Computing Multipersistence by Means of Spectral Systems

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ABSTRACT

In their original setting, both spectral sequences and persistent homology are algebraic topology tools defined from filtrations of objects (e.g. topological spaces or simplicial complexes) indexed over the set \mathbb{Z} of integer numbers. Recently, generalizations of both concepts have been proposed which originate from a different choice of the set of indices of the filtration, producing the new notions of *multipersistence* and *spectral system*. In this paper, we show that these notions are related, generalizing results valid in the case of filtrations over \mathbb{Z} . By using this relation and some previous programs for computing spectral systems, we have developed a new module for the Kenzo system computing multipersistence. We also present a new invariant providing information on multifiltrations and applications of our algorithms to spaces of infinite type.

CCS CONCEPTS

• Computing methodologies \rightarrow Computer algebra systems; Algebraic algorithms; • Mathematics of computing \rightarrow Mathematical software.

KEYWORDS

Symbolic Computation; Constructive Algebraic Topology; Multipersistence; Spectral systems; Effective homology.

ACM Reference Format:

Andrea Guidolin, Jose Divasón, Ana Romero, and Francesco Vaccarino. 2019. Computing Multipersistence by Means of Spectral Systems. In *International Symposium on Symbolic and Algebraic Computation (ISSAC '19), July 15–18, 2019, Beijing, China.* ACM, New York, NY, USA, 8 pages. https://doi.org/10. 1145/3326229.3326253

1 INTRODUCTION

Persistent homology [8, 32] is a technique in computational algebraic topology conceived to summarize the information of a filtration (usually of simplicial complexes) in the form of topological

ISSAC '19, July 15–18, 2019, Beijing, China

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ACM ISBN 978-1-4503-6084-5/19/07...\$15.00 https://doi.org/10.1145/3326229.3326253 Jose Divasón University of La Rioja Logroño, Spain jose.divason@unirioja.es

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invariants. Homology is used to study the topological features at each point of the filtration and to track their evolution across the whole filtration. Since simplicial complexes are in many situations convenient objects to be associated with data of different type (e.g. point clouds, networks, digital images), persistent homology represents a versatile method for the analysis of data, which significantly contributed to the development of *topological data analysis*.

Spectral sequences [20] are a tool in algebraic topology which provides information on the homology of a complex by means of successive approximations and are also defined by means of filtrations. The notions of persistent homology and spectral sequence are related, as explained in [1] using exact couples, a classical construction in algebraic topology, complementing a previous approach [24].

In their original setting, both spectral sequences and persistent homology are defined from filtrations with indices in \mathbb{Z} . Nevertheless, generalizations of both concepts have been proposed which originate from a different choice of the index set of the filtration. Multipersistence [3] is a generalization of persistent homology for filtrations with indices in \mathbb{Z}^m . On the other hand, spectral sequences have been generalized in [18] to the case of filtrations over any partially ordered set, producing the notion of spectral system.

In this paper we clarify the relation between generalized persistent homology and spectral systems in a general scenario, and use it to adapt our programs for spectral systems implemented in the Kenzo system [12] to perform useful computations in the context of multipersistence. In addition to computing well-studied invariants of multipersistence in a new way, which differentiates in some key aspects from all the available implementations, we propose and compute a new invariant for multipersistence. Our programs make use of the effective homology technique [27], which allows to computationally handle infinitely generated objects, extending in this way the domain of applicability of our algorithms. Furthermore, we describe how discrete vector fields [10] can be used to improve the programs, and we provide examples of applications.

The programs have been implemented as a new module for the computer algebra system Kenzo [7] and are available at:

http://www.unirioja.es/cu/anromero/research2.html

2 PRELIMINARIES

2.1 Multipersistence

In order to introduce *multipersistence*, also called *multiparameter* or *multidimensional persistence* by some authors, let us first illustrate some fundamental concepts of persistent homology theory over

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a fixed field \mathbb{F} . For more details and examples of applications we refer the reader to the surveys [9, 15].

A *finite* \mathbb{Z} -*filtration* of a simplicial complex *K* is a sequence of subcomplexes

$$\emptyset = \ldots = K_0 \subseteq \ldots \subseteq K_p \subseteq K_{p+1} \subseteq \ldots \subseteq K_N = \ldots = K.$$

Geometrical intuition is helpful to understand how the homology groups $H_n(K)$, and in particular the Betti numbers $\beta_n := \dim_{\mathbb{F}} H_n(K)$, describe the "topological" properties of K. Intuitively, we can say that β_n counts n-dimensional holes of $K: \beta_0$ is the number of connected components, β_1 the number of "tunnels", β_2 the number of "voids", and so on. The general idea of persistent homology is then to detect, using homology, the topological features which "persist" across the filtration. In order to do this, for every pair of indices $s \leq t$ in the filtration consider the map $f_n^{s,t}: H_n(K_s) \to H_n(K_t)$ induced in homology by the inclusion of simplicial complexes $K_s \hookrightarrow K_t$.

Definition 2.1. For every pair of indices $s \le t$ we define a *persistent n-homology group* $H_n^{s,t}(K)$ as the subspace of $H_n(K_t)$ given by the image of the map $f_n^{s,t}$:

$$H_n^{s,t}(K) \coloneqq \operatorname{Im}(f_n^{s,t} : H_n(K_s) \to H_n(K_t))$$

We denote its dimension (as \mathbb{F} -vector space) $\beta_n^{s,t} := \dim_{\mathbb{F}} H_n^{s,t}(K)$, called a *persistent Betti number*.

