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Elder-Rule-Staircodes for Augmented Metric Spaces*

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Abstract. An augmented metric space is a metric space (X, d_X) equipped with a function $f_X : X \to \mathbb{R}$. This type of data arises commonly in practice, e.g., a point cloud X in $\mathbb{R}^D$ where each point $x \in X$ has a density function value $f_X(x)$ associated to it. An augmented metric space (X, d_X, f_X) naturally gives rise to a 2-parameter filtration $\mathcal{K}$. However, the resulting 2-parameter persistent homology $\mathrm{H}_\bullet(\mathcal{K})$ could still be of wild representation type and may not have simple indecomposables. In this paper, motivated by the elder-rule for the zeroth homology of 1-parameter filtration, we propose a barcode-like summary, called the *elder-rule-staircode*, as a way to encode $\mathrm{H}_0(\mathcal{K})$. Specifically, if $n = |X|$, the elder-rule-staircode consists of n number of staircase-like blocks in the plane. We show that if $\mathrm{H}_0(\mathcal{K})$ is interval decomposable, then the barcode of $\mathrm{H}_0(\mathcal{K})$ is equal to the elder-rule-staircode. Furthermore, regardless of the interval decomposability, the fibered barcode, the dimension function (a.k.a. the Hilbert function), and the graded Betti numbers of $\mathrm{H}_0(\mathcal{K})$ can all be efficiently computed once the elder-rule-staircode is given. Finally, we develop and implement an efficient algorithm to compute the elder-rule-staircode in $O(n^2 \log n)$ time, which can be improved to $O(n^2\alpha(n))$ if X is from a fixed dimensional Euclidean space $\mathbb{R}^D$, where $\alpha(n)$ is the inverse Ackermann function.

Key words. multiparameter persistent homology, hierarchical clustering, persistence diagram, elder-rule

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1. Introduction.

Several ideas connected to the notion of what is nowadays known as *persistent homology* arose in the work by Frosini and collaborators [29, 30, 37], in Robins's Ph.D. thesis [47], in the work of Barannikov about smooth functions on manifolds [4], in Edelsbrunner and collaborators [23, 27], and in Zomorodian and Carlsson [53]. In many practical applications, persistence is applied to simplicial filtrations constructed over finite metric spaces (see, e.g., [17, 49]). In this paper, we work in the more general setting of *augmented metric spaces.*

An augmented metric space is a metric space (X, d_X) equipped with a function $f_X : X \to \mathbb{R}$ [5, 11, 18]. This type of data arises commonly in practice, e.g., a point cloud X in $\mathbb{R}^D$ where each point has a density function value f_X associated to it. Studying hierarchical clustering methods induced in this setting has attracted much attention starting with [11] and more

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recently with [5, 9, 16, 41]. Another example is where $X = V$ equals the vertex set of a graph $G = (V, E)$, d_X represents a certain graph-induced metric on X (e.g., the diffusion distance induced by G), and f_X is some descriptor function (e.g., discrete Ricci curvature) at graph nodes. This graph setting occurs often in practice for graph analysis applications, where G can be viewed as a skeleton of a hidden domain. When summarizing or characterizing G, one wishes to take into consideration both the metric structure of this domain and the node attributes. Given that persistence-based summaries from only the edge weights or from only node attributes have already shown promise in graph classification (see, e.g., [8, 13, 32, 52]), it would be highly desirable to incorporate (potentially more informative) summaries encoding both types of information to tackle such tasks. In brief, we wish to develop topological invariants induced from such augmented metric spaces.

On the other hand, an augmented metric space naturally gives rise to a 2-parameter filtration (by filtering both via f_X and via distance d_X; see Definition 3.2). However, while a standard (1-parameter) filtration and its induced persistence module have a persistence diagram as a complete discrete invariant, multiparameter persistence modules do not have such a complete discrete invariant [12, 21]. The 2-parameter persistence module induced from an augmented metric space may still be of wild representation type and may not have simple indecomposables [5]. Instead, several recent works consider informative (but not necessarily complete) invariants for multiparameter persistence modules [25, 31, 33, 39, 42, 43, 51]. In particular, RIVET [39] provides an interactive visualization of barcodes associated to 1-dimensional slices of an input 2-parameter persistence module M, which are called the *fibered barcodes*. For implementing the interactive aspect, RIVET makes efficient use of *graded Betti numbers* of M, another invariant of the 2-parameter persistence module M.

Our contributions. We propose a barcode-like summary, called the *elder-rule-staircode*, as a way to encode the zeroth homology of the 2-parameter filtration induced by a finite augmented metric space. Specifically, given a finite $\mathcal{X} = (X, d_X, f_X)$, its elder-rule-staircode consists of $n = |X|$ number of staircase-like blocks of $O(n)$ descriptive complexity in the plane. The development of the elder-rule-staircode is motivated by the elder-rule behind the construction of persistence pairing for a 1-parameter filtration [26]. For the 1-parameter case, *barcodes* [53] can be obtained by the decomposition of persistence modules in the realm of commutative algebra or, equivalently, by applying the elder-rule which is flavored with combinatorics or order theory. As we describe in section 4, our elder-rule-staircodes are obtained by adapting the elder-rule for treegrams arisen from 1-parameter filtration.

Interestingly, we show that our elder-rule-staircode encodes much of the topological information of the 2-parameter filtration $\mathcal{K}$ induced by $\mathcal{X}$. In particular, the fibered barcodes, the fibered treegrams, and the graded Betti numbers associated to $\mathrm{H}_0(\mathcal{K})$ can all be efficiently computