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TOPOLOGICAL INVARIANTS OF WEIGHTED SIMPLICIAL COMPLEXES AND THEIR APPLICATIONS IN DATA CLUSTERING

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ABSTRACT

Clustering algorithms built on distance thresholds or centroid geometry often fail when data lies on curved manifolds, contains multi-scale structure, or exhibits noise that distorts local density estimates. This paper investigates whether topological invariants derived from weighted simplicial complexes - specifically Betti numbers, persistence diagrams, and Euler characteristics computed across a filtration of edge weights - can serve as a more stable basis for cluster identification than conventional distance-based methods. A weighted Vietoris-Rips complex was constructed from five benchmark datasets spanning synthetic and real-world domains, and persistent homology was computed at successive filtration values to extract zeroth and first-order Betti numbers. These invariants were then used to define a topological clustering criterion, compared against k-means, DBSCAN, and spectral clustering using adjusted Rand index and silhouette scores. Results indicate that topology-based clustering achieved a mean adjusted Rand index of 0.81 across the five datasets, compared with 0.64 for k-means and 0.71 for DBSCAN, with the largest gains observed on datasets containing non-convex or nested cluster shapes. Persistence diagrams also proved more resistant to Gaussian noise injection, retaining stable Betti-1 counts up to a noise variance of 0.15 where distance-based methods degraded sharply. These findings support the proposition, stated at the outset, that weighted simplicial complexes encode structural information about data shape that persists across scale and noise in ways centroid- or density-based methods cannot capture, and they suggest a practical pathway for incorporating topological data analysis into standard clustering pipelines without prohibitive computational cost for datasets under approximately 2,000 points.

Keywords: *Persistent homology[1]; Weighted simplicial complex[2]; Betti numbers[3]; Topological data analysis[4]; Data clustering[5]; Vietoris-Rips filtration[6]; Euler characteristic[7].*

1. INTRODUCTION

1.1 BACKGROUND AND MOTIVATION

Clustering remains one of the oldest problems in exploratory data analysis, yet the algorithms in widest use - k-means, hierarchical agglomeration, DBSCAN - rest on assumptions about geometry that real data frequently violates. k-means assumes roughly spherical, equally sized clusters in Euclidean space; DBSCAN depends on a

single density threshold that struggles when clusters vary in density; spectral methods require a well-chosen similarity kernel whose bandwidth is rarely obvious in advance. When data has intrinsic curvature, when clusters are nested inside one another, or when the boundary between groups is defined by connectivity rather than proximity, these methods can misclassify structure that is visually obvious to a human observer. Topological data analysis (TDA) offers a different starting point. Rather than asking how close points are to each other in a fixed metric, TDA asks what shape the data traces out as a similarity threshold is varied continuously, and it records which features of that shape - connected components, loops, voids - persist across a wide range of thresholds rather than appearing only briefly. Persistent homology, the central tool of TDA, has been applied to sensor networks, protein folding, and neural activity, but its use as a direct clustering criterion, rather than as a preprocessing or visualization step, is comparatively underexplored, and that gap motivates the present study.

1.2 THE ROLE OF WEIGHTED SIMPLICIAL COMPLEXES

A simplicial complex generalizes a graph: where a graph has vertices and edges, a simplicial complex also has triangles, tetrahedra, and higher-dimensional simplices, each one representing a group of points that are mutually close under some criterion. Assigning weights to these simplices - typically the pairwise distances that generated them - turns the complex into a filtered object: at a low threshold only, the nearest neighbors are connected, and as the threshold increases, edges and higher simplices are added until the complex becomes a single connected blob. Tracking the birth and death of topological features across this filtration produces a persistence diagram, and the features that survive across a long range of thresholds are generally interpreted as genuine structure rather than noise. The zeroth Betti number, Beta-0, counts connected components and directly corresponds to a partition of the data into clusters at each threshold; the first Betti number, Beta-1, counts independent loops, which can indicate ring-shaped or annular substructure that centroid-based methods routinely miss. This paper treats the sequence of Beta-0 values across a filtration, together with their persistence lengths, as the primary clustering signal, an approach that shifts the clustering decision from a single fixed parameter to a multi-scale topological summary.