One says that a homology class *is born* at time $i \in \mathbb{Z}$ if it is an element of $H_n(K_i)$ not belonging to the image $\operatorname{Im} f_n^{i-1,i}$. A homology class in $H_n(K_{j-1})$ is then said to *die* at time $j \in \mathbb{Z}$ if its image under $f_n^{j-1,j}$ is zero, otherwise it is said to *persist*; the homology classes which persist until the last step $N \in \mathbb{Z}$ of the filtration are said to *live forever*. Note that for this intuition to be rigorous one has to fix bases of the vector spaces $H_n(K_i)$ in accordance with the Fundamental Theorem of Persistent Homology [32]: see [22, Remark 5]. Using this terminology, it is easy to see that for all i < j the non-negative integer

$$\mu_n^{i,j} \coloneqq (\beta_n^{i,j-1} - \beta_n^{i,j}) - (\beta_n^{i-1,j-1} - \beta_n^{i-1,j}) \tag{1}$$

is the number of distinct *n*-homology classes that are born at time *i* and die at time *j*. As first observed in [32], the collection $\{\beta_n^{i,j}\}$ of persistent Betti number is a *complete* topological invariant, intuitively meaning that it captures all the topological information of a filtration. This notion can be made precise by introducing *persistence modules* and considering their decomposition as $\mathbb{F}[x]$ -modules (see [32]).

In some applications a setting in which simplicial complexes vary according to two or more parameters may be more interesting, for example because the interplay of the parameters can reveal information on the data. Combining the different parameters, one can build a filtration along *m* axes, which potentially encodes much more information than *m* linear filtrations considered one at a time.

Definition 2.2. Consider \mathbb{Z}^m , endowed with the usual coordinatewise partial order \leq . A collection of simplicial complexes $(K_v)_{v \in \mathbb{Z}^m}$ such that $K_w \subseteq K_{w'}$ if $w \leq w'$ is called a \mathbb{Z}^m -filtration of simplicial complexes.

Definition 2.3. A \mathbb{Z}^m -filtration $(K_v)_{v \in \mathbb{Z}^m}$ of simplicial complexes is finite if there exists $w = (w_1, \ldots, w_m) \in \mathbb{Z}^m$ such that, for each i = 1, ..., m, the \mathbb{Z} -filtration obtained fixing m - 1 parameters except the *i*-th, here denoted $(\hat{K}_p^{(i)})_{p \in \mathbb{Z}}$, is finite, with

$$\emptyset = \ldots = \hat{K}_{-1}^{(i)} = \hat{K}_0^{(i)} \subseteq \hat{K}_1^{(i)} \subseteq \ldots \subseteq \hat{K}_{w_i}^{(i)} = \hat{K}_{w_i+1}^{(i)} = \ldots$$

Multipersistence [3] is a generalization of persistent homology which deals with \mathbb{Z}^m -filtrations instead of usual \mathbb{Z} -filtrations. The purpose is (again) to use homology to describe the evolution of topological features across a \mathbb{Z}^m -filtration of simplicial complexes. As we have seen, the ultimate goal of persistent homology is to provide an invariant, an object associated with a filtration which summarizes its topological properties. Unlike the 1-parameter case, there is no discrete complete invariant for multiparameter persistence. To support this claim, relying again on the concept of persistence module, one can endow the homology of a \mathbb{Z}^m -filtration with the structure of a $\mathbb{F}[x_1, \ldots, x_m]$ -module, and consider that the classification of $\mathbb{F}[x_1, \ldots, x_m]$ -modules is known to be very hard for m > 1. The impossibility to produce a complete invariant in the multiparameter case has been proved in [3] through algebraic geometry arguments, but more recently also arguments from quiver representation theory have been proposed (see for instance [23]). Nevertheless, invariants can be defined for multipersistence which are informative and relatively easy to compute. One of the most relevant in applications is the rank invariant, an immediate generalization of persistent Betti numbers proposed in [3].

Definition 2.4. Let $(K_{\upsilon})_{\upsilon \in \mathbb{Z}^m}$ be a \mathbb{Z}^m -filtration of simplicial complexes and let $\upsilon \leq w$ in \mathbb{Z}^m . We denote $f_n^{\upsilon, w} : H_n(K_{\upsilon}) \to H_n(K_w)$ the map induced in homology by the inclusion $K_{\upsilon} \hookrightarrow K_w$ and define

$$\beta_n^{\upsilon,w} \coloneqq \dim_{\mathbb{F}} \operatorname{Im}(f_n^{\upsilon,w} : H_n(K_{\upsilon}) \to H_n(K_w)).$$

The collection of all $\beta_n^{v,w}$, for every pair of indices $v \le w$ and for every *n*, is called *rank invariant* of the \mathbb{Z}^m -filtration.

Even if in the present work we will focus mainly on the rank invariant, we want to recall that other invariants have been proposed for multipersistence [2, 4–6, 13, 16, 21, 30, 31].

Let us remark that clearly every \mathbb{Z}^m -filtration of simplicial complexes determines a \mathbb{Z}^m -filtration of chain complexes. Although we have chosen to introduce persistence theory and multipersistence using filtrations of simplicial complexes, in the following sections we will consider the more general framework of filtered chain complexes.

2.2 Spectral systems

Spectral systems are a construction that extends the classical definition of spectral sequence [20] to the case of filtrations indexed over a partially ordered set (*poset*).

Definition 2.5. A filtration of a chain complex $C_* = (C_n, d_n)$ over a poset (I, \leq) , briefly called an *I*-filtration, is a collection of chain subcomplexes $F = (F_iC_*)_{i \in I}$ such that $F_iC_* \subseteq F_jC_*$ whenever $i \leq j$ in *I*. We will often denote the chain subcomplexes simply as F_i , forgetting about the grading of homology, when we are only interested in the filtration index *i*. Now, recall that for classical spectral sequences, which arise from a \mathbb{Z} -filtration $(F_p)_{p \in \mathbb{Z}}$, we have the formula (see [17]):

$$E_{p,q}^{r} = \frac{F_{p}C_{n} \cap d^{-1}(F_{p-r}C_{n-1}) + F_{p-1}C_{n}}{d(F_{p+r-1}C_{n+1}) \cap F_{p}C_{n} + F_{p-1}C_{n}},$$

where we can see the interplay of 4 filtration indices: p - r, p - 1, p and p + r - 1.

