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Survey of Antihomology Research

BA Jefferson

September 2017



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Pacific Northwest National Laboratory
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Abstract

Homology has been gaining traction as a tool for studying patterns in real-world datasets. During the past year, I have sought to understand a slight variant on the typical computation of homology of a metric space which we term *antihomology*. This exposition will survey that work. In section 2, I begin with findings from computations on samples from common spaces (the circle, the disc, and the square). Section 3 presents one conjecture and one lemma regarding 1-dimensional cycles on the circle with evenly space points and the circle with random sampling. In section 4, I applied antihomology to power grid datasets and compared results with more traditional data reduction techniques. Lastly, section 5 reveals the connection between antihomology and location covering problems.

1 Introduction

To the author's awareness, this is the first time homology has been systematically explored (or even computed) with the space described below. We seek to gain a better understanding of what the computation is capturing with respect to abstract spaces and data alike. Of particular interest is how to interpret the result. Ordinarily, homology roughly finds voids in a space (think of bubbles in pancake batter, or a hole punched in a sheet of paper). In our application, we construct an "anti-space" from proximity data, where points that are normally far apart in proximity are represented as being close. The homology of this anti-space is what we deem *antihomology*.

Some of the spaces described in this paper are straightforward and don't require explicit construction (the circle for example). In other instances, we are required to construct a space for the homology and antihomology calculations. The reader should be somewhat familiar with *simplicial complexes*, although a complete comprehension is not required. We construct the Vietoris-Rips complex in all our computations (homology and antihomology alike). For this complex, each point in the space is a "0-cell" in the Vietoris-Rips complex. Higher dimensional cells (or cliques in graph theoretical conceptions) are added whenever k points are sufficiently close to one another. That is, $k + 1$ points form a k -cell if all pairwise distances are less than some threshold t . This space is used for homology. To compute the anti-space, rather than k -cells being formed from distances less than t , a k -cell is formed from distances *greater* than t . Thus, a 1-cell (a line segment) in the anti-space connects two points that are very far from each other.

For each threshold, t we have a new space and anti-space by following the Vietoris-Rips construction. Homology can be computed on each space for each threshold. There are natural functions relating the homologies from this family of spaces. The collection of homologies for different thresholds is called *persistent homology*. The relationship between homology groups across thresholds is described in Carlsson (2008). We will see how the notion of persistence aids in extracting robust findings for antihomology.

For both antihomology and homology, the output is a collection of "voids," varying in dimension. A 1-dimensional void, (think of a loop or a hole in a doughnut), may coexist with other dimensional voids in a space. We call a k -dimensional void, a *k-cycle*. In our computation, points from the sampled space are provided to describe each k -cycle (for example the 1-cycle, $[1,2] [2,3] [3,4] [1,4]$ has points 1, 2, 3, 4, and 5). For all of the following investigations we are only concerned with 1-cycles. All results, if not explicit, should be assumed to be with about 1-cycles.

2 Patterns with Antihomology

Antihomology cycles appear to intimate information possibly related to the convex hull of a space. A cycle is created when several points are long distances from adjacent points, but close to all other points. To gain a better handle on what this pattern should look like, here we will compute the antihomology of familiar spaces and discuss findings.

2.1 Method

Points were sampled uniformly from the circle ($x^2 + y^2 = 9$), ellipse ($.25x^2 + 9y^2 = 2.25$), line, and square ($[0, 1] \times [0, 1]$). The antihomology of each space was computed and observational notes were recorded. These notes included the total number of cycles, most frequent cycle length, and the maximum cycle length. Since the spaces are 2-dimensional, an image was produced and points included in the same cycle are highlighted.

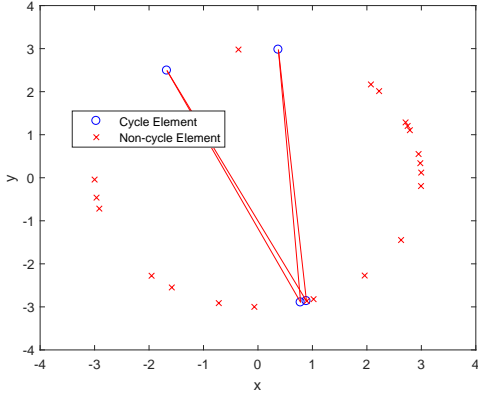
2.2 Beginning Statistics

We uniformly sampled 25 points from a circle 50 times. For each sample, the threshold was varied and persistent antihomology computed. We found that the average number of 1-dimensional cycles were 84 and that the most frequent cycle length was four. Cycle length is the number of unique points named in a cycle. On average, length four cycles accounted for 62% of all cycles from antihomology for the circle. The average maximum length of a cycle was 14. From construction, the minimum length of a cycle must be 4. These calculations can be found for all spaces in table 1.