1.3 SCOPE AND CONTRIBUTION OF THIS STUDY

This study restricts itself to five datasets of moderate size, chosen to represent a spread of geometric difficulty: two synthetic sets with known non-convex cluster shapes, two tabular real-world datasets from public repositories, and one dataset drawn from sensor-style time-aligned measurements. The contribution is threefold. First, it provides a reproducible procedure for constructing weighted Vietoris-Rips complexes and extracting Betti-number sequences suitable for clustering rather than purely descriptive analysis. Second, it proposes a concrete decision rule - selecting the filtration value at which Beta-0 stabilizes over the longest interval - for converting a persistence diagram into an actual partition of the data, addressing a practical gap in much of the TDA literature, which stops at visualization. Third, it benchmarks this rule quantitatively against three widely used clustering algorithms on the same five datasets under identical noise conditions, giving a direct empirical answer to whether the added computational and conceptual overhead of TDA is justified in practice, at least at the data sizes tested here.

2. SURVEY OF RELATED WORK

Persistent homology entered mainstream data science through the work of Edelsbrunner and Harer, who formalized the notion of a persistence diagram as a multiset of birth-death pairs summarizing the topological evolution of a filtered simplicial complex; their treatment established most of the algorithmic machinery - boundary matrices, reduction algorithms, and the stability theorem bounding how much a diagram can change under small perturbations of the input - that later applied work relies on.Carlsson's survey extended this into an argument for TDA as a general-purpose tool for qualitative data analysis, emphasizing that topological summaries are invariant under smooth deformation and therefore capture structure that resists simple rescaling or projection artifacts, a property directly relevant to clustering where the correct metric is often unknown.Ghrist provided an accessible geometric treatment of simplicial homology aimed at engineers and applied scientists, and this framing - homology as a way of counting holes rather than as pure algebra - underlies much of the applied TDA literature that followed, including the present paper's use of Betti numbers as an interpretable clustering signal rather than an abstract invariant.

Within clustering specifically, several authors have proposed hybrid approaches. Chazal et al. developed a framework connecting persistence-based clustering to mode-seeking methods, showing that a cluster tree derived from the sublevel sets of a density estimator can be stabilized using persistence, effectively filtering out spurious modes that arise from sampling noise. this line of work is close in spirit to the present paper but operates on density functions rather than directly on the simplicial complex of pairwise distances. Rieck and Leitte examined the sensitivity of persistence diagrams to parameter choices in high-dimensional data and cautioned that naive application of Vietoris-Rips filtrations to high-dimensional point clouds can produce misleading results because of the curse of dimensionality affecting distance concentration. a caution this paper takes seriously by restricting its real-world datasets to low or moderately reduced dimensionality. Singh, Memoli, and Carlsson introduced the Mapper algorithm, which builds a simplified topological skeleton of high-dimensional data using overlapping clusters within filtered bins. And Mapper has since become one of the most widely deployed TDA tools in applied settings, though it depends on several user-chosen parameters - filter function, resolution, overlap - that can materially change the resulting graph, a dependency this paper's Betti-number approach attempts to reduce by relying on a single filtration parameter, edge weight.

More recent work has attempted direct comparison between topological and conventional clustering. Kovacev-Nikolic et al. applied persistent homology to protein conformational data and found that topological summaries distinguished conformational states that Euclidean clustering conflated, an early demonstration that geometry-based clustering can fail on manifold-valued data even when the underlying groups are well separated in a topological sense.Umeda applied persistence-based features as inputs to a downstream classifier for time-series data rather than as a clustering rule in its own right, illustrating a common pattern in the literature: topology as a feature-engineering step feeding a separate learning algorithm, rather than as the clustering mechanism itself. This paper departs from that pattern by using the Betti-number sequence directly as the partitioning criterion. Weighted simplicial complexes specifically, as opposed to the more common unweighted or binary adjacency versions, have received comparatively less systematic benchmarking against standard clustering baselines using paired metrics such as adjusted Rand index across multiple dataset types.and it is this specific comparison -

weighted-complex topology versus k-means, DBSCAN, and spectral clustering, on the same data, under controlled noise - that the present study is designed to fill.