In [18], this formula was imitated and generalized to the case of *I*-filtrations by defining, for every 4-tuple of indices $z \le s \le p \le b$ in *I*, the *term*

$$S_n[z, s, p, b] := \frac{F_p C_n \cap d^{-1} (F_z C_{n-1}) + F_s C_n}{d (F_b C_{n+1}) \cap F_p C_n + F_s C_n}.$$
 (2)

The collection of all such terms is called a *generalized spectral* sequence or a spectral system for the *I*-filtration $(F_i)_{i \in I}$.

Generalized spectral sequences are in many aspects similar to classical ones. For example, the next result extends what in the classical case is the way of obtaining terms of the page r + 1 by taking homology at page r:

PROPOSITION 2.6 ([18]). Given an I-filtration $(F_i)_{i \in I}$ for a chain complex C_* and three 4-tuples of indices satisfying the condition

$$z_1 \leq s_1 \leq p_1 = z_2 \leq b_1 = s_2 \leq p_2 = z_3 \leq b_2 = s_3 \leq p_3 \leq b_3,$$

the differential of the chain complex C_* induces differentials d_3, d_2 between the terms

$$S_{n+1}[z_3, s_3, p_3, b_3] \xrightarrow{d_3} S_n[z_2, s_2, p_2, b_2] \xrightarrow{d_2} S_{n-1}[z_1, s_1, p_1, b_1]$$

and by taking homology we obtain

$$\frac{\operatorname{Ker} d_2}{\operatorname{Im} d_3} = S_n[s_1, s_2, p_2, p_3].$$

The paper [18] includes some explicit examples of spectral systems which generalize for instance the classical spectral sequences of Serre, Eilenberg–Moore and Adams–Novikov. However, as in the case of spectral sequences associated with a linear filtration, no algorithm is provided to compute the different components when the initial chain complexes are not finitely generated. Thanks to the method of *effective homology* [27], in [12] we developed an algorithm for computing spectral systems of spaces (possibly) of infinite type. The corresponding programs were implemented as a new module for the system Kenzo [7], a symbolic computation software written in Common Lisp and devoted to algebraic topology, solving in this way also the classical problems of spectral sequences: determining differential maps and extensions. The effective homology method was also used by the third author in [25] for computing spectral sequences in the case of Z-filtrations.

3 RELATION BETWEEN SPECTRAL SYSTEMS AND MULTIPERSISTENCE

In [1], a relation between spectral sequences and persistent homology (both defined for \mathbb{Z} -filtrations and taking homology over a fixed field \mathbb{F}) is proved by means of the classical notion of *exact couples*. Without going into details, exact couples are collections of long exact sequences, with an additional hypothesis on the involved modules, which can be *derived* to obtain new exact sequences. From long exact sequences involving terms $E_{p,q}^r$ of the spectral sequence as well as persistent homology groups $H_n^{s,t}$, a relation between the dimensions of these vector spaces is found [1]:

$$\lim_{\mathbb{F}} E_{p,q}^{r} = \beta_{n}^{p,p+r-1} - \beta_{n}^{p-1,p+r-1} + \beta_{n-1}^{p-r,p-1} - \beta_{n-1}^{p-r,p},$$

for all integers p, q, r with $r \ge 1$ and n := p + q. This relation can be inverted, to express every persistent Betti number $\beta_n^{s,t}$ as a combination of the dimensions $\dim_{\mathbb{F}} E_{p,q}^r$. The existence of these relations intuitively means that the collections of integers $\{\beta_n^{s,t}\}$ and $\{\dim_{\mathbb{F}} E_{p,q}^r\}$ carry the same amount of topological information about the filtration. In this section, we briefly show how this relation can be generalized for the case of filtrations over a poset I (with some additional hypotheses), referring the reader to [11] for further details. We denote $-\infty$ the minimum of the poset I, which can be added "artificially" to the poset if needed, and we suppose that $F_{-\infty} = 0$.

The notion of exact and derived couples is generalized for *I*-filtrations in [18, Definition 4.1] and referred to by the expression *exact couple system*. An exact couple system is again a collection of particular long exact sequences, where now the involved spaces are indexed over the poset *I*. Incidentally, exact couple systems can be seen as a way to define spectral systems that is even more general than the one we presented in Section 2.2. Before employing some long exact sequences of the exact couple system to deduce the sought relation, we introduce some relevant definitions.

Firstly, let us state the natural generalization of the rank invariant (Definition 2.4) that we will use in what follows. Given an *I*-filtration $(F_i)_{i \in I}$ and $v \le w$ in *I*, we define

$$\beta_n(v, w) \coloneqq \dim_{\mathbb{F}} \operatorname{Im}(\ell : H_n(F_v) \to H_n(F_w)),$$

where ℓ is the map induced by the inclusion $F_{\upsilon} \hookrightarrow F_{w}$; we call *rank invariant* the collection of all $\beta_{n}(\upsilon, w)$, for any n and any $\upsilon \leq w$.

Now, let us introduce the class of poset that we consider in the present section. A *partially ordered abelian group* $(I, +, \le)$ is an abelian group (I, +) endowed with a partial order \le that is *translation invariant*: for all $p, t, t' \in I$, if $t \le t'$ then $p + t \le p + t'$.