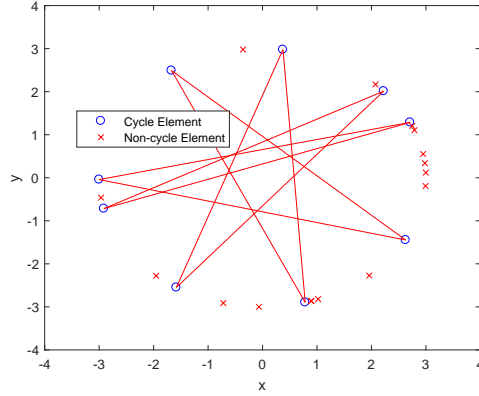
Space	# of Cycles	Mst. Freq. Lth.	Percent Mst. Freq.	Max Lth.
Circle	85.96 \pm 7.2589	4	64.545 \pm 6.7193	14.3 \pm 2.0127
Ellipse	98.72 \pm 13.208	4	97.807 \pm 3.7012	4.86 \pm 1.2124
Line	82.24 \pm 19.328	4	98.001 \pm 3.2383	4.84 \pm 1.1493
Square	50.28 \pm 12.058	4	61.799 \pm 10.351	7.94 \pm 1.3463

Table 1: Averages on Cycle Results

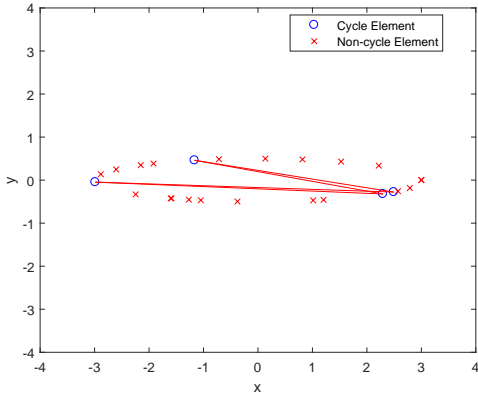
The measures ‘number of cycles’, ‘percent of most frequent length’, and ‘maximum length’ provide a means for distinguishing these spaces. The circle has the longest cycles, while the ellipse has the largest number of cycles. Figure 1 shows example cycles for both the circle and ellipse. Cycles seem to occur at points furthest away in both spaces. A cycle oscillates across the space. For the ellipse, we find that two points that lie close together near the vertex create a cycle with another two points close to the opposite vertex. for a given pair of neighboring points, since the ellipse (as compared to the circle) has more points on the opposite vertex, there are more length 4 cycles. Thus, the pictured cycles match some intuition about the absolute number of cycles. Almost all cycles are of length 4 in the ellipse and line. Only about half of the cycles are of length 4 in the square.