3. METHODOLOGY

Five datasets were selected to test the clustering procedure across a spread of geometric difficulty: two synthetic two-dimensional sets (concentric rings and interleaving crescents, generated with controlled Gaussian noise), two tabular datasets from public repositories (a customer-segmentation dataset with eight numeric features and an iris-style morphological dataset), and one dataset of accelerometer-style time-windowed sensor readings aggregated into feature vectors. For each dataset, points were embedded in their native feature space (or a PCA-reduced two- to five-dimensional space where the native dimensionality exceeded ten, following the caution raised in the survey regarding distance concentration), and pairwise Euclidean distances were computed to serve as edge weights. A weighted Vietoris-Rips complex was then built incrementally: starting from a filtration value of zero, edges were added in order of increasing weight, and higher-order simplices (triangles, tetrahedra) were added whenever all their constituent edges were already present in the complex, following the standard Vietoris-Rips construction rule. At each filtration step, the number of connected components (Beta-0) and independent one-dimensional cycles (Beta-1) were recorded using a union-find structure for Beta-0 and a boundary-matrix reduction for Beta-1, implemented following the standard persistent homology reduction algorithm. This produced, for each dataset, a persistence diagram summarizing the birth and death filtration values of every topological feature.

Cluster assignment was derived from this diagram using a stability rule: the filtration interval over which Beta-0 remained constant for the longest stretch was identified, and the connected components at the midpoint of that interval were taken as the final cluster labels. This choice avoids the need to pre-specify the number of clusters, in contrast to k-means, while still producing a single partition rather than a hierarchy. Noise robustness was tested by injecting Gaussian perturbations of increasing variance (0.05 to 0.30 in steps of 0.05) into each dataset and repeating the full pipeline, recording at what noise level the stable Beta-0 interval collapsed to fewer than three filtration steps. All comparison algorithms - k-means (with k fixed to the ground-truth cluster count), DBSCAN (with epsilon selected via k-distance elbow), and spectral clustering (with an RBF kernel, bandwidth chosen via median heuristic) - were run on the identical noise-perturbed datasets to keep the comparison controlled.

3.1 THEORETICAL FOUNDATIONS: STABILITY AND BETTI NUMBER COMPUTATION

The empirical robustness of persistence-based clustering documented in Section 4 follows from a precise stability property of persistent homology, stated and proved here, together with the combinatorial basis for computing Betti numbers from the Vietoris-Rips filtration. Definition. Given a finite point set X with a filtration function $f: X \times X \to \mathbb{R}$ (here, pairwise distance), the weighted Vietoris-Rips complex at scale t, $\mathrm{VR}_t(X)$, has a k-simplex {x_0..., x_k} whenever all pairwise distances among x_0, x_k are at most t. The persistence diagram D(X) records the birth and death scale of each homological feature (connected component for degree 0, independent loop for degree 1) as t increases from 0 to infinity. Proposition 1 (Betti-0 as Graph Connectivity). For any fixed t, the zeroth Betti number $\beta_0\big(\mathrm{VR}_t(X)\big)$ equals the number of connected components of the 1-

skeleton graph $G_t = (X, \{\text{edges } (x_i, x_j) : d(x_i, x_j) \leq t\})$, independent of the higher-dimensional simplices in $\text{VR}_t(X)$.

Proof. The zeroth simplicial homology group H_0 of any simplicial complex K is generated by the vertices of K modulo the boundary relations induced by its edges: two vertices lie in the same homology class if and only if they are connected by a path of edges in the 1-skeleton of K, since the boundary map partial_1 sends an edge to the difference of its two endpoint vertices, and the image of partial_1 exactly identifies vertices joined by an edge. Because higher-dimensional simplices of $\text{VR}_t(X)$ (triangles, tetrahedra) have boundary maps that only involve edges and vertices already present in the 1-skeleton, they contribute no additional relations to H_0. Hence $H_0(\text{VR}_t(X))$ has rank equal to the number of connected components of the 1-skeleton graph G_t, which is precisely $\beta_0(\text{VR}_t(X))$, establishing the claim and justifying the paper's practice of tracking Beta_0 directly as a partition of the data into clusters at each filtration value.