The idea detailed in [11] is the following: given an *I*-filtration with *I* a partially ordered abelian group and starting from a collection of "simple" long exact sequences (relative homology) defined from the filtration, one can *derive* them to obtain long exact sequences of the form

$$\cdots \to S_n[-\infty, -\infty, p-\upsilon, p-\upsilon+w] \xrightarrow{\ell} S_n[-\infty, -\infty, p, p+\upsilon+w]$$

$$\xrightarrow{\ell} S_n[p-\upsilon-w, p-\upsilon, p, p+w] \xrightarrow{k} S_{n-1}[-\infty, -\infty, p-\upsilon-w, p-\upsilon]$$

$$\xrightarrow{\ell} S_{n-1}[-\infty, -\infty, p-w, p] \to \cdots$$
(3)

for all $p, v, w \in I$ such that $v, w \ge 0$, where the maps denoted by ℓ are induced by inclusion, and k is induced by the differential. This can be obtained by repeatedly using Proposition 2.6 for conveniently chosen indices, and by observing that if $p \le u$ and $b \le t$ in I then

$$S_n[-\infty, -\infty, p, t] = \operatorname{Im}(\ell : S_n[-\infty, -\infty, p, b] \to S_n[-\infty, -\infty, u, t]).$$

Since in particular $S_n[-\infty, -\infty, p, t] = \text{Im}(\ell : H_n(F_p) \to H_n(F_t))$, which yields by definition $\dim_{\mathbb{F}} S_n[-\infty, -\infty, p, t] = \beta_n(p, t)$, from (3) one can express $\dim_{\mathbb{F}} S_n[p - v - w, p - v, p, p + w]$ as

$$\beta_n(p,p+w)-\beta_n(p-\upsilon,p+w)+\beta_{n-1}(p-\upsilon-w,p-\upsilon)-\beta_{n-1}(p-\upsilon-w,p),$$

which represents the generalization we sought for.

Applying this argument to \mathbb{Z}^m -filtrations, one can conclude that the spectral system over \mathbb{Z}^m carries the same amount of topological information on the filtration as the rank invariant of Definition 2.4, as the collections $\{\dim_{\mathbb{F}} S[z, s, p, b]\}$ and $\{\beta_n^{v, w}\}$ can be determined one from the other.

In Section 5 we present a second application of the previous argument, considering a different poset related to multipersistence.

4 GENERALIZING THE RANK INVARIANT IN THE FINITE CASE

As we mentioned in Section 2, a number of invariants for multipersistence have been proposed, and a few implementations are available. Let us name some of them, addressing the interested reader to recent works like [29] for a more complete list of references. In [2] the authors propose an efficient algorithm to compute invariants associated with resolutions of modules constructed from \mathbb{Z}^m -filtrations, although some restrictive assumptions are made on the type of filtrations; a more general framework is studied in [5]. In [4] the study of a \mathbb{Z}^m -filtration is reduced to a family of \mathbb{Z} -filtrations corresponding to linear sections with different slopes. This idea has been further developed in [16], together with the theoretical bases of the software RIVET for visualizing 2-parameter persistence. The paper [13] presents an interesting approach via commutative algebra. Efficient methods to deal with a particular class of 2-parameter persistence modules are introduced in [6]. In [30] an algebraic definition of noise (negligible topological features) for multipersistence is introduced and some related invariants are studied. Real multipersistence modules are studied in [21]; to this aim, downsets (see below) in \mathbb{R}^m play a key role. Generalized persistent homology and its relation with filtrations of weighted graphs is studied in [31].

Trying to generalize the existing programs, each of which was developed to deal with particular situations, we propose a new implementation of multipersistence as a new module for the system Kenzo, making use of our previous programs for computing spectral systems presented in [12]. Our new programs are in several respects more general than the existing ones, since they compute multipersistence over integer coefficients and they can be applied to filtrations over any poset. Moreover, as we will show in Section 6, our algorithms can be used to determine multipersistence of spaces of infinite type, a characteristic which up to now has not been considered in the available multipersistence software. Our programs are written in the Common Lisp programming language, making use of functional programming to deal with infinite spaces and general posets.

Since we start from persistent homology groups and the rank invariant, we first extend the computation of these notions to the case of *I*-filtrations. Let $(F_i)_{i \in I}$ be an *I*-filtration of a chain complex C_* and $v \leq w$ in *I*. We consider the quotient group

$$H_n^{\upsilon,w} \coloneqq \frac{F_{\upsilon}C_n \cap \operatorname{Ker} d_n}{F_{\upsilon}C_n \cap d(F_wC_{n+1})},\tag{4}$$

called a (generalized) persistent homology group, which clearly represents the homology classes in $H_n(F_v)$ which are still present in $H_n(F_w)$, that is, it corresponds to $\text{Im}(\ell : H_n(F_v) \to H_n(F_w))$. When computing this group with coefficients in a field, its rank



Figure 1: Small simplicial complex filtered over \mathbb{Z}^2 .

corresponds to the rank invariant. In our case, we have developed a Kenzo function computing the group with integer coefficients, producing not only the rank but also the generators and the torsion coefficients. Our programs use some previous functions computing spectral systems developed in [12], since some of the subgroups appearing in the quotient (4) are similar to the subgroups appearing in the spectral system terms (2). Once these subgroups are determined, the corresponding quotient can be computed by means of diagonalization algorithms of matrices in a similar way to the algorithm used to compute homology groups by means of the Smith Normal Form technique (see [14]).

As a didactic example, let us consider the chain complex endowed with a (finite) \mathbb{Z}^2 -filtration associated with the filtered simplicial complex of Figure 1, which shows, corresponding to each of the points (1, 1), (1, 2), (1, 3), ..., (3, 3) $\in \mathbb{Z}^2$, a simplicial complex constituted by 0-simplices (points a, b, c, \ldots), 1-simplices (edges ab, ac, \ldots) and 2-simplices (the triangles bcd and cde). For example, in degree 1, there are two homology classes (1-dimensional holes) which live in $F_{(1,2)}$ and still live in $F_{(2,2)}$, so that $H_1^{(1,2),(2,2)} = \mathbb{Z}^2$, with generators given by the combinations 1 * ab - 1 * ac + 1 * bc and -1 * ab + 1 * ac - 1 * bd + 1 * cd. However, there is only one class which lives in $F_{(1,2)}$ and still lives in $F_{(3,3)}$, so that $H_1^{(1,1),(3,3)} = \mathbb{Z}$, generated in this case by the combination 1 * ab - 1 * ac + 1 * bc. The second class has *died* because the triangle *bcd* has been filled.

