The Theory of Multidimensional Persistence*

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ABSTRACT

Persistent homology captures the topology of a filtration – a one-parameter family of increasing spaces – in terms of a complete discrete invariant. This invariant is a multiset of intervals that denote the lifetimes of the topological entities within the filtration. In many applications of topology, we need to study a multifiltration: a family of spaces parameterized along multiple geometric dimensions. In this paper, we show that no similar complete discrete invariant exists for multidimensional persistence. Instead, we propose the *rank invariant*, a discrete invariant for the robust estimation of Betti numbers in a multifiltration, and prove its completeness in one dimension.

Categories and Subject Descriptors

F.2.2 [**Analysis of Algorithms and Problem Complexity**]: Nonnumerical Algorithms and Problems—*Computations on discrete structures*

General Terms

Algorithms, Theory

Keywords

computational topology, multidimensional analysis, persistent homology

1. INTRODUCTION

In this paper, we introduce the theory of *multidimensional persistence*, the extension of the concept of *persistent homology* [7, 17]. Persistence captures the topology of a *filtration*, a one-parameter increasing family of spaces. Filtrations arise naturally from many processes, such as multiscale analyses of noisy datasets. Given a filtration, persistent homology provides a small description in terms of a multiset of intervals we call the *barcode*. The intervals correspond to the lifetimes of the topological attributes. Since features have long lives, while noise is short-lived, a quick examination of the intervals enables a robust estimation of the topology of a dataset. This is the key reason for the current popularity of persistent homology for solving problems in diverse disciplines, such as shape description [4], denoising volumetric density data [13], detecting holes in sensor networks [6], and analyzing the structure of natural images [5].

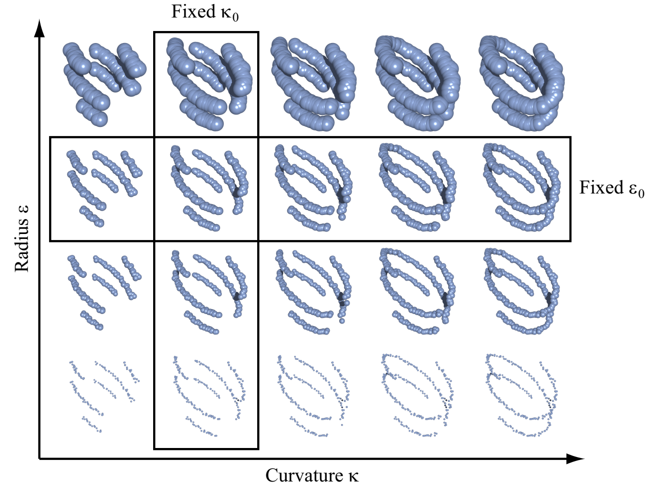

Figure 1: A bifiltration, parameterized along curvature κ and radius ϵ. We can only apply persistent homology to a filtration, so we must either fix ϵ or κ.

We often encounter richer structures that are parameterized along multiple geometric dimensions. These structures may be modeled by *multifiltrations*, as the bifiltration shown in Figure 1. In previous work, we provided the theoretical foundations for persistent homology, obtaining a simple classification over fields in terms of the barcode [17]. Significantly, we showed that the barcode was *complete*, capturing all the topological information within a filtration. In this paper, we show that a similar result is unattainable for multidimensional persistence: there exists no small complete description, like the barcode, in higher dimensions. Given this negative theoretical result, we still desire a discriminating invariant that enables detection of persistent features in

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a multifiltration. To this end, we propose the *rank invariant*. In one dimension, this invariant is equivalent to the barcode and consequently complete. Unlike the barcode, however, the rank invariant extends to higher dimensions, where it still captures persistent features, making it useful for practical applications.

1.1 Motivation

Filtrations arise naturally whenever we attempt to study the topological invariants of a space computationally. Often, our knowledge of a space is limited and imprecise. Consequently, we utilize a multiscale approach to capture the connectivity of the space, giving us a filtration.

Example 1 (radius ϵ) We often have a finite set of noisy samples from a subspace $X \subset \mathbb{R}^n$, such as the point set at the bottom of the vertical box in Figure 1. If the sampling is dense enough, we should be able to compute the topological invariants of X directly from the points [2]. To do so, we approximate the original space as a union of balls by placing ϵ-balls around each point. As we increase ϵ, we obtain a family of nested spaces or a filtration, as shown in the vertical box in Figure 1.

This example states the central idea behind many methods for computing the topology of a point set, such as *Čech*, *Rips-Vietoris* [12], or *witness* [5] complexes.

Often, the space under study is filtered to begin with. And the filtration contains important information that we wish to extract.

Example 2 (density ρ) Suppose we have a probability density function δ on $X \subset \mathbb{R}^n$. We can define

$$X_\rho = \{x \in X \mid 1/\delta(x) \leq \rho\}.$$

Clearly, $X_{\rho_1} \subseteq X_{\rho_2}$ for $\rho_1 \leq \rho_2$, so $\{X_\rho\}_\rho$ is a filtration. We can obtain information about δ from this filtered space. For instance, the number of persistent connected components gives an estimate of the number of the modes of δ. In higher dimensions, one may uncover even more interesting structure, as was demonstrated for the nine-dimensional *Mumford dataset* [5].

Example 3 (curvature κ) In prior work, we develop a methodology for obtaining compact shape descriptors for manifolds by examining the topology of derived spaces [1]. Our approach constructs the *tangent complex*, the closure of the tangent bundle, and filters it using curvature, as shown in the horizontal box in Figure 1. We show that the persistence barcodes of the filtered tangent complex are useful shape descriptors.

In practice, we often have a finite set of samples from our space, giving us a filtered point set in the last two examples. Given a point set, we may employ the technique in Example 1 to capture topology, constructing a filtration based on increasing the radius ϵ. But when the point set itself is filtered, our solution lies within the persistent homology along other geometric dimensions, such as density ρ in Example 2, or curvature κ in Example 3. We now have multiple dimensions along which our space is filtered, that is, we have a *multifiltration*. Of course, we could apply persistent homology along any single dimension by fixing the value of the other parameters, as indicated by the boxes the figure [4]. However, persistent homology itself was motivated by our inability to robustly estimate values for these parameters. To eliminate the need for fixing values, we wish to apply persistence along all dimensions at once. Our goal is to be able to identify persistent features by examining the entire multifiltration. We call this problem *multidimensional persistence*. Variants of this problem have appeared in other contexts, such as the *first size homotopy groups* [10].

1.2 Approach

To understand the structure of multidimensional persistence, we utilize a general algebraic approach consisting of three steps: *correspondence*, *classification*, and *parameterization*. In the first step, we identify the algebraic structure that corresponds to our space of interest. In the second step, we obtain a complete classification of the structure, up to isomorphism. In the third step, we parameterize the classification.

Our parameterization will be in the form of invariants. An *invariant* is a map that assigns the same object to isomorphic structures. For example, the *trivial* invariant assigns the same object to all structures and is therefore useless. A *complete* invariant, on the other hand, assigns different objects to structures that are not isomorphic. Complete invariants are the most powerful type of invariant and we naturally search for them. If complete invariants do not exist, we search for incomplete invariants that have enough discriminating power to be useful.

Our goal is to obtain a useful parameterization consisting of a small set of invariants whose description is finite in size. We utilize terminology from algebraic geometry to distinguish between invariants. We seek invariants that correspond to discrete images of points in algebraic varieties and are not dependent on the underlying field of computation. The former condition enables them to have finite parameterizations. The latter means that our invariant always comes from the same set, similar to the Betti numbers, which are always integers regardless of the coefficient ring. For brevity, we call these invariants *discrete*, and other invariants *continuous*. Continuous invariants may be uncountable in size or depend on the underlying field of computation. Naturally, these invariants are not viable from a computational point of view. Therefore, our objective is a complete discrete invariant for multidimensional persistence. We note that our notation has nothing to do with whether the underlying field of computation is continuous, such as $\mathbb{R}$, or discrete, such as $\mathbb{F}_p$ for a prime p.

1.3 One-Dimensional Persistence

In a previous paper, we follow the algebraic approach above and obtain a complete discrete invariant for one-dimensional persistence [17]:

1. Correspondence: We show a correspondence between the homology of a filtration in any dimension and a graded $R[t]$-module, where $R[t]$ is the ring of polynomials with indeterminate t over ring R.

2. Classification: Over fields k, $k[t]$ is a principal ideal domain, so a consequence of the standard structure theorem for graded $k[t]$-modules gives the full

classification:

$$\bigoplus_{i=1}^{n} \Sigma^{\alpha_i} k[t] \;\oplus\; \bigoplus_{j=1}^{m} \Sigma^{\gamma_j} k[t]/(t^{n_j}),$$

where Σ^α denotes an α-shift upward in grading.

3. Parameterization: The classification gives us n half-infinite intervals $[\alpha^i, \infty)$ and m finite intervals $[\gamma_j, \gamma_j + n_j)$. The multiset of $n + m$ intervals is a complete discrete invariant. We call this multiset the *persistence barcode* [1].

In essence, we are able to complete all our steps for one-dimensional persistence and get everything we could possibly wish for.

1.4 Contributions

In this paper, we show that multidimensional persistence has an essentially different character from its one-dimensional version. We devote a major portion of this paper to the following theoretical contributions:

- We identify the algebraic structure that corresponds to multidimensional persistence to be a finitely-generated multigraded module over the field of multivariate polynomials.
- We establish a full classification of this structure in terms of the set of the orbits of the action of an algebraic group on an algebraic variety.
- We reveal that this classification has discrete and continuous portions. The former is canonically parameterizable, but the latter has no precise parameterization.

Our results imply that no complete discrete invariant exists for multidimensional persistence, unlike its one-dimensional counterpart. Given this negative result, we conclude the paper by describing a practical invariant:

- We propose a discrete invariant, the rank invariant, that is computable, compact, and useful for extracting persistence information from multifiltrations.
- We prove the rank invariant is equivalent to the persistence barcode in one dimension, making it complete for one-dimensional persistence, the only type for which it can be complete.

Our work has both theoretical and practical components, the former being a full understanding of multidimensional persistence, and the latter being a practical invariant that is useful for computation. In Section 2, we review concepts from algebra, algebraic topology, and algebraic geometry, and invent some notation. The next three sections detail the three steps of our approach, respectively. In Section 6, we propose our discrete invariant for multidimensional persistence and show its completeness in one dimension.

2. BACKGROUND

Let $\mathbb{N}$ be the set of non-negative integers, also called the *natural numbers*. Intuitively, a multiset is a set within which an element may appear multiple times, such as $\{a, a, b, c\}$. Formally, a *multiset* is a pair (S, μ), where S is the *underlying set of elements* and $\mu\colon S \to \mathbb{N}$ specifies the *multiplicity* $\mu(s)$ of each element $s \in S$. We often characterize a multiset via the set-theoretic definition of μ: $\{(s, \mu(s)) \mid s \in S\}$. For the example, we get $\{(a, 2), (b, 1), (c, 1)\}$. We define $(s, i) \in (S, \mu)$ iff $s \in S$ and $1 \le i \le \mu(s)$, that is, i indexes the multiple copies of s.

For $u, v \in \mathbb{N}^n$, we say $u \lesssim v$ if $u_i \le v_i$ for $1 \le i \le n$. Let (S, μ) be any multiset where $S \subseteq \mathbb{N}^n$. Then, the relation $\lesssim$ is a *quasi-partial order* on (S, μ): it is *reflexive* and *transitive*, but not *anti-symmetric*, since elements appear with multiplicity.

A *monomial* in $x_1, \ldots, x_n$ is a product of the form

$$x_1^{v_1} \cdot x_2^{v_2} \cdots x_n^{v_n}$$

with $v_i \in \mathbb{N}$. We denote it x^v, where $v = (v_1, \ldots, v_n) \in \mathbb{N}^n$. A *polynomial* f in $x_1, \ldots, x_n$ and *coefficients* in field k is a finite linear combination of monomials, $f = \sum_v c_v x^v$, with $c_v \in k$. We denote the set of all polynomials $k[x_1, \ldots, x_n]$. For example, $5x_1x_2^2 - 7x_1^3 \in k[x_1, x_2]$ has two non-zero coefficients: $c_{(1,2)} = 5$ and $c_{(3,0)} = -7$.

An *algebraic variety* is the set of common zeros of a collection of polynomials. One variety we encounter in this paper is the *Grassmannian* $\mathrm{Gr}_k(V)$, the set of k-dimensional subspaces of a vector space V. An *algebraic group* is an algebraic variety endowed with group structure, so that the group operation is a morphism of the variety. The *automorphism group* $\mathrm{GL}(V)$ of a system of objects V is the set of invertible linear transformations on V, where the group operation is function composition.

Let S be a set and G be a group. An *action of G on S* is a binary operation $*\colon G \times S \to S$ such that for the identity element $e \in G$, we have $e * s = s$ for all $s \in S$, and $(g_1g_2) * s = g_1 * (g_2 * s)$ for all $s \in S$ and $g_1, g_2 \in G$. Given a group action, we define $s_1 \sim s_2$ iff there exists $g \in G$ such that $g * s_1 = s_2$. Then, $\sim$ is an equivalence relation on S and partitions it. Each cell in the partition is an *orbit in S under G*.

An *n-graded ring* is a ring R equipped with a decomposition of Abelian groups $R \cong \oplus_v R_v, v \in \mathbb{N}^n$ so that multiplication has the property $R_u \cdot R_v \subseteq R_{u+v}$. The set of polynomials $A_n = k[x_1, \ldots, x_n]$ forms the *polynomial ring*. A_n is graded by $A_v = kx^v, v \in \mathbb{N}^n$ and is the prototype for n-graded rings. We may visualize the 2-graded ring A_2 on the integer grid $\mathbb{N}^2$, as shown in Figure 3(a), where each bullet is a grade that contains an element from k. Our example polynomial $5x_1x_2^2 - 7x_1^3$ has non-zero elements in grades $(1, 2)$ and $(3, 0)$. An *n-graded module* over an n-graded ring R is an Abelian group M equipped with a decomposition $M \cong \oplus_v M_v, v \in \mathbb{N}^n$ together with a R-module structure so that $R_u \cdot M_v \subseteq M_{u+v}$.

3. CORRESPONDENCE

In this section, we carry out the first step of the approach enumerated in Section 1.2: identifying the algebraic structure underlying our problem. The abstraction for our input is a multifiltered space. A space X is *multifiltered* if we are given a family of subspaces $\{X_v \subseteq X\}_{v \in \mathbb{N}^n}$ with inclusions

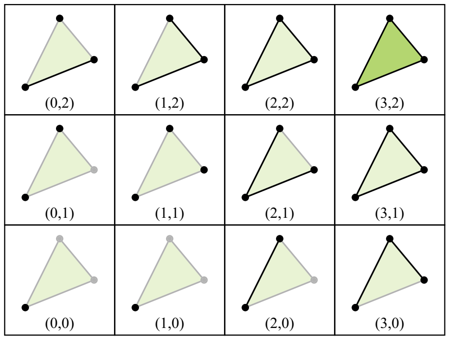


Figure 2: A bifiltration of a triangle.

$X_u \subseteq X_w$ whenever $u \lesssim w$, so that the diagrams

$$\begin{tikzcd} X_u \arrow[r] \arrow[d] & X_{v_1} \arrow[d] \\ X_{v_2} \arrow[r] & X_w \end{tikzcd} \tag{1}$$

commute for $u \lesssim v_1, v_2 \lesssim w$. We showed an example of a bifiltration in Figure 1.

In practice, our input is often a finite complex K along with a function $F\colon \mathbb{R}^n \to K$ that gives a subcomplex K_v for any value $v \in \mathbb{R}^n$, such as the bifiltered triangle in Figure 2. This input converts naturally to a multifiltered complex. Since the complex is finite, there is a finite set of *critical* coordinates $C = \{v_i \in \mathbb{R}^n\}_i$ at which new simplices enter the complex. Projecting C onto each coordinate axis gives us a finite set of critical values C_d in each dimension d. We now restrict ourselves to the discrete set of the Cartesian product $\prod_{d=1}^n C_d$ of the critical values, parameterizing the resulting grid using $\mathbb{N}$ in each dimension. This gives us a multifiltered complex, provided the function F makes the induced diagrams (1) commute.

Given a multifiltered space X, the homology of each subspace X_v over a field k is a vector space. For instance, the bifiltered complex in Figure 2 has zeroth homology vector spaces isomorphic to

k^2	k	k	k
k^2	k^3	k	k
k	k	k	k

where the dimension of the vector space counts the number of components of the complex. We also have inclusion maps relating the subspaces, inducing maps at the homology level.

Definition 1 (persistence module) A *persistence module* M is a family of k-modules $\{M_v\}_v$ together with homomorphisms $\varphi_{u,v}\colon M_u \to M_v$ for all $u \lesssim v$ such that $\varphi_{u,v} \circ \varphi_{v,w} = \varphi_{u,w}$ whenever $u \lesssim v \lesssim w$.

The homology of a multifiltration in each dimension is a persistence module. To capture the structure of the maps in a persistence module, we define a multigraded module, following our treatment in the one-dimensional case [17].

Definition 2 (structure) Given a persistence module M, we define an n-graded module over A_n by

$$\alpha(M) = \bigoplus_v M_v,$$

where the k-module structure is the direct sum structure and we require that $x^{v-u}\colon M_u \to M_v$ is $\varphi_{u,v}$ whenever $u \lesssim v$.

That is, we incorporate the relationships given by the homomorphisms into the structure of an n-graded module. Our treatment is consistent with, and an extension of, the one-dimensional case, where the corresponding structure is a 1-graded or *singly-graded* module [17].

Theorem 1 (correspondence) *The correspondence α defines an equivalence of categories between the category of finite persistence modules over k and the category of finitely generated n-graded modules over $A_n = k[x_1, \ldots, x_n]$.*

To recap, the homology of a finite multifiltered complex is a finite persistence module, and the structure of a persistence module is a finitely generated n-graded module.

One may ask, however, about the reverse relationship: Is every finite persistence module realizable as the homology of a multifiltration? More specifically, can we realize every such module as the homology of a finite multifiltered simplicial complex, since that is our usual representation of a space in practice? The following theorem answers this question in the affirmative.

Theorem 2 (realization) *Every finite persistence module may be realized as the homology, in any dimension greater than zero, of a finite multifiltered space, or a finite multifiltered simplicial complex.*

The proof is constructive and we omit it here.

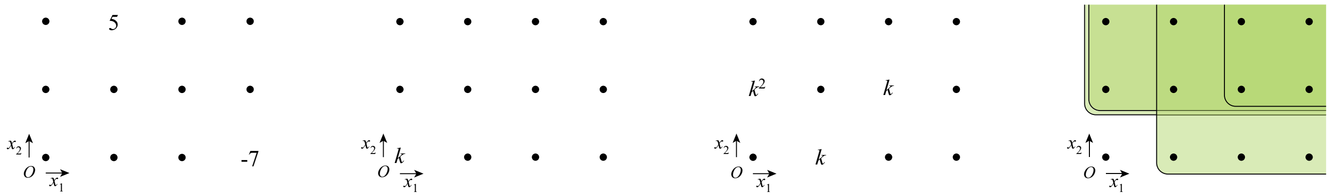
We end this section with an aside on our choice of input. The grid-like filtrations we study arise naturally in practice. Nevertheless, filtrations arising from other partial orders may also be interesting and produce algebraic invariants. However, this would take us out of the realm of commutative algebra, perhaps into non-commutative algebra, and definitely into another paper.

4. CLASSIFICATION

We have now identified the algebraic structures that correspond to our problem: finitely generated n-graded modules over A_n. In this section, we focus on our second task: finding a complete classification for this structure. We begin with a classification of finitely generated free graded objects. Next, we utilize these free objects to describe two discrete invariants for the modules. Finally, we examine the relationship between the two invariants to complete our classification. Our approach is entirely in the spirit of the representation theory of finite dimensional algebras [11]. We have chosen to present a complete argument for clarity and explicitness.

4.1 Free Graded Objects

Intuitively, a free object is a generalization of a vector space: a number of *generators* are *free* to create an infinite number of unique elements. Consequently, a free object has a simple structure and parameterization. In this section, we develop graded versions of free objects to provide discrete



(a) $5x_1x_2^2 - 7x_1^3$ (b) Module k (c) k-vector space V (d) Free A_2-module F

Figure 3: 2-graded objects: (a) Polynomial $5x_1x_2^2 - 7x_1^3$ in the 2-graded ring $A_2 = k[x_1, x_2]$ visualized on $\mathbb{N}^2$. (b) Field k endowed with graded module structure (Definition 3). (c) A k-vector space V with generators at $(1,0)$ and $(2,1)$, and two generators at $(0,1)$ (Definition 5). (d) A free A_2-module F with same type as (b) (Definition 6).

invariants for our input. We begin by endowing a field k with a graded A_n-module structure.

Definition 3 (k) For a field k, we define k to be the n-graded A_n-module with grading $k_0 = k$ and $k_v = \{0\}$ for $v \neq 0$. The A_n-structure is given by setting the action of all the variables identically to zero.

We show the module k in Figure 3(b). To construct more complicated modules, we introduce the concept of shifting.

Definition 4 (shift) Given an n-graded object M and $v \in \mathbb{N}^n$, the *shifted object* $M(v)$ is defined by $M(v)_u = M_{u-v}$ for all $u \in \mathbb{N}^n$.

In other words, the object $M(v)$ is identical to M, but its direct sum decomposition is shifted upwards in grading by v. We use shifted objects to create graded vector spaces.

Definition 5 (vector space) Let ξ be a multiset of elements from $\mathbb{N}^n$. A *finitely generated n-graded k-vector space with basis* ξ is a finite direct sum of shifted copies of k:

$$V(\xi) = \bigoplus_{(v,i)\in\xi} k(v).$$

Note that we enumerate the elements with multiplicity using our notation for multisets. Figure 3(c) displays a 2-graded k-vector space defined by multiset

$$\{((1,0),1),((0,1),2),((2,1),1)\}.$$

In a vector space, a generator's scope is a single grade. In a free module, we extend its scope via the action of the the variables.

Definition 6 (free module F) Let ξ be a multiset of elements from $\mathbb{N}^n$. The *free n-graded A_n-module with basis* ξ is the direct sum of shifted copies of A_n:

$$F(\xi) = \bigoplus_{(v,i)\in\xi} A_n(v) = \bigoplus_{(v,i)\in\xi} k[x_1,\ldots,x_n](v).$$

Compare this definition with the previous one. Our construction has the usual universal mapping property defining a free module [16]. Figure 3(d) displays the free module with the same defining multiset as our example vector space. Each shaded region indicates the scope of a generator in its corner.

Lemma 1 (type ξ, isomorphism) *Any finitely-generated n-graded k-vector space may be written uniquely, up to isomorphism, with a basis as in Definition 5. Similarly, any free n-graded A_n-module may be written uniquely, up to isomorphism , with a basis as in Definition 6. The basis is the type $\xi(M)$ of the object M. Two objects of the same type are isomorphic.*

The lemma gives a full classification, establishing ξ as a complete discrete invariant, up to isomorphism, for each of the two free structures. A free module has a vector space in each grade. We use the quasi-partial order $\lesssim$ to formalize this next.

Lemma 2 (grade) *$F(\xi)_v$ is a k-vector space with dimension equal to* $\operatorname{card}\{(u,i) \in \xi \mid u \lesssim v\}$*, where* card *denotes cardinality.*

In Figure 3(d), the dimension of M_v is simply the number of regions that cover grade v. For example, $\dim M_{(2,1)} = 4$ as $(2,1)$ is contained in all four regions. Finally, we extend the notion of an automorphism to free graded modules by requiring it to respect the grading.