Theorem 1 (Stability of Persistence Diagrams). Let f, g: X -> R be two filtration functions on the same underlying simplicial complex (for instance, distances computed under two slightly different metrics or after a bounded perturbation of the data), and let D(f), D(g) denote the resulting persistence diagrams. Then the bottleneck distance between the diagrams satisfies $d_B(D(f), D(g)) \leq \|f - g\|_\infty$ infinity, where $\{f \leq t - \epsilon\}$ infinity is the supremum norm of the difference between the two filtration functions over all simplices. Proof sketch. This is the celebrated stability theorem of Cohen-Steiner, Edelsbrunner, and Harer, whose argument proceeds by constructing an explicit epsilon-matching between the two diagrams using the interleaving of the sublevel-set filtrations induced by f and g: since $|f(\sigma) - g(\sigma)| \leq \|f - g\|_\infty$infinity for every simplex sigma, the sublevel-set complex $\{g \leq t\}$ is contained in {g <= t} which is contained in {f <= t + epsilon} for $\{f \leq t + \epsilon\}$ for $\epsilon = \|f - g\|_\infty$ infinity, and this sandwich relation propagates through the persistence modules via the algebraic stability of interleaved persistence modules, yielding a matching between the diagrams' points that moves each point by at most epsilon in the plane, which is by definition an upper bound of epsilon on the bottleneck distance. Applied to the present setting, this theorem is precisely why Betti-1 counts remain stable up to a Gaussian noise variance of 0.15 as reported in the abstract: since Gaussian perturbation of the point cloud changes pairwise distances, and hence the filtration function, by an amount controlled in expectation by the noise standard deviation, the resulting persistence diagram moves by a correspondingly bounded amount in bottleneck distance, explaining the observed noise-resistance of topology-based clustering relative to distance-threshold methods that lack any comparable stability guarantee.

Proposition 2 (Euler Characteristic Consistency Check). At every filtration value t, the alternating sum of simplex counts in VR_t(X) equals the alternating sum of Betti numbers: $\chi(\text{VR}_t(X)) = \#\text{vertices} - \#\text{edges} + \#\text{triangles} - \cdots = \beta_0(t) - \beta_1(t) + \beta_2(t) - \cdots$, and this identity was used throughout Section 4 as an internal consistency check on the computed persistence diagrams, since any discrepancy between the directly counted alternating simplex sum and the alternating sum of computed Betti numbers at a given t signals either a numerical error in the boundary-matrix reduction algorithm or an incomplete simplex enumeration, and no such discrepancy was observed across the five benchmark datasets at any tested filtration value.

4. DATA COLLECTION AND ANALYSIS

Data for the two synthetic sets were generated programmatically (500 points per set, ground-truth labels retained for scoring); the two tabular datasets were drawn from public repositories with sample sizes of 440 and 300 respectively after removing rows with missing values; the sensor dataset comprised 620 windows of aggregated accelerometer features. Table 1 summarizes the raw structural properties of each dataset prior to any clustering being applied.

Table 1. Dataset characteristics

Dataset	Points (n)	Features (native)	Features (used)	Ground-truth clusters	Shape complexity
Concentric rings (synthetic)	500	2	2	2	Non-convex, nested
Interleaving crescents (synthetic)	500	2	2	2	Non-convex
Customer segmentation	440	8	4 (PCA)	4	Mixed density
Morphological (iris-style)	300	4	4	3	Mildly overlapping
Sensor windows	620	12	5 (PCA)	3	High noise floor

The five datasets differ enough in shape and dimensionality that no single baseline algorithm would be expected to dominate across all of them, which is precisely the point of including them together. Table 2 reports the Betti-number persistence summary extracted for each dataset - specifically, the longest stable Beta-0 interval and the number of Beta-1 features whose persistence exceeded 10% of the filtration range, treated as a proxy for genuine loop structure rather than noise.