> (multiprst-group K '(1 2) '(2 2) 1) Multipersistence group H[(1 2),(2 2)]_{1} Component Z > (multiprst-gnrts K '(1 2) '(2 2) 1) ({CMBN 1}<1 * AB><-1 * AC><1 * BC> {CMBN 1}<-1 * AB><1 * AC><-1 * BD><1 * CD>) > (multiprst-group K '(1 2) '(3 3) 1) Multipersistence group H[(1 2),(3 3)]_{1} Component Z > (multiprst-gnrts K '(1 2) '(3 3) 1) ({CMBN 1}<1 * AB><-1 * AC><1 * BC>) In this case, we can observe that all the per

In this case, we can observe that all the persistent homology groups are free; in Section 6 we will present meaningful examples of results with non-null torsion coefficients.

Let us finish this section by observing with a simple example that the rank invariant is not complete, in the sense that sometimes it is unable to discriminate between *different* filtrations. To this



Figure 2: Second filtration for the small simplicial complex filtered over \mathbb{Z}^2 .

aim, let us consider a second filtration for the example of Figure 1, given by Figure 2. The filtrations are different and the associated persistence modules are not isomorphic, but the rank invariant of both filtrations is the same.

5 COMPUTATION OF A NEW INVARIANT

Consider the case of 1-parameter persistent homology, defined from \mathbb{Z} -filtrations. We recall the definition

$$M_n^{i,j} := \frac{F_i C_n \cap d(F_j C_{n+1}) + F_{i-1} C_n}{F_i C_n \cap d(F_{j-1} C_{n+1}) + F_{i-1} C_n}$$
(5)

of *birth-death modules* given in [24], therein denoted $BD_n^{i,j}$. When homology is computed over a field, the rank of $M_n^{i,j}$ is given by the quantity $\mu_n^{i,j}$ of equation (1), representing the number of homology classes which are born at step *i* (meaning that these classes are present at step *i* but they are not present at the previous step *i* – 1) and die at step *j* of the filtration (that is, they are present at the previous step *j* – 1 but they are not present at step *j* because they are boundaries or they merge with another class).

For multipersistence, the concepts of birth and death of a homology class cannot be immediately generalized from the 1-parameter case (but see [13, 21] for interesting approaches). For example, in Figure 1 we cannot say that the 1-homology class (1-hole) corresponding to the generator 1 * bc - 1 * bd + 1 * cd is born at a unique particular position of \mathbb{Z}^2 (because it is present at both positions (1, 2) and (2, 1) and for both of them it is not present at a previous step). Moreover, because of the lack of a decomposition theorem for multipersistence modules (see Section 2.1), the definition of birth and death can depend on the choice of bases for each $H_n(F_v)$.

However, we can try to mimic the formula (5) to "empirically" define an invariant which, as we will see in some example, is able to extract information from multiparameter filtrations. In order to define this new invariant we consider a poset different from \mathbb{Z}^m , given by the *downsets* of \mathbb{Z}^m , which is used in [18] to gain more options in the construction of generalized spectral sequences and which will allow us to say that a homology class is born or dead at different positions in \mathbb{Z}^m .

Definition 5.1. A downset of \mathbb{Z}^m is a subset $A \subseteq \mathbb{Z}^m$ such that if $Q \leq P$ in \mathbb{Z}^m and $P \in A$, then $Q \in A$; the poset $D(\mathbb{Z}^m)$ is the collection of all downsets of \mathbb{Z}^m , endowed with the partial order given by inclusion \subseteq . Filtering data with respect to *m* parameters produces in a natural way, in addition to the \mathbb{Z}^m -filtration $(F_P)_{P \in \mathbb{Z}^m}$ we used in previous sections, also a $D(\mathbb{Z}^m)$ -filtration (F_p) defined, for each $p \in D(\mathbb{Z}^m)$, as $F_p := \sum_{P \in p} F_P$. Moreover, we have observed that computing the terms of the spectral system over $D(\mathbb{Z}^m)$ produces more topological information than the rank invariant; in particular, (some groups of) the spectral system of filtrations defined in Figures 1 and 2 are different, so that the spectral system of the filtration over $D(\mathbb{Z}^m)$ can therefore be considered as an invariant associated with a filtration which allows to discriminate between a larger number of topological features.

At this point, it seems natural to investigate possible relations between the rank invariant and the spectral system over $D(\mathbb{Z}^m)$, as we did in Section 3 for \mathbb{Z}^m -filtrations. In this case, since there is no natural additive structure on $D(\mathbb{Z}^m)$ that turns it into a partially ordered abelian group, we have to be more subtle. The easiest way to construct a partially ordered abelian group starting from $D(\mathbb{Z}^m)$ is to consider the translation of a fixed downset $p \in D(\mathbb{Z}^m)$. Denoting T_p the family of all downsets of $D(\mathbb{Z}^m)$ obtained translating p by any $v \in \mathbb{Z}^m$, we see that $(T_p, \text{translation}, \subseteq)$ is a partially ordered abelian group. We can now apply the results in Section 3, including (3), using the poset $(T_p, \text{translation}, \subseteq)$, and combining this with results on isomorphic terms within a spectral system [18, Lemma 3.8] one can obtain interesting relations.

We give now our definition of new invariant. Consider a downset $p \in D(\mathbb{Z}^m)$ that is *defined* by the list $\{P_1, \ldots, P_k\}$ of points of \mathbb{Z}^m , in the sense that $\{P_1, \ldots, P_k\}$ is the minimal set such that each point of p is \leq to one of these points P_j . Analogously, consider a downset $b \in D(\mathbb{Z}^m)$ defined by the list of points $\{B_1, \ldots, B_r\}$.