Lemma 3 ($\mathrm{GL}_{\lesssim}$) *Let $\mu \in \mathrm{GL}(V(\xi))$ be an automorphism of $V(\xi)$. We say μ* respects the grading *if for any $(v,i) \in \xi$, $\mu(v)$ lies in the span of elements $(v',i') \in \xi$ such that $v' \lesssim v$. We define $\mathrm{GL}_{\lesssim}(V(\xi))$ to be the set of all such automorphisms. Then, $\mathrm{GL}_{\lesssim}(V(\xi))$ is an (algebraic) subgroup of $\mathrm{GL}(V(\xi))$. Moreover, the automorphism group of $F(\xi)$ is isomorphic to $\mathrm{GL}_{\lesssim}(V(\xi))$ and therefore algebraic, so we denote it by $\mathrm{GL}(F(\xi))$.*

4.2 Two Discrete Invariants

In the remainder of this section, we use M to denote our input: a finitely generated n-graded A_n-module. We cannot use the invariant ξ directly since M is not free in general. But we could look at free objects related to it. Let $I_n = (x_1,\ldots,x_n)$ be the n-graded ideal in A_n that is generated by $x_1,\ldots,x_n$. Dividing out the elements in M with coefficients in I_n, we derive a vector space that contains M's generators.

Definition 7 (ξ) The space $V(M) = M/I_nM = k \underset{A_n}{\otimes} M$ is a vector space. We define $\xi(M) = \xi(V(M))$.

$\xi(M)$ is our first discrete invariant for M. For the zeroth homology module for our bifiltration in Figure 2, we get:

$$\xi(M) = \{((0,0),1), ((0,1),1), ((1,1),1)\}.$$

The invariant $\xi(M)$ has an intuitive meaning in the context of one-dimensional persistence (see Section 1.3). What we capture with $\xi(M)$ corresponds to the left endpoints of barcode intervals. Applying Definition 6, we may construct the free graded module $F(\xi(M))$. This module has the same generators as M, but allows them to be free. In one dimension, the construction corresponds to starting half-infinite intervals at the left endpoints, as we have not located the right endpoints.

The invariant $\xi(M)$ is not complete. The module $F(\xi(M))$ is a free approximation of M: it lacks the set of relations that constrain M. So, we may begin our classification by computing $\xi(M)$, and then refine it by studying classification of all modules with a fixed value of $\xi(M)$. For this refinement, we use a canonical isomorphism $k \otimes_{A_n} F(\xi(M)) \cong k \otimes_{A_n} M = V(M)$.

Lemma 4 (φ) *There exists a surjection $\varphi_M \colon F(\xi(M)) \to M$, unique up to automorphism of $F(\xi(M))$, such that the induced homomorphism*

$$k \underset{A_n}{\otimes} \varphi_M \colon k \underset{A_n}{\otimes} F(\xi(M)) \to k \underset{A_n}{\otimes} M$$

is the canonical isomorphism given above.

The surjection is the *free hull* of M, dual to the notion of *injective hull* in the literature [8, Page 628]. Its existence is entirely analogous to the existence of the first stage of a *minimal free resolution for local rings* [9, Section 1B]. The kernel $\ker \varphi_M$ of surjection φ_M consists precisely of the relations defining M and is called the *ideal of relations*. Generally, the kernel is not free, but we may use our technique from Definition 7 to capture its generators. This construction gives us our second discrete invariant for M: $\xi(\ker \varphi_M)$. Intuitively, what we capture with $\xi(\ker \varphi_M)$ corresponds to the right endpoints of barcode intervals in one-dimensional persistence. We end this section by naming our two discrete invariants.

Definition 8 (ξ_0, ξ_1) We define $\xi_0(M) = \xi(M)$ and $\xi_1(M) = \xi(\ker \varphi_M)$ as two discrete invariants for a finitely generated n-graded A_n-module M.

For the zeroth homology module for our bifiltration in Figure 2, we get:

$$\xi_1(M) = \xi(\ker \varphi_M) = \{((1,2),2), ((2,1),2)\}.$$

4.3 Complete Classification

We now have the locations of the births and deaths of generators in M inside two multisets $\xi_0(M)$ and $\xi_1(M)$, respectively. The two invariants together are not complete, so we next study the classification of all modules with fixed values for the invariants. In one-dimensional persistence, we were able to establish a significant result that we can pair births and deaths to get the barcode intervals [17]. To complete the classification for multidimensional persistence, we need

$$\begin{aligned} K &= \ker \varphi_M \\ F_0 &= F(\xi_0(M)) = F(\xi(M)) \\ F_1 &= F(\xi_1(M)) = F(\xi(K)) \\ \varphi_K &\colon F_1 \to K \end{aligned}$$

(a) Notation

$$\begin{tikzcd} & K \arrow[d, hook, "i"] & \\ F_1 \arrow[ur, "\varphi_K"] \arrow[r, "\psi_M"] & F_0 \arrow[r, two heads, "\varphi_M"] & M \end{tikzcd}$$

(b) Diagram

Figure 4: Notation and diagram for complete classification.

to study the relationship between the free graded modules associated to our two invariants. For notational sanity, we define the notation in Figure 4(a). The free graded modules F_0 and F_1 have our two discrete invariants as generators, and the surjection φ_K is asserted by Lemma 4. Since K includes in M, we have the diagram in Figure 4(b), where we define $\psi_M = i \circ \varphi_K$, so the diagram commutes. Since $\operatorname{im} \psi_M = \ker \varphi_M$ by construction, the sequence at the bottom of the diagram, $F_1 \to F_0 \to M$, is *exact*. The homomorphism $\psi_M \colon F_1 \to F_0$ relates our two free modules. To understand this map, we begin by modeling any relationship between any two free graded modules.

Definition 9 (relation family RF, $\mathfrak{RF}$) Let $F(\xi_0)$ and $F(\xi_1)$ be free graded modules. A *relation family* $\mathrm{RF}(\xi_0, \xi_1)$ is a family $\{V_v\}_{v \in \xi_1}$ of vector spaces such that

1. $V_v \subseteq F(\xi_0)_v$,
2. $\dim V_v = \dim F(\xi_1)_v$,
3. for $u, v \in \xi_1, u \lesssim v$, we have $\theta_{v-u}(V_u) \subseteq V_v$, where θ_w is multiplication by x^w.

The collection $\mathfrak{RF}(\xi_0, \xi_1)$ consists of all possible relation families $\mathrm{RF}(\xi_0, \xi_1)$.