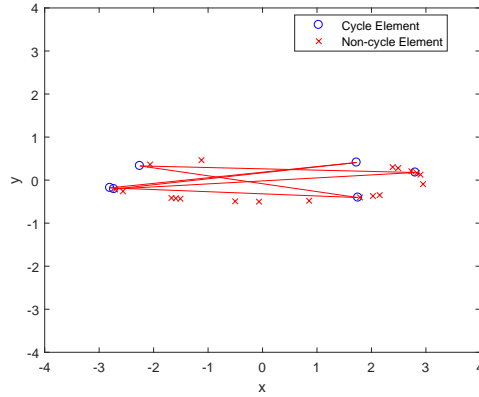
(a) Circle: 4-cycle



(b) Circle: 9-cycle



(c) Ellipse: 4-cycle

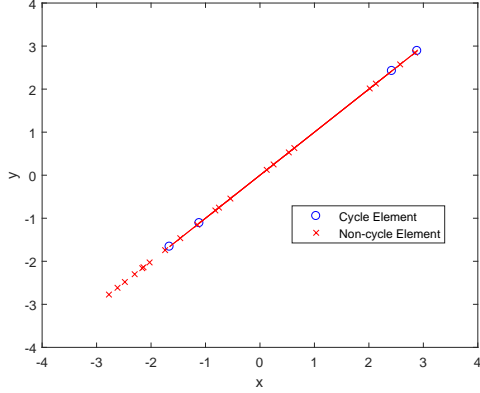


(d) Ellipse: 6-cycle

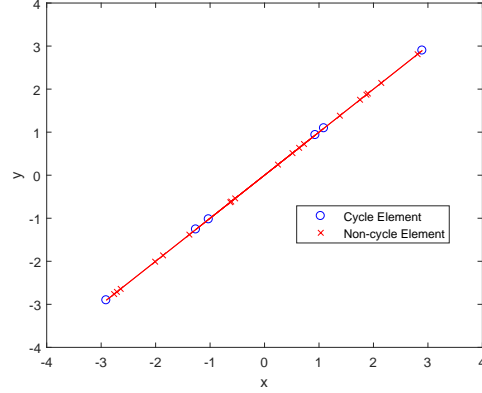
Figure 1: Antihomology Cycles for Circle and Ellipse

Figures 1 and 2 show the longest cycle and a length 4 cycle for each of the four sample spaces for the fiftieth sample. Cycles for the square depicted, show a pattern that was pervasive in all simulations. Namely, the points that are named in 1-cycles may include several points that exist on the hull of that space. For these contrived examples, we can see that the longer a cycle naming is, the spread of those named points across the space also seems to increase. We also note that no two cycle names will be the same in a given antihomology. The collection of all points named on a cycle may be a slightly larger superset to the hull of the space. Consequently, the total number of 1-cycles may be a heuristic for the density of the space. The square contains the fewest number of cycles on average, and has the highest density of the four spaces. Although, this is

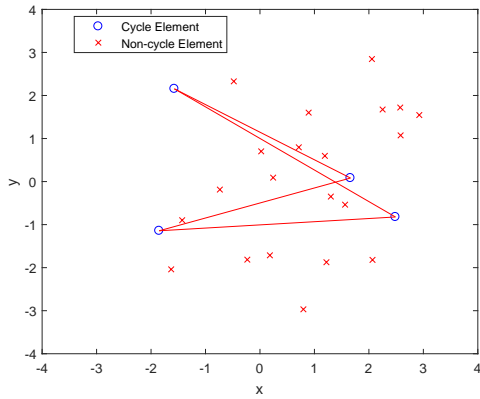
speculative, we believe that these statistics from a topological measure are capturing particular geometric patterns in the space that ordinary homology cannot.



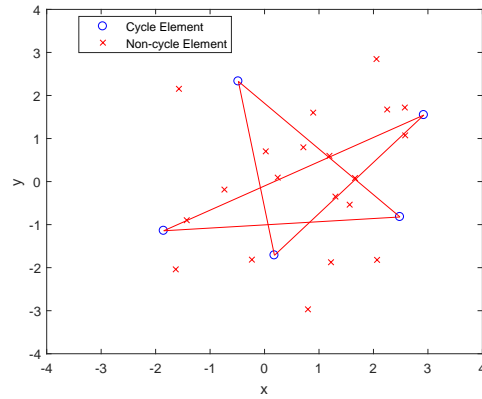
(a) Line: 4-cycle



(b) Line: 6-cycle



(c) Square: 4-cycle



(d) Square: 5-cycle

Figure 2: Antihomology Cycles for Line and Square

2.3 Comparisons Across Known Spaces

Also of interest to the authors was the capability of persistent antihomology (like ordinary homology) to distinguish spaces. The notion of persistence proves useful when considering data, that is often noisy and not precise. Under persistent homology, we create a family of related complexes and compute homology for each complex in order to determine homological structures that exist over a wide range of scale values

for the space. When considering antihomology, the number of cycles increases to a level where individual cycles are likely not a sufficient characteristic of the space. Rather, we must look at the collective number of cycles over varying scale values as provided by persistent antihomology.

We randomly sampled 25 points from one of four spaces (random points on the circle, evenly spaced points on the circle, the disc - or filled in circle, and the square). For that sample, we computed the function relating scale value (threshold at which the simplicial complex was created) with number of 1-cycles from antihomology computations. A population of these functions was created by repeating this procedure 50 times with the choice in which space to sample from also being random. A complete-linkage clustering procedure was applied to the normed differences of all pairs of functions to provide a clustering of the spaces based on antihomology.

For the clustering procedure, we varied the number of clusters from 2 to 5. Frequency tables are included below. For all clusterings, the evenly spaced circle and randomly sampled circle clustered together. For the 3 and 4 cluster solutions, all disc samples clustered together, but 3 of the square samples were intermixed in that cluster. The majority of the square samples clustered together consistently. The separation of the disc and square is a result that ordinary persistent homology cannot produce. Thus, persistent antihomology can distinguish noisy spaces to a fairly good degree, even with small (25 point) samples.