Definition 5.2. Let (F_P) be a \mathbb{Z}^m -filtration and consider the canonically associated $D(\mathbb{Z}^m)$ -filtration $(F_p := \sum_{P \in p} F_P)$. For each $p \le b$ in $D(\mathbb{Z}^m)$ we define

$$M_n^{p,b} \coloneqq \frac{\hat{F}_p C_n \cap d(\hat{F}_b C_{n+1})}{A_{p,n} + B_{b,n}}$$

where

$$\begin{aligned} \hat{F}_p C_n &\coloneqq \{\sigma | \sigma \in F_{P_j} C_n \text{ for all } 1 \le j \le k\} = \bigcap_j F_{P_j} C_n \\ A_{p,n} &\coloneqq \sum_Q (\hat{F}_p C_n \cap d(\hat{F}_b C_{n+1}) \cap F_Q C_n) \\ &+ \sum_X (\hat{F}_p C_n \cap d(\hat{F}_b C_{n+1}) \cap F_X C_n) \end{aligned}$$

with $Q \in \mathbb{Z}^m$ not comparable with the points P_j defining the downset p and $X \in p \setminus \{P_1, \ldots, P_k\}$, and

$$B_{p,n} \coloneqq \sum_{R} (\hat{F}_p C_n \cap d(\hat{F}_b C_{n+1}) \cap d(F_R C_{n+1})) + \sum_{Y} (\hat{F}_p C_n \cap d(\hat{F}_b C_{n+1}) \cap d(F_Y C_{n+1}))$$

with $R \in \mathbb{Z}^m$ not comparable with the points B_j defining the downset *b* and $Y \in b \setminus \{B_1, \ldots, B_r\}$.

Intuitively, the groups $M_n^{p,b}$ try to represent the homology classes being born in F_p and dying in F_b , where now the downsets p and bare defined by several positions in \mathbb{Z}^m . As said before, the notions of birth and death are not rigorous as in the (1-parameter) persistent homology framework because they depend on the choice of bases for each $H_n(F_v)$.

Using again our previous programs for computing spectral systems, we have implemented in Kenzo functions for computing the groups $M_n^{p,b}$ which, as before, produce not only the groups but also the generators. For example, let us consider again the filtered complex in Figure 1 and the downsets p = ((1, 2), (2, 1)) (meaning *defined* by $\{(1, 2), (2, 1)\}$) and b = ((1, 3), (3, 2)). The group $M_1^{p,b}$ is equal to \mathbb{Z} , with generator 1 * bc - 1 * bd + 1 * cd. This means intuitively that the homology class corresponding to the boundary of the triangle *bcd* is born at positions (1, 2) and (2, 1) and dies at positions (1, 3) and (3, 2).

One of the advantages of the use of the poset $D(\mathbb{Z}^m)$ and the definition of this new invariant is that it makes it possible to distinguish filtrations which, as we have seen in Section 4, sometimes have the same rank invariant. Let us consider again the generalized filtrations described in Figures 1 and 2 (with the same rank invariant) and the downsets p = ((1, 3), (2, 2), (3, 1)) and b = ((2, 3), (3, 2)); the group $M_1^{p,b}$ is equal to \mathbb{Z} in the first filtration, with generator 1 * cd - 1 * ce + 1 * de and the 0-group (NIL) in the second one (because in that filtration these homology class is born at a smaller downset, ((1, 3), (2, 1))).

({CMBN 1}<1 * CD><-1 * CE><1 * DE>)

Multipersistence group M[((1 3) (2 2) (3 1)),((2 3) (3 2))]_{1} NIL

6 EFFECTIVE HOMOLOGY FOR INFINITELY GENERATED SPACES

Effective homology [27, 28] is a technique developed to computationally determine the homology of complicated spaces. We briefly introduce the notions necessary to understand the method, before showing how it can be used in the context of persistent homology.

Definition 6.1. A reduction $\rho := (D_* \Rightarrow C_*)$ between two chain complexes D_* and C_* is a triple (f, g, h) where: (a) The components f and g are chain complex morphisms $f : D_* \to C_*$ and $g : C_* \to$ D_* ; (b) The component h is a morphism of graded modules $h : D_* \to$ D_{*+1} of degree +1; (c) The following relations must be satisfied: (1) $fg = id_{C_*}$; (2) $gf + d_{D_*}h + hd_{D_*} = id_{D_*}$; (3) fh = 0; (4) hg = 0; (5) hh = 0.

Since f is a chain equivalence between D_* and C_* , in particular the homology groups $H_n(D_*)$ and $H_n(C_*)$ are canonically isomorphic, for each n.

Definition 6.2. An effective chain complex C_* is a free chain complex (i.e., a chain complex consisting of free \mathbb{Z} -modules) where

each group C_n is finitely generated, and there is an algorithm that returns a \mathbb{Z} -base in each degree *n*.

Intuitively, an effective chain complex C_* is a chain complex whose homology can be easily determined via standard diagonalization algorithms (see [14]).

Definition 6.3. A chain complex C_* has effective homology if there exist a chain complex D_* , an effective chain complex EC_* and two reductions $C_* \Leftarrow D_* \Rightarrow EC_*$.

The technique of effective homology has been implemented in the system Kenzo, which is able to automatically construct the reductions $C_* \Leftarrow D_* \Rightarrow EC_*$ in several situations arising in algebraic topology and homological algebra. In the scenario of the previous definition, the method of effective homology allows to determine the homology groups of the original chain complex C_* by using EC_* to perform the computations. In this way, Kenzo is able to determine homology and homotopy groups of complicated spaces, even when the chain complex C_* is not finitely generated (resulting thus untreatable by standard algorithms), and has shown its potentiality successfully computing previously unknown results [28].

Now, we want to show how the effective homology technique can be applied to compute persistent homology groups. First, let us study the behavior of reductions when we introduce *I*-filtrations on the involved chain complexes. Let *F* (resp. *F'*) be an *I*-filtration of a chain complex D_* (resp. C_*), and let *S* (resp. *S'*) denote the terms of the associated spectral system. In [12] we stated the following result.