Note that in this definition, we treat ξ_1 as a set, disregarding the multiplicities. Now, automorphisms $\mu \in \mathrm{GL}(F(\xi_0))$ induce automorphisms of the exact sequence at the bottom of the diagram in Figure 4(b) and therefore of M. In particular, μ maps a relation family into another relation family, giving us the following.

Lemma 5 $\mathrm{GL}(F(\xi_0))$ *is a (left) group action on the collection* $\mathfrak{RF}(\xi_0, \xi_1)$.

Recall the homomorphism $\psi_M \colon F_1 \to F_0$ from the diagram. In each grade v, ψ_M maps vector space $(F_1)_v$ to a vector space within $(F_0)_v$. That is, we get a relation family.

Lemma 6 ($\eta(\psi_M)$) *The homomorphism ψ_M yields a relation family $\eta(\psi_M) \in \mathfrak{RF}(\xi_0(M), \xi_1(M))$, where for $v \in \xi_1(M)$, $\eta(\psi_M)_v = \psi_M(F_1)_v$.*

We may now state a primary result of the paper.

Theorem 3 (classification) *Let ξ_0, ξ_1 be multisets of elements from $\mathbb{N}^n$ and $[M]$ be the isomorphism class of finitely generated n-graded A_n-modules M with $\xi_0(M) = \xi_0$ and $\xi_1(M) = \xi_1$. Then, the assignment $[M] \mapsto \eta(\psi_M)$ is a bijection from the collection of isomorphism classes to the set of orbits*

$$\mathcal{RF}(\xi_0, \xi_1) / \operatorname{GL}(F(\xi_0)). \tag{2}$$

In other words, each module M is classified, up to isomorphism, by three invariants: $\xi_0(M)$, $\xi_1(M)$, and the orbit $\eta(\psi_M)$ under the action of the automorphisms of the associated free graded module $F(\xi_0)$.

5. PARAMETERIZATION

Having established a complete classification of the graded modules, we now turn our attention to the third step of our approach: parameterizing the classification. The two discrete invariants are already parameterized as multisets. The remaining invariant is the set of orbits described by Theorem 3. In this section, we examine the structure of the orbits using concepts in algebraic geometry. The general picture that emerges is that this portion of the classification is a continuous invariant. To appreciate its nature, we next detail an example in two dimensions. We end this section with possible strategies for coping with the continuous invariant.

5.1 Algebraic Action

We begin by endowing the collection of relation families $\mathcal{RF}(\xi_0, \xi_1)$ with the structure of an algebraic variety. Note first that $\mathcal{RF}(\xi_0, \xi_1)$ is a subset of the variety

$$\prod_{(v,i) \in \xi_1} \operatorname{Gr}_{\dim F(\xi_1)_v}(F(\xi_0)_v) \tag{3}$$

where Gr is the Grassmannian. It is now easy to verify that the containment conditions that define the collection $\mathcal{RF}(\xi_0, \xi_1)$ are algebraic on this variety, giving us the following.

Theorem 4 (algebraic action) *$\mathcal{RF}(\xi_0, \xi_1)$ is a variety in a natural way, and the action of the algebraic group $\operatorname{GL}(F(\xi_0))$ on it is an algebraic action.*

Unfortunately, the set of orbits of the action of an algebraic group on an algebraic variety is not, in general, an algebraic variety [14]. The number of orbits may be uncountable, giving us a continuous invariant.

5.2 The Continuous Invariant

To further appreciate the complexity of the continuous invariant, we show its structure for a simple two-dimensional example. Suppose we have a set of modules for which

$$\xi_0 = \{((0,0),2)\},$$
$$\xi_1 = \{((3,0),1),((2,1),1),((1,2),1),((0,3),1)\},$$

as visualized on $\mathbb{N}^2$ in Figure 5. It is easy to build a bifiltered simplicial complex whose first homology groups correspond to this picture. At $(0,0)$, we have a complex composed of

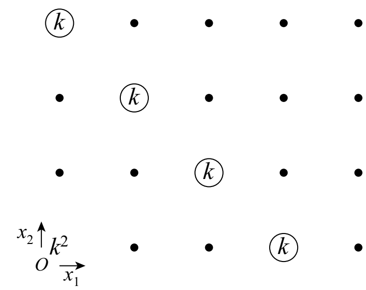


Figure 5: Visualization of ξ_0 and ξ_1 on $\mathbb{N}^2$ for our example, with the elements of the latter circled.

two loops, giving us k^2. In each of the circled coordinates, we choose a sew a surface between the two loops such that no two complexes are sewn the same. For example, we could sew a cylinder at $(3,0)$, a punctured crosscap at $(2,1)$, and so on. Observe that the discrete invariants ξ_0, ξ_1 cannot discern the difference between the resulting complexes.

To obtain the classification, we apply Theorem 3. The generators of $F(\xi_0)$ are co-located, so we have the full group of automorphisms

$$\operatorname{GL}(F(\xi_0)) = \operatorname{GL}(k^2) = \operatorname{GL}_2(k),$$

where $\operatorname{GL}_2(k)$ is the group of invertible 2×2 matrices with elements from k. We use Equation (3) to endow $\mathcal{RF}(\xi_0, \xi_1)$ with a variety structure. For each $(v,i) \in \xi_1$, $F(\xi_0)_v$ is isomorphic to k^2 and $\dim F(\xi_1)_v = 1$, so $\operatorname{Gr}_{\dim F(\xi_1)_v}(F(\xi_0)_v) = \operatorname{Gr}_1(k^2) = \mathbb{P}^1(k)$, where $\mathbb{P}^1(k)$ denotes *projective line*, the set of lines in k^2 going through the origin. Then, the variety is simply $\mathbb{P}^1(k)^4$ as there are no containment conditions. The classification is given by the orbit space

$$\mathbb{P}^1(k)^4 / \operatorname{GL}_2(k), \tag{4}$$

where elements $g \in \operatorname{GL}_2(k)$ act in the evident way on the four lines, transforming each line to another.