	Random Circ.	Even Spcd. Circ	Square	Disc
Cluster 1	9	15	0	0
Cluster 2	0	0	19	7

Table 2: 2 Cluster Solution

	Random Circ.	Even Spcd. Circ	Square	Disc
Cluster 1	0	0	3	7
Cluster 2	0	0	16	0
Cluster 3	9	15	0	0

Table 3: 3 Cluster Solution

	Random Circ.	Even Spcd. Circ	Square	Disc
Cluster 1	0	0	1	0
Cluster 2	0	0	15	0
Cluster 3	0	0	3	7
Cluster 4	9	15	0	0

Table 4: 4 Cluster Solution

	Random Circ.	Even Spcd. Circ	Square	Disc
Cluster 1	0	0	2	3
Cluster 2	0	0	1	4
Cluster 3	0	0	1	0
Cluster 4	0	0	15	0
Cluster 5	9	15	0	0

Table 5: 5 Cluster Solution

2.4 Remarks on the Calculations

Although we’ve gathered some evidence as to what antihomology reflects about a given space, the method should not be applied without considerations. First, there are situations where the antihomology calculation will yield no results. Consider a sample of points from the unit square plus an additional point at (50, 50). Since every point forms a 1-simplex with the point (50,50), any cycle in the square is contractible, so thus, there are no cycles for this space! In addition to this, when cycles are produced, the name of a cycle is up to homotopy equivalence. This means that any one cycle could have different properties based on which, of potentially many, equivalent names are chosen. Another naming concern stems from the fact that homology is a vector space. Given a basis for a vector space, we can always find another basis. The new basis may be described as linear combinations of the original basis elements. This is problematic for our goals because we are interested in describing single 1-cycles, and not the sum of 1-cycles. Figure 3 is one basis element that was named from the javaplex homology calculation for a sample of the square. This ‘cycle’ is visibly the sum of two disjoint cycles. The perpendicular orientation of the two cycles is purely coincidental and should not be misinterpreted as meaningful.

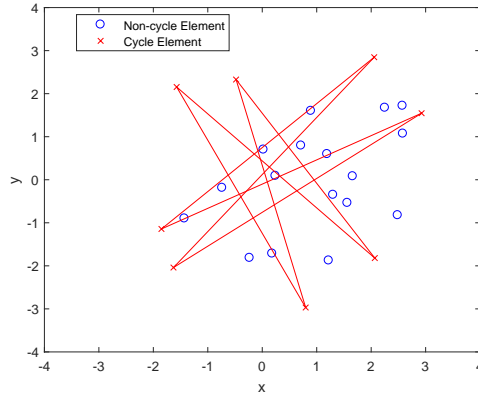


Figure 3: Undesirable Cycle Naming

2.5 Summary

Antihomology was calculated for small samples from simple 2-dimensional spaces. The number of cycles and length of cycles provided a means of distinguishing these spaces. Interpreting these measures is difficult, although some geometric patterns appear to correlate with the measures. Visualizations of the samples and cycles allowed further confirmation of the relationship between geometry and antihomology. A broader range of sample spaces and larger sample sizes is encouraged.

3 Antihomology of the Circle

Two questions are explored with respect to antihomology:

1. Given that we are computing persistent homology, how do specific threshold values relate to the number of 1-cycles for a given space?
2. In what conditions can the length of a cycle be predicted?

By explicitly relating the threshold value to the length and number of cycles, we seek to work toward an interpretation of cycles in the context of scaling data or spaces. Connecting these themes in a simple space is the first step toward antihomology providing a robust geometric descriptor for large datasets.

3.1 Method

With varying sample sizes, we compute the antihomology of samples from the circle of radius 3. A variety of measures are extracted. We sample both uniformly and consider regularly spaced points along the circle.

3.2 Results

For brevity we state the results concisely here. All results assume that N is larger than 4.

Lemma 1. *Given N regularly spaced points around the circle of any radius, r , and threshold, t , with*

$$t = \sqrt{2r^2 \left(1 - \cos \left(\frac{2\pi \left(\left\lfloor \frac{N}{2} \right\rfloor \right)}{N} \right) \right)},$$

if N is odd, then there is exactly one 1-cycle for antihomology and the cycle has length N .