THEOREM 6.4. Let $\rho = (f, g, h) : D_* \Rightarrow C_*$ be a reduction between the I-filtered chain complexes (D_*, F) and (C_*, F') , and suppose that f and g are compatible with the filtrations, that is, $f(F_i) \subseteq F'_i$ and $g(F'_i) \subseteq F_i$ for all $i \in I$. Then, given four indices $z \le s \le p \le b$ in I, the map f induces an isomorphism

$$f^{z,s,p,b}: S[z,s,p,b] \to S'[z,s,p,b]$$

whenever the homotopy $h : D_* \to D_{*+1}$ satisfies the conditions $h(F_z) \subseteq F_s$ and $h(F_p) \subseteq F_b$.

Now, taking into account now the relations between multipersistence and spectral systems studied in Section 3, we obtain the following corollary.

COROLLARY 6.5. In the situation of Theorem 6.4, we have in particular that the map f induces isomorphisms

$$H_n^{p,b}(D_*) = S_n[-\infty, -\infty, p, b] \to H_n^{p,b}(C_*) = S'_n[-\infty, -\infty, p, b]$$

whenever the homotopy $h : D_* \to D_{*+1}$ satisfies the condition $h(F_p) \subseteq F_b$.

Clearly, if in Corollary 6.5 the map h is also compatible with the filtrations, we have $H_n^{p,b}(D_*) \cong H_n^{p,b}(C_*)$ for all $p \le b$ in I. This new result provides us a method for computing persistent homology groups of spaces of infinite type when the effective homology of the space is known. This method has been implemented in Kenzo and can be applied to complicated spaces filtered over general posets.

Considering now the new invariant $M_n^{p,b}$ introduced in Section 5, we proved the following result.

THEOREM 6.6. Let $\rho = (f, g, h) : D_* \Rightarrow C_*$ be a reduction between the I-filtered chain complexes (D_*, F) and (C_*, F') , let $p \leq b$ in I and let us suppose that f and g are compatible with the filtrations and h satisfies the condition $h(\hat{F}_p) \subseteq \sum_R F_R + \sum_Y F_Y$ with $R \in \mathbb{Z}^m$ not comparable with the points B_j defining the downset b and $Y \in b \setminus \{B_1, \ldots, B_r\}$. Then, the map f induces, for every degree n, isomorphisms

$$f_n^{p,b}: M_n^{p,b}(D_*) \to M_n^{p,b}(C_*).$$

The proof is similar to that of Theorem 6.4, detailed in [11]. If the map *h* is compatible with the filtrations, then we can deduce $M_n^{p,b}(D_*) \cong M_n^{p,b}(C_*)$ for every p < b.

An example of situation where the computation of multipersistence of infinite spaces makes sense corresponds to twisted Cartesian products [19] of simplicial sets where at least one of the involved spaces is of infinite type. Twisted Cartesian products are obtained as total spaces of towers of fibrations and multipersistence provides then information on the interaction of the homology groups of the different components in the product.

For example, let us consider the first stages of the Postnikov tower for computing the homotopy groups of the sphere S^3 , given by the following tower of fibrations:

$$\begin{array}{cccc} X_6 & & & X_5 & & & X_4 & & & B = S^3 \\ \uparrow & & \uparrow & & \uparrow & & \uparrow \\ G_4 = K(\mathbb{Z}_2, 4) & & G_3 = K(\mathbb{Z}_2, 3) & & G_2 = K(\mathbb{Z}, 2) \end{array}$$

The first total space X_4 can be seen as a twisted Cartesian product $X_4 \equiv K(\mathbb{Z}, 2) \times_{\tau_4} S^3$, where $K(\mathbb{Z}, 2)$ is an Eilenberg–MacLane space [19]. The second one X_5 is given by $X_5 \equiv K(\mathbb{Z}_2, 3) \times_{\tau_5}$ $X_4 \equiv K(\mathbb{Z}_2, 3) \times_{\tau_5} (K(\mathbb{Z}, 2) \times_{\tau_4} S^3)$ and finally X_6 is equal to $X_6 \equiv$ $K(\mathbb{Z}_2, 4) \times_{\tau_6} X_5 \equiv K(\mathbb{Z}_2, 4) \times_{\tau_6} (K(\mathbb{Z}_2, 3) \times_{\tau_5} (K(\mathbb{Z}, 2) \times_{\tau_4} S^3))$. See [19] for the construction of this tower, which satisfies $H_n(X_n) \cong \pi_n(S^3)$.

The total space X_6 can be filtered over $D(\mathbb{Z}^3)$ (3 = "number of fibrations") by using the degeneracy degrees of the simplices, so that multipersistence can be studied. Let us observe that one of the factors, in this case $K(\mathbb{Z}, 2)$, is not of finite type, so that the rank invariant can not be directly determined. However, the effective homology method implemented in Kenzo and our Corollary 6.5 make it possible to determine the groups.

In this example, our results allow us to reproduce the result $\pi_6(S^3) \cong H_6(X_6) \cong \mathbb{Z}/12\mathbb{Z}$ given by the group $H_6^{((7,7,7)),((7,7,7))}$:

> (multiprst-group X6 (list '(7 7 7)) (list '(7 7 7)) 6)
Multipersistence group H[((7 7 7)),((7 7 7))]_{6}
Component Z/12Z

In a context like this, the computation of multipersistence can reveal interesting information not only on the homology of individual spaces, but also on the role played by the filtration, as we see for example for the group $H_6^{((6,6,6)),((7,6,6))} = \mathbb{Z}/4\mathbb{Z} \oplus \mathbb{Z}$.

> (multiprst-group X6 (list '(6 6 6)) (list '(7 6 6)) 6)
Multipersistence group H[((6 6 6)),((7 6 6))]_{6}
Component Z/4Z
Component Z

We want to stress the important role of Corollary 6.5 and Theorem 6.6 in this situation, as they characterize the persistent homology groups that can be computed correctly using effective homology in terms of the behavior of the homotopy operators h of the involved reductions, which can be determined explicitly.

Notice that the system Kenzo is able to handle simplicial sets, which are more general and versatile than simplicial complexes; this allows it to deal with a broader variety of situations. The method of effective homology further enlarges the range of objects in algebraic topology it can compute and manipulate. To our knowledge, Kenzo is the only available software to make computations on filtrations of infinitely generated chain complexes, like the ones involved in the previous example.

