over a filter functions which are established to stratifiably smooth, by Proposition 1, we are guaranteed this will converge to a stationary point. The set $\mathbb{F}' = \{F'_1, \cdots, F'_{\mathcal{P}}\}$ can be regarded as the cycle barycenters. These barycenters (centroids) can be used to construct cycle communities in a similar fashion as k-means clustering.

3.3 Cycle Communities Construction

We now present an algorithm for obtaining the cycle communities based on the optimization problem stated in (9). The algorithm construction follows similar dynamics as in k-means clustering. A full-blown convergence analysis is required to establish any convergence results but a cursory glance indicates that it will always converge to local stationary point. Further observe that this algorithm assumes a single homology group. However, it can easily be extended to multiple homology across for comparison across objects by simply combining the homology groups. We now demonstrate the application of this concept cycle communities construction through a simulation study.

Algorithm 2 Cycles Communities Construction

Require: Cycle basis or homology basis generators $\mathcal{C}_K \in \mathcal{H}_1$, $k = 1, \cdots, \mathcal{Q}$. Choose initial centroids $\mathcal{C}'_r$, $r = 1, \cdots, \mathcal{P}$, numerical stopping criteria w.

Ensure: $\mathcal{P} \leq \mathcal{Q}$, and $w > 0$

while $\sum_{r=1}^{\mathcal{P}} \sum_{k=1}^{\mathcal{Q}} W_p \left(PH(F'_r, \mathcal{C}'_r), PH(F_k, \mathcal{C}_k^{(r)}) \right) > w$ **do**

  Register the $\mathcal{Q}$ cycles to centroid simplex $\mathcal{C}_k^{(r)} \leftarrow W_p \left(PH(F'_r, \mathcal{C}'_r), PH(F_k, \mathcal{C}_k^{(r)}) \right)$

  Assign the cycles to centroid groups where $\sum_{r=1}^{\mathcal{P}} W_p \left(PH(F'_r, \mathcal{C}'_r), PH(F_k, \mathcal{C}_k^{(r)}) \right)$ is minimal

end while

4 Experiments

We demonstrate our cycle community construction concept through a simulation study by comparing . The three topological spaces used in this simulation are modelled after the skeletons of Tropaeolum, Chardonnay and Cabernet (Figure 3-top). Eighteen points were specifically chosen at cordinates (Figure 3-bottom) along

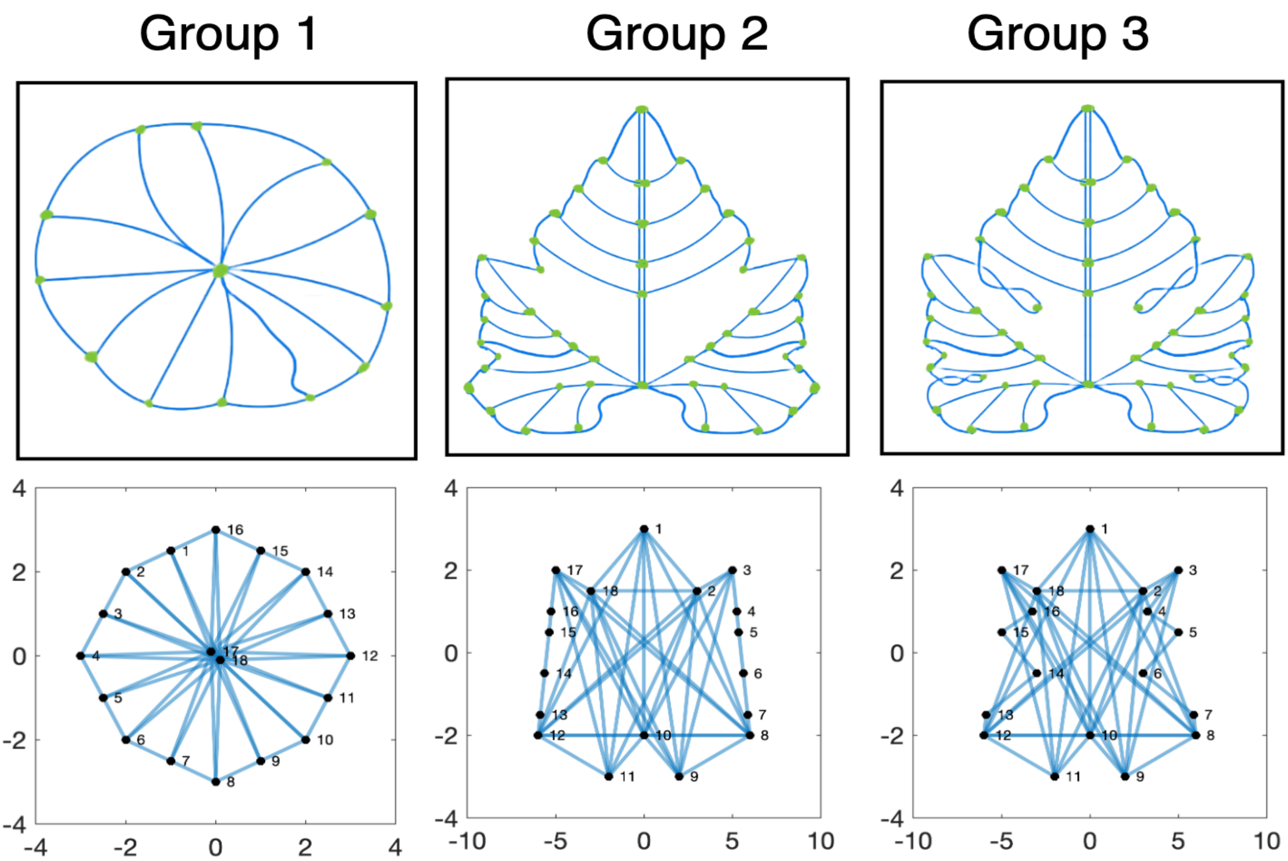

Fig. 3: The topological spaces used in the simulation. Group 1 (Tropaeolum) is topologically different from Group 2 and Group 3. Group 2 (Chardonnay) is topologically equivalent to Group 3 (Cabernet).

these skeletons and perturbed with noise $N(0, 0.025)$, and seven networks were generated in each group. Group 1 is expected to have much different first homology group $\mathcal{H}_1$ (cycles) compared to Group 2 and Group 3. Group 2 and Group 3 will however have similar cycles since their first homology generators will be quite close by the construction of the simulation. In running the experiment, we expect two distinct communities with the potential for a non-influential third community. The first major community should primarily be made up of the cycles in Group 1 and the second major community should primarily be made up of the cycles in Group 2 and Group 3.

Partial results confirm the clustering pattern expected in our experimental design.

5 Conclusion

This project demonstrates the power of combining gradient descent, subsampling methods to the novel concept of cycle communities construction. Preliminary experimental results demonstrates the efficacy of the proposed methodology. A much elaborate theoretical development and experimental runs will more reinforce these realizations and it will be an exciting area of exploration in the future.

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