Proof. For any N , this threshold corresponds to the largest threshold where a 1-simplex can exist. For N odd, at this threshold, there are exactly two 1-simplices attached to each point. Choose any base point, x_0 and consider an adjacent point on the circle, x_1 . By the regular spacing of the circle there exists a unique third point y , so that $\{x_0, y\}$ and $\{x_1, y\}$ are 1-simplices. Since all points can be reached by a sequence of 1-simplices connecting adjacent points, there exists a cycle with all points. Note that this is the only cycle, because there does not exist any 2-simplices. \square

Conjecture 1 (Antihomology Threshold). *Given regularly spaced points around the circle of radius, r , a lower bound on thresholds such that there 1-cycles exist is*

$$t = \sqrt{2r^2 \left(1 - \cos \left(\frac{2\pi \left(\left\lfloor \frac{N}{4} \right\rfloor \right)}{N} \right) \right)}$$

the distance approximating the length of a side of the square inscribed in the circle.

The above lemma and conjecture concerned points spaced uniformly around the circle. However, real data may be noisy. As an initial study of variation and antihomology, we investigate points sampled randomly (uniform distribution) from the circle. We estimate the probability that four random points form a cycle on the circle. Let a threshold be given, t . Let x_i be a point on the circle. We use the notation ϵ_i to be the arc corresponding to t and x_i such that points on the circle a distance of t from x_1 fall on the arc, ϵ_i . For convenience, we will use measure theory notation, μ to denote the length of the arc, $\mu(\epsilon_1)$.

The relationship between four points $\{x_1, x_2, x_3, x_4\}(= C)$ forming a cycle must adhere to the following:

1. (a) $d(x_1, x_3) < t$ and (b) $d(x_2, x_4) < t$,
2. (a) $d(x_1, x_2) > t$, (b) $d(x_2, x_3) > t$, (c) $d(x_3, x_4) > t$, and (d) $d(x_1, x_4) > t$, and
3. There is no point, y such that $d(y, x_i) > t$ for $i \in \{1..4\}$

Consider the construction sequentially with index. Then assuming x_1 is given, the probability that C forms a cycle is equal to the probability that

1. $x_2 \in \epsilon_1$,
2. $x_3 \in \epsilon_2 \cap \{y | d(y, x_1) < t\}$ (given x_2 as above),
3. $x_4 \in \epsilon_1 \cap \epsilon_3 \cap \{y | d(y, x_2) < t\}$ (given x_3 as above), and
4. $y \notin \left(\bigcup_{i=1..4} \epsilon_i \right)^c$ (given previous conditions hold).

Since x_1 is given, the first inclusion corresponds to 2(a) above. The second inclusion corresponds to 1(a) and 2(b). The final inclusion corresponds to 1(b), 2(b), and (c), assuming the previous 2 conditions. The final condition on other points implies that the cycle cannot deformation retract to a point. Given t , the above four conditional probabilities can be computed and multiplied to give the probability that four points constitute a cycle. This expression is too cumbersome to include here.

4 Power Grid Problem

Consider several power generators on an electric power grid. Each generator provides a different amount of power depending on several factors including time of day, type of generator, other generators being off-line, etc. Suppose that we can measure the output summary for a given generator at time, t , as a real value. We are interested in identifying those generators that are most instrumental in providing power and most representative of similar generators. Using methods like singular value decomposition or cluster analysis, one can reduce the set of generators to a smaller representative set and express the output of each generator as a linear combination of the output from those in the representative set. These methods are well-established and provide useful solutions for these questions. We want to see how using antihomology and homology techniques compare to these methods by fitting a linear model of the reduced set to the full set.

4.1 Method

We were provided with five datasets of simulated power generators. Each dataset contains 34 power generators and to each power generator there is an associated time-series of 381 real values. We treat each dataset independently. For our approach we consider each power generator in a single dataset as one point in \mathbb{R}^{381} and the Euclidean distance between any two points, $d(g_i, g_j)$. The set of distances allow us to construct a simplicial complex. Each power generator is a 0-cell in the Vietoris-Rips complex. Higher dimensional cells (or cliques in graph theoretical conceptions) are added whenever k power generators have sufficiently similar performance outputs. We compute persistent homology for each dataset.