We claim that no discrete invariant is possible for this bifiltration. Consider the subspace Ω of the orbit space containing pairwise-distinct lines. That is, we have four tuple of lines (l_1, l_2, l_3, l_4) where $l_i \neq l_j$ for $i \neq j$. The subspace Ω is clearly invariant under the $\operatorname{GL}_2(k)$ action and hence the orbit space $\Omega / \operatorname{GL}_2(k)$ is a subspace of our orbit space in Equation (4). Using matrices from $\operatorname{GL}_2(k)$, we transform the lines so that

1. l_1 becomes the x-axis,
2. l_2 becomes the y-axis,
3. and l_3 becomes the *diagonal* line spanned by $(1,1)$.

These transformations exist as l_1, l_2 span k^2, being nonzero and distinct, and l_3 cannot be zero or either axis after the first two transformations. We now have a tuple $(x\text{-axis}, y\text{-axis}, \text{diagonal}, \lambda_4)$, where λ_4 is l_4 after the transformations. While there are different matrices in $\operatorname{GL}_2(k)$ that can transform the original tuple to this tuple, the matrices differ by multiplication by a diagonal matrix, since the only matrices that preserve the axes and the diagonal line are diagonal matrices. Consequently, λ_4 is determined uniquely, and we may identify the orbits $\Omega / \operatorname{GL}_2(k)$ with the lines in $\mathbb{P}^1(k)$ with the axes and the diagonal removed. Each such line is determined by its slope which cannot be 0, ∞, or 1, according to the discussion. Therefore, $\Omega/\operatorname{GL}_2(k)$ can be identified with $\mathbb{P}^1(k) - \{0, 1, \infty\} = k - \{0, 1\}$.

Now, note that this classification is dependent on the field of coefficients k. If k is uncountable, so is the subspace, and in turn, the full orbit space. If k is a finite field, such as $\mathbb{F}_p$ for p a prime, we get a finite solution for the subspace Ω we have chosen, but we still have not detailed the full picture for the orbit space. However, we already see the field-dependence problem: Changing the field not only changes the classification, but also the target of the classification: We not only get different values, we get values from different sets altogether. This is analogous to getting Betti numbers in $\mathbb{Z}_2$ when computing over $\mathbb{Z}_2$, Betti numbers in $\mathbb{Z}_3$ when computing over $\mathbb{Z}_3$, and so on. Therefore, we cannot get a discrete invariant for our example.

5.3 Refinement

We have illustrated that our goal – obtaining a complete discrete invariant – is not attainable for multigraded objects. Intuitively, the continuous invariant captures subtle second-order information about the complicated transitions in a multigraded module. This information may be worthy of study and we end this section by suggesting possible avenues of attack.

Our two discrete invariants may be viewed as the first two in a family of discrete invariants. We may develop standard homological algebra in the category of graded modules over an n-graded k-algebra A_n, with the resulting derived functors $\underset{A_n}{\otimes}$ and Hom_{A_n} now being equipped with the structure of an n-graded A_n-module [16]. In particular, the functor $\operatorname{Tor}_i^{A_n}(M, k)$ makes sense and we now define a family of n discrete invariants by

$$\xi_i = \xi\left(\operatorname{Tor}_i^{A_n}(M, k)\right).$$

The first two invariants in the family match our two discrete invariants in Definition 8. It may be interesting to study the rest of this family as each invariant will make our classification finer. However, the existence of the continuous invariant indicates that no matter how many of these invariants we include, there will still be a residual continuous component in the classification.

While the set of orbits is not a variety, we conjecture that additional structure exists in the following form. Let $G = \operatorname{GL}(F(\xi_0))$ and suppose there is a family of closed subvarieties $\mathcal{RF}_n \subseteq \mathcal{RF}(\xi_0, \xi_1)$ such that

1. $\mathcal{RF}_n \subseteq \mathcal{RF}_{n+1}$ for all n,
2. $\mathcal{RF}_n$ is closed under the action of G,
3. $\mathcal{RF}_n$ eventually becomes equal to $\mathcal{RF}(\xi_0, \xi_1)$,
4. the set of orbits of the G-action on $\mathcal{RF}_n - \mathcal{RF}_{n-1}$ is an algebraic variety in a natural way.

This kind of structure is called an *equivariant stratification* of the variety in question, with the difference $\mathcal{RF}_n - \mathcal{RF}_{n-1}$ being a *stratum*. The orbit varieties are called *moduli spaces* in classification problems for which the invariant lies in a given stratum. The result is known to hold in some special cases by the work of Cohen and Orlik [3] and Terao [15].

6. THE RANK INVARIANT

Our study of multigraded objects shows that no complete discrete invariant exists for multidimensional persistence. We still desire a discriminating invariant that captures persistent information, that is, homology classes with large persistence. This information is not contained in our two discrete invariants, ξ_0 and ξ_1, as they capture birth and death coordinates of the generators in the complexes. What we need lies within the relationship between the two invariants or in the maps between the complexes. In this section, we propose and advocate a small and computable invariant that identifies persistent features in a multifiltration. Our invariant is equivalent to persistence barcodes, and therefore complete, for one-dimensional filtrations.

The persistent information is contained in the relating homomorphisms $\varphi_{u,v}$ in Definition 1. Recall that we incorporated these maps into a multigraded module through the action of the variables, requiring that $x^{v-u}\colon M_u \to M_v$ to be $\varphi_{u,v}$ in Definition 2. To analyze this family of maps, we begin by defining their domains.

Definition 10 ($\mathbb{D}^n$) Let $\dot{\mathbb{N}} = \mathbb{N} \cup \{\infty\}$ with $u \leq \infty$ for all $u \in \dot{\mathbb{N}}$. Let $\mathbb{D}^n \subset \mathbb{N}^n \times \dot{\mathbb{N}}^n$ be the subset above the diagonal, $\mathbb{D}^n = \{(u, v) \mid u \in \mathbb{N}^n, v \in \dot{\mathbb{N}}^n, u \lesssim v\}$. For $(u, v), (u', v') \in \mathbb{D}^n$, we define $(u, v) \preceq (u', v')$ if $u \lesssim u'$ and $v' \lesssim v$.

It is easy to check that $\preceq$ is a quasi-partial order on $\mathbb{D}^n$. With this notation, our parameterization of singly-graded modules in Section 1.3 is a multiset from $\mathbb{D}^1$, and $\preceq$ indicates the first pair contains the second, when the pairs are viewed as intervals.