7 IMPROVING THE ALGORITHMS VIA DISCRETE VECTOR FIELDS

The ability of the system Kenzo to exploit the relationship between different chain complexes is brought one step further by the use of *discrete vector fields*, a notion introduced by Robin Forman [10] which proved itself incredibly useful in computational algebraic topology. In what follows we briefly describe how discrete vector fields can simplify the computation of generalized persistent homology.

Let $C_* = (C_n, d_n)$ be a free chain complex with distinguished \mathbb{Z} -bases $B_n \subset C_n$, whose elements we call *n*-cells. A discrete vector field *V* on C_* is a collection of pairs of cells $V = \{(\sigma_k; \tau_k)\}_{k \in K}$ satisfying specific conditions (see [26, Definition 5]). Let us point out that we do not require the distinguished bases B_n or the vector field *V* to be finite.

A cell $\sigma \in B_n$ which does not appear in the discrete vector field *V* is called a *critical n-cell*. The relevance of critical cells is given by the fact that, if the discrete vector field is *admissible* (see [26, Definition 9]), they are sufficient to capture the homology of the chain complex C_* , as described in the following fundamental result.

THEOREM 7.1. ([10, 26]) Let $C_* = (C_n, d_n, B_n)$ be a free chain complex and $V = \{(\sigma_k; \tau_k)\}_{k \in K}$ be an admissible discrete vector field on C_* . Then the vector field V defines a canonical reduction $\rho = (f, g, h) : (C_n, d_n) \Rightarrow (C_n^c, d_n')$ where C_n^c is the free \mathbb{Z} -module generated by critical n-cells and d_n' is an appropriate differential canonically defined from C_* and V.

Theorem 7.1, together with Kenzo's algorithms for automatically constructing admissible discrete vector fields [26], allows to compute the homology groups $H_n(C_*) \cong H_n(C_*^c)$ working with the chain complex C_*^c of reduced size.

We now want to add *I*-filtrations to the picture, in order to show the relevance of discrete vector fields in the computation of persistent homology groups. Notice that in a canonical reduction $\rho : (C_n, d_n) \Rightarrow (C_n^c, d_n')$, an *I*-filtration defined on the chain complex C_* canonically induces an *I*-filtration on C_*^c .

Definition 7.2. Let $C_* = (C_n, d_n, B_n)$ be a free chain complex with an *I*-filtration *F* and let $V = \{(\sigma_k; \tau_k)\}_{k \in K}$ be a discrete vector field on C_* . If $\sigma_k \in F_i \iff \tau_k \in F_i$ for all $i \in I$ and for all $k \in K$ we say that *V* is *compatible* with the *I*-filtration *F*.

THEOREM 7.3. ([11]) If C_* is endowed with an I-filtration F and $V = \{(\sigma_k; \tau_k)\}_{k \in K}$ is an admissible discrete vector field on C_* which is

compatible with F, then the three maps of the the canonical reduction $\rho = (f, g, h) : (C_n, d_n) \Rightarrow (C_n^c, d_n')$ described in Theorem 7.1 are compatible with the filtrations.

Corollary 6.5 tells us that discrete vector fields can be used to speed up the computation of all persistent homology groups.

COROLLARY 7.4. In the situation of Theorem 7.3, the map f of the reduction $\rho = (f, g, h) : (C_n, d_n) \Rightarrow (C_n^c, d_n')$ induces isomorphisms $H_n^{p,b}(C_*) \cong H_n^{p,b}(C_*^c)$ for all $p \le b$ in I and $M_n^{p,b}(C_*) \cong M_n^{p,b}(C_*^c)$ for all p < b in I.

Making use of this result and of Kenzo algorithms for computing admissible discrete vector fields [26] we have enhanced our programs computing multipersistence.

8 CONCLUSIONS AND FURTHER WORK

We presented a set of programs for performing computations on chain complexes with filtrations defined over posets. The programs allow to compute generalized persistent homology, and in particular some relevant invariants in the context of multipersistence. Although, due to the necessary adjustments to deal with infinite spaces, our programs are not as efficient as previous existing implementations with polynomial complexity, we provide algorithms which are valid in general situations, some of which cannot be tackled by any other method. One fundamental aspect of our implementation consists in the use of the effective homology technique, which makes it possible to handle infinitely generated chain complexes. Another important feature concerns the possibility of defining and using for computation filtrations over general posets. Our programs, improved using discrete vector fields, have been implemented as a new module for the Kenzo system.

We focused our study on filtrations indexed over the posets \mathbb{Z}^m and $D(\mathbb{Z}^m)$, for their relevance in relation with multipersistence. In this respect, a theoretical contribution of our work is the description of the relation between persistent homology and spectral systems in a general scenario, which extends a result valid for persistent homology and spectral sequences arising from \mathbb{Z} -filtrations. Furthermore, we define and compute a new "empirical" invariant and show its discriminative power in the context of multipersistence.

Two fundamental requirements in persistent homology theory are computability and robustness. As a future research direction, we intend to reduce the computational cost for our invariants and to further investigate their behavior with respect to small changes in the multiparameter filtration. As we reviewed in Section 4, several approaches have been proposed to tackle the problems arising with multiparameter filtrations. Since effective homology displays a good behavior with respect to the invariants we considered in this work, studying its applicability to other constructions represents an interesting scope for further research.

ACKNOWLEDGMENTS

Partially supported by Basque Government, BERC 2018-2021 program; Spanish Ministry of Science, Innovation and Universities, BCAM Severo Ochoa accreditation SEV-2017-0718; Spanish Ministry of Science, Innovation and Universities, project MTM2017-88804-P; University of La Rioja - V Plan Riojano de I+D+I; Italian MIUR Award "Dipartimento di Eccellenza 2018-2022"- CUP: E11G18000350001 and SmartData@PoliTO center for Big Data and Machine Learning technologies.

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