Homology captures a summary of the topological structures present in a space. These structures are not limited by dimensionality or complexity. The computation of persistent homology on the power generator datasets provides two useful characteristics in our view. First, the so called 0-cycles correspond to connected components of the space. The persistent 0-cycles provide a hierarchical clustering of the generators based on similarity of the outputs. Second, we view the generators as existing in some Euclidean space. As such, when an n -dimensional void (or n -cycle) is found, it indicates that as a Euclidean embedding, we need at least n -dimensions to describe the space. Our analysis focused on this point. For example, suppose generators ‘4,’ ‘5,’ ‘9,’ ‘17,’ and ‘29’ formed a 1-cycle. We would interpret this result as the entire set of power

generators exists in at least a 2-dimensional space since there is at least one 1-cycle. We use the generators listed in a 1-cycle to approximate a basis for the entire set of generators. First, since we are computing persistent homology, the cycles are ordered based on the number of thresholds they survive (more thresholds survived = more reliable cycle). The generators named in each 1-cycle are added to a ‘potential basis set’ in order of cycle and a linear model is tested. A second method for deriving a basis set involved ordering power generators by number of 1-cycles each was named in. Each generator is added one at a time to the basis set and the reduced model was tested.

To supplement this method, we also analyzed the homology of the anti-space of power generators. A cycle in antihomology tends to include points that are mutually most distant, while each having many nearby points. In the previously mentioned preliminary experiments, we find that 1-cycles come close to approximating the convex hull of 2-dimensional spaces. Thus, the generators named in cycles from antihomology may represent different time series characteristics of the entire set of power generators. Antihomology is assessed with the power generator data with the goal of reducing the number of generators. After producing antihomology for each dataset, the five basis sets were derived using the two methods above. For details on the methods we compared homology methods to, see Purvine et. al. (2017).

Analysis Procedure

1. Each dataset was analyzed independently. For a given basis set size, all methods that were able to produce a basis set was counted.
2. For each basis set in this collection, a linear model was tested against the entire time series for all power generators in that dataset.
3. The methods were ranked within the given basis set size.

4.2 Results

The homology methods were especially sensitive to differences across the datasets and set size. With dataset 1, the homology methods performed poorly at providing a basis set of generators. Table 6 provides rankings for homology and antihomology methods for dataset 1. For set sizes where the methods could produce a basis, the methods ranked near last in most cases. The most frequent named generator method under homology performed the best for a basis set size of 6. This was comparatively the best performance of the method.

Basis Size	AH: Freq	H: Freq	AH: Srt Cycles	H: Srt Cycles	# of Mthds
4	7	10	8	11	11
5	16	15	13	0	18
6	25	15	0	0	25
7	29	21	28	0	29
8	35	30	33	0	35
9	21	20	23	16	23
10	39	33	41	0	41
11	30	23	26	24	30
12	17	0	14	0	17
13	26	0	0	0	28
14	18	0	0	0	20
15	18	0	0	0	19

Table 6: Table of Homology and Antihomology Data Reduction Method Rankings. Two methods were used for each homology and antihomology. Rankings of 0 indicate that method couldn't produce a basis of the given size. These rankings are for dataset 1.

In other datasets, the methods performed better for particular set sizes. In particular, the most frequent antihomology generator method ranked first on three occasions (dataset 5, set sizes: 4 and 17; dataset 3, set size 5). There didn't appear to be any systematic reasoning to the success or failure of our homology methods for a given set size. Despite the methods' ability to reduce the set of power generators to a representative set, there were several times the homology methods performed poorly by comparison. However, it should be noted that most methods ranked last for some dataset and some basis set size. Considering the fact that the antihomology methods outperformed established data reduction methods for many set sizes, we have further reason to consider antihomology as a useful tool in taming large datasets.

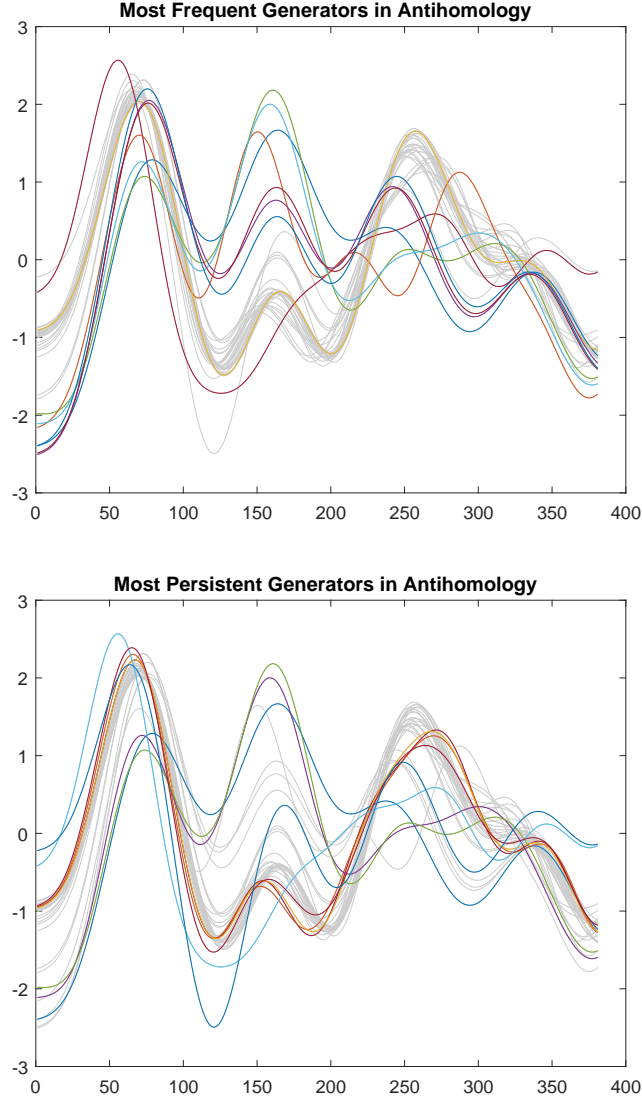


Figure 4: Antihomology Methods for Dataset 5 with 9 Generators

For this exploratory analysis, it is useful to see the time series for the basis generators from the methods. Figure 4 shows the time series for dataset 5 with colored indicators for basis elements under the two instantiations of antihomology methods. The first method (depicted in the top figure) was ranked 9th out of 18 methods (set size = 9) and the second was ranked first. As the cardinality of the basis set increases, the two

methods will converge, but one goal of data reduction is to acquire an interpretable number of dimensions. To that end, differences between the two instantiations can have meaningful implications in small set sizes (as observed by the goodness of fit measure employed here). Figure 5 shows the basis generators for a set size of 5 for both antihomology methods in dataset 3. Comparing the two figures, the most persistent generators antihomology method may be capturing outliers earlier than the most frequent generators antihomology method. More analysis is required.

4.3 Summary

In this project we proposed a new method for deriving an approximation to a linear basis for datasets. This method was tested against several other conventional means of deriving linear basis approximations and proved comparable. In particular, it outperformed the other methods on more than one occasion. During this test phase, we employed four variants of our topological analysis techniques. Not discussed here, we also provided our basis elements to the power engineer that provided the data sets who tested the basis as a reduced order model (accounting for power generator derivations that were not included here) in a related simulation. The engineer reported that the reduced order simulation resulting from our basis elements was a very good approximation to the original full simulation.

Since our antihomology method provided good approximations, the authors seek to answer related questions. The antihomology approaches used here have some built in redundancies in deciding basis elements. The most pertinent goal remains to find an efficient way of eliminating those redundancies without compromising the integrity of the result. We also seek to test the methods with a larger array of datasets.