Table 2. Persistent homology summary per dataset

Dataset	Stable Beta-0 interval (% of range)	Beta-0 at stable interval	Significant Beta-1 features	Interpretation
Concentric rings	38%	2	2	Two nested loops correctly separated
Interleaving crescents	29%	2	0	Non-convex arcs resolved, no loop artifact
Customer segmentation	22%	4	1	Matches ground truth; one spurious minor loop
Morphological	31%	3	0	Clean match to known species groupings
Sensor windows	14%	3	3	Shortest stable interval; reflects sensor noise floor

The shortest stable interval belongs to the sensor dataset, consistent with the residual jitter present in aggregated accelerometer windows - the topological method is not immune to noise, only more resistant to it up to a point, a distinction developed further in the discussion. Table 3 presents the primary comparative result: adjusted Rand index (ARI) and silhouette score for the proposed topological method against the three baselines, computed on the clean (non-perturbed) versions of each dataset.

Table 3. Clustering performance comparison (clean data)

Dataset	Topological ARI	k-means ARI	DBSCAN ARI	Spectral ARI	Topological Silhouette
Concentric rings	0.94	0.31	0.88	0.9	0.61
Interleaving crescents	0.89	0.42	0.79	0.85	0.55
Customer segmentation	0.77	0.71	0.68	0.74	0.48
Morphological	0.83	0.8	0.76	0.81	0.57
Sensor windows	0.62	0.58	0.44	0.55	0.39
Mean	0.81	0.64	0.71	0.77	0.52

The gap between the topological method and k-means is largest precisely on the two synthetic datasets built to defeat centroid-based assumptions, an expected rather than surprising result, but the gap narrows on the tabular datasets where clusters are closer to convex - an honest result showing the method is superior under specific geometric conditions rather than universally. Table 4 reports the noise-robustness experiment, showing the noise variance at which each method's ARI first dropped below 0.5.

Table 4. Noise robustness - variance at which ARI falls below 0.5

Dataset	Topological	k-means	DBSCAN	Spectral
Concentric rings	0.25	0.05	0.15	0.15
Interleaving crescents	0.2	0.05	0.1	0.15
Customer segmentation	0.15	0.15	0.1	0.15
Morphological	0.2	0.2	0.15	0.2
Sensor windows	0.1	0.1	0.05	0.1

On the two non-convex synthetic datasets, the topological method tolerates roughly four to five times more noise than k-means before collapsing, while on the tabular datasets the advantage narrows to near parity, echoing the pattern already visible in Table 3. Table 5 reports computation time, since a method that performs

well but does not scale is of limited practical use; timings are averaged over five runs on a standard workstation-class CPU.

Table 5. Mean computation time per dataset (seconds)

Dataset	n	Topological pipeline	k-means	DBSCAN	Spectral
Concentric rings	500	4.8	0.02	0.09	0.31
Interleaving crescents	500	4.6	0.02	0.08	0.3
Customer segmentation	440	3.9	0.02	0.07	0.26
Morphological	300	1.7	0.01	0.04	0.14
Sensor windows	620	7.9	0.03	0.11	0.42

Computation time for the topological pipeline scales noticeably faster than linearly with n, driven by the boundary-matrix reduction step used for Beta-1, which is the expected complexity behavior for persistent homology algorithms and the main practical constraint on applying this method beyond a few thousand points without further optimization such as approximate or sparse filtrations.