Definition 11 (rank invariant ρ_M) Let M be a finitely generated n-graded A_n-module. We define $\rho_M\colon \mathbb{D}^n \to \mathbb{N}$ to be $\rho_M(u, v) = \operatorname{rank}(x^{v-u}\colon M_u \to M_v)$.

The function ρ_M is clearly a discrete invariant for M.

Lemma 7 (order-preserving) *If* $(u, v) \preceq (u', v')$*, then* $\rho_M(u, v) \leq \rho_M(u', v')$*, that is,* ρ_M *is an* order preserving *function from* $(\mathbb{D}^n, \preceq)$ *to* $(\mathbb{N}, \leq)$*.*

Proof: Immediate using the fact that given any composite $f \circ g$ of linear transformations, we have

$$\operatorname{rank}(f \circ g) \leq \operatorname{rank} f, \operatorname{rank} g.$$

□

We now state the rank invariant's completeness in one dimension through its equivalence to barcodes. We note that the following theorem is the converse of the *k-triangle Lemma* [7, 17].

Theorem 5 (completeness) *The rank invariant* ρ_M *is complete for singly-graded modules* M*.*

Proof: To prove completeness, we show equivalence via a bijection ϑ between the set of barcodes and the set of rank invariants. According to the classification theorem for a graded module M recalled in Section 1.3, the intervals in its barcode ξ capture the lifetimes of the generators of M. Therefore, the corresponding rank function is $\vartheta(\xi)(t, s) = \operatorname{card}\{((t', s'), i) \in \xi \mid (t, s) \subseteq (t', s')\}$. Figure 6 illustrates

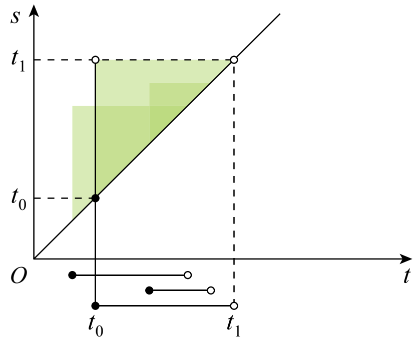


Figure 6: The intervals of a barcode ξ are drawn below the t-axis. Each interval (t_0, t_1) defines a triangle as shown. The rank function $\vartheta(\xi)(t, s)$ is the number of triangles that contain (t, s).

this correspondence. The barcode intervals are drawn below the t axis and the rank function's domain, $\mathbb{D}^1$, exists above the diagonal in the (t, s)-plane. Each interval $[t_0, t_1)$ has a triangular region defined by inequalities $t \geq t_0$, $s < t_1$, and $s \geq t$, with corner vertex (t_0, t_1) and vertices (t_0, t_0) and (t_1, t_1) on the diagonal. Half-infinite intervals correspond to degenerate triangles, but they are handled easily, so we do not discuss them here. The rank function $\vartheta(\xi)(t, s)$ is simply the number of triangles that contain (t, s). As an aside, we note that the map $(t, s) \mapsto (t, s - t)$ gives the index-persistence figures in the previous papers [7, 17].

Clearly, we can construct each triangle from its corner by projecting the corner vertically and horizontally onto the diagonal. Moreover, there is a trivial bijection between the corner (t_0, t_1) and the interval $[t_0, t_1)$. Given a barcode ξ, we know how to build the rank function $\vartheta(\xi)$ by the equation above. Given a rank function ρ, we need to identify the corner points to build the corresponding barcode. We begin by first walking along the diagonal until the rank function is nonzero at $t_0 = \operatorname{argmin}_t \rho(t, t) \neq 0$. By Lemma 7, the function $s \mapsto \rho(t_0, s)$ is a non-increasing function, so we walk vertically up until t_1 where $\rho(t_0, t_1) < \rho(t_0, t_0)$. The point (t_0, t_1) is a corner, so we subtract its triangle from ρ. The proof follows by induction. □

When the module is the persistence module associated to the ith homology of a multifiltration, we can define the rank invariant directly in terms of the input.

Definition 12 ($\rho_{X,i}$) Let $X = \{X_v\}_{v \in \mathbb{N}^n}$ be a multifiltration. We define $\rho_{X,i} \colon \mathbb{D}^n \to \mathbb{N}$ over field k to

$$\rho_{X,i}(u, v) = \operatorname{rank}(H_i(X_u, k) \to H_i(X_v, k)).$$

The function $\rho_{X,i}$ is a homeomorphism invariant of the multifiltered space, deriving its invariance from the invariance of ρ_M. Intuitively, Theorem 5 means that the rank invariant for one-dimensional filtrations may be separated into a set of overlapping triangles whose thickness at any point is the rank. These triangles, in turn, carry the same information as a set of intervals or the barcode. Our classification theorem, on the other hand, implies that a similar result is not possible for higher dimensions. As our example in Section 5.2illustrates, the picture is much more complicated: It is not possible to separate the rank invariant into overlapping "regions" to extend the barcode. However, the rank invariant does extend as an incomplete invariant and we may utilize it to identify persistent features by the following procedure. Given a rank invariant, we look for points $(u, v) \in \mathbb{D}^n$ that are far from the diagonal and have a neighborhood of constant value. The first condition corresponds to the persistence of the features. The second condition indicates the stability of our choice (u, v). With this procedure, the rank invariant emerges as a practical tool for reliable estimation of the Betti numbers of multifiltered spaces.

7. CONCLUSION

We believe the primary contribution of this paper is the full theoretical understanding of the structure of multidimensional persistence: We identify the corresponding algebraic structure, classify it, and undertake its parameterization. Our theory reveals that a complete discrete invariant does not exist for multidimensional persistence, unlike its one-dimensional counterpart. A second practical contribution of our paper is the rank invariant, a tool for robust estimation of the Betti numbers. We prove that the rank invariant is equivalent to the persistent barcode in one dimension, so it is complete when it can be. Unlike the barcode, the rank invariant extends to higher dimensions as an incomplete but useful invariant.

We have developed an algorithm for computing the rank invariant. For bifiltrations, the rank invariant is already four-dimensional, so we are examining possible interfaces for visualizing and exploring the rank invariant. We plan to apply our work toward automatic identification of features in multifiltrations, such as the filtered tangent complex [4].

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