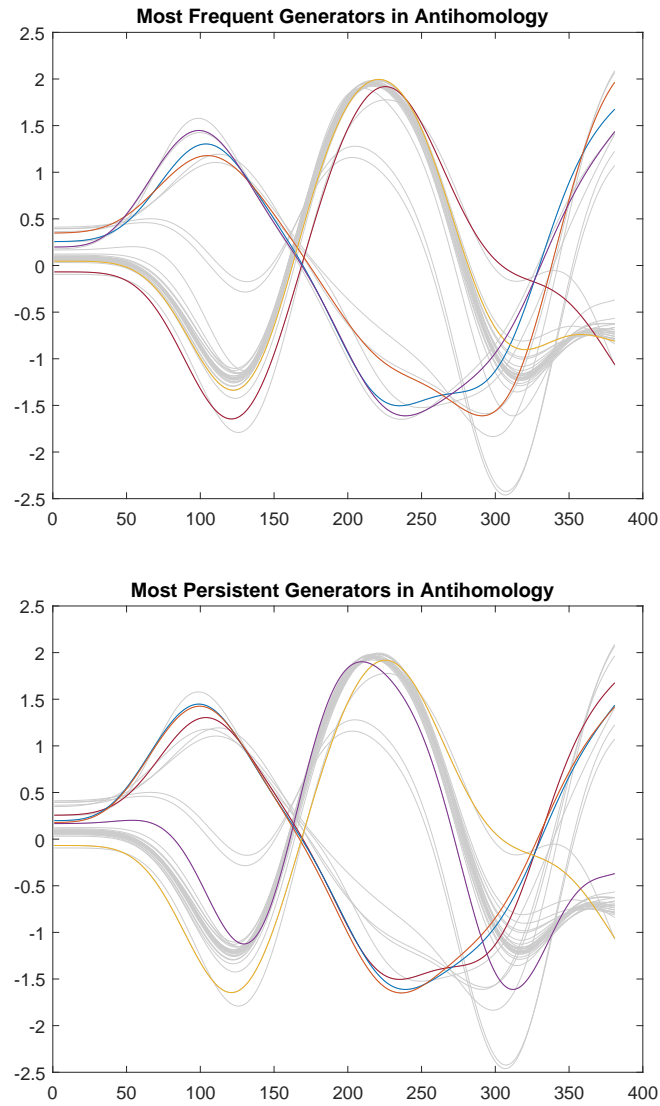


Figure 5: Antihomology Methods for Dataset 3 with 5 Generators

5 Open Cover

I briefly present main findings that relate antihomology to covering spaces.

Fact 1 (N-cover Existence). *Suppose there exists a 1-cycle, $AG(p_0, \dots, p_{N-1})$. Then there exists a N -cover such that each neighborhood is a Euclidean ball of radius T , where T is the threshold used to create the simplicial complex.*

Proof. Consider the union of balls based at points p_0, \dots, p_{N-1} of radius T . Suppose there is a point, q not covered by this union. Then q forms an edge with each p_i in the simplicial complex. Also, for adjacent points, p_i, p_{i+1}, q forms a 2-simplex $\{p_i, p_{i+1}, q\}$. Thus each edge in $AG(p_0, \dots, p_{N-1})$ contracts to the point q . So the 1-cycle is not a 1-cycle. \square

Lemma 2 (3-cover). *Given X_T with smallest irreducible and non-decomposable 1-cycle, $AG(p_0, \dots, p_N)$ with $N > 3$, then a 3-cover is always possible.*

Proof. Let X_T be as in the statement of the lemma. Consider points p_1, p_2 , and p_4 . We show that the union of balls $\cup_{i \in \{1,2,4\}} B_T(p_i)$ cover X_T . First, we know that all points of the 1-cycle are contained in one of the three neighborhoods since $AG(p_0, \dots, p_N)$ is non-decomposable. Let $p \in X_T$. If p is not in $\cup_{i \in \{1,2,4\}} B_T(p_i)$, then 1-simplices, $\{p, p_2\}$ and $\{p, p_4\}$ are formed since the respective proximities are greater than T . The proximity between p and p_3 or p and p_0 is less than T by Fact 1 (assume the former is true). Then p forms a 1-cycle, $AG(p_2, p_3, p_4, p)$. But the smallest generator has length greater than 4. $\rightarrow \circ \leftarrow$ \square

Lemma 3 (2-cover). *Given X_T with smallest irreducible and non-decomposable 1-cycle, $AG(p_0, \dots, p_N)$ with $N > 4$, then a 2-cover is always possible.*

Proof. Let X_T be as in the statement of the lemma. Consider points p_1 and p_4 . We show that the union of balls $\cup_{i \in \{1,4\}} B_T(p_i)$ cover X_T . Suppose q is not covered by the union. Since there is no $p_i \in AG$ so that $\{p_1, p_i\}$ and $\{p_i, p_4\}$ are in X_T [length of the generator is more than 5, non-decomposable], then $q \neq p_i$ for all i . But $\{q, p_1\}$ and $\{q, p_4\}$ are in X_T and the set of 1-simplices $\{\{q, p_1\}, \{p_1, p_2\}, \{p_2, p_3\}, \{p_3, p_4\}, \{p_4, q\}\}$ forms a 1-cycle of length shorter than N . $\rightarrow \circ \leftarrow$ \square

Fact 2. *For the simplicial complex, X_T , if $k \in \mathbb{N}$ is such that there is a $k - 1$ simplex in X_T not contained by any other simplex in X_T , then there exists a k -cover of X_T .*

Proof. Consider the $k - 1$ simplex, σ , in X_T not contained by another simplex. That simplex consists of k points. By definition, for points not in σ , q , there must be a point in σ , p so that the distance $d(p, q) \leq T$. If not, then the $k - 1$ simplex is contained in $\{q\} \cup \sigma$. Thus σ provides the base points of a k -cover. \square