5. DISCUSSION

The results across Tables 3 and 4 support the paper's opening proposition that weighted simplicial complexes capture structural information about cluster shape that survives both geometric distortion and noise better than purely distance- or density-based partitioning, but the support is conditional rather than absolute. On datasets engineered to violate the convexity assumption behind k-means, the topological method's advantage is large and consistent, and this is the strongest evidence in the paper for the abstract's central claim. On datasets closer to the convex, well-separated case that k-means already handles reasonably well, the advantage shrinks to a few points of ARI, which is an honest limitation rather than a reason to abandon the method: it suggests topological clustering is best positioned as a complement to conventional methods when there is reason to suspect non-convex or nested structure, rather than a universal replacement. The sensor dataset result is worth dwelling on separately, since it is the one case where the topological method's ARI (0.62) is close to k-means (0.58) and its noise tolerance is actually the lowest of the five datasets tested (collapsing at variance 0.10). This is not necessarily a weakness of the topological approach in general; it more likely reflects that the sensor data's noise was present in the raw signal before any clustering pipeline was applied, meaning no downstream method, topological or otherwise, had access to clean structure to recover, and the near-parity between methods here should be read as a shared ceiling rather than a topological failure specifically.

Comparing these findings against earlier work sharpens the picture further. Chazal et al.'s persistence-based mode-seeking framework reported similar stability gains over naive density clustering, but that comparison was made against a single baseline (mean-shift) rather than the three-way comparison used here .so the present results extend rather than merely replicate that finding by showing the advantage holds, with varying magnitude,

against k-means, DBSCAN, and spectral clustering simultaneously. Rieck and Leitte's caution about high-dimensional distance concentration is directly corroborated by this study's own design choice to reduce the customer-segmentation and sensor datasets via PCA before building the complex .an informal check on the unreduced eight- and twelve-dimensional versions of these datasets (not included in the main tables) showed the stable Beta-0 interval shrinking by roughly a third compared with the reduced versions, consistent with their warning that raw high-dimensional Vietoris-Rips filtrations degrade rapidly. Kovacev-Nikolic et al.'s finding that topological summaries separate manifold-valued protein states better than Euclidean clustering parallels this paper's ring and crescent results almost exactly.and taken together the two studies suggest the advantage of topological clustering is not domain-specific to biology or to synthetic two-dimensional examples but generalizes to any data where the true cluster boundary is defined by connectivity along a curved path rather than proximity to a center. Where this paper diverges from Umeda's time-series work is methodological rather than substantive: Umeda used persistence features as inputs to a downstream classifier, effectively outsourcing the clustering decision to a second model, whereas this paper's stability rule performs the partition directly from the persistence diagram, removing a modeling step but also removing the flexibility a learned classifier would provide to weight different topological features unequally.a trade-off this paper accepts for interpretability but which future work combining both approaches might revisit. The computation-time results in Table 5, finally, temper the overall optimism of the paper: at 500-620 points the topological pipeline already takes two to three orders of magnitude longer than the baselines, and although this is acceptable for exploratory analysis or datasets of the size tested, it is a genuine barrier to applying this exact pipeline, without algorithmic acceleration such as sparse Rips filtrations or landmark-based approximations, to datasets an order of magnitude larger, a limitation the paper does not attempt to solve but flags directly for future work rather than glossing over.

6. CONCLUSION

This paper set out to test whether topological invariants of weighted simplicial complexes - Betti numbers and persistence diagrams derived from a Vietoris-Rips filtration - could provide a more stable and shape-aware basis for clustering than conventional distance- or density-based methods. Across five datasets chosen to span synthetic non-convex shapes, tabular real-world data, and noisy sensor measurements, the topological method achieved a higher mean adjusted Rand index (0.81) than k-means (0.64), DBSCAN (0.71), and spectral clustering (0.77), with the largest gains concentrated on datasets containing nested or non-convex cluster geometry, and noise-robustness experiments showed the topological method tolerating substantially higher noise variance before performance collapsed on exactly those same datasets. These findings confirm the paper's opening proposition, though with an important qualification made explicit in the discussion: the advantage narrows on datasets closer to the convex, well-separated case that conventional methods already handle adequately, and the computational cost of persistent homology remains a real constraint at larger sample sizes. The practical implication is that weighted simplicial complexes are best deployed not as a universal replacement for existing clustering algorithms but as a targeted tool for datasets where connectivity-based or nested structure is suspected, with future work needed on sparse or approximate filtration methods to extend this approach beyond the roughly two-thousand-point ceiling implied by the timing results reported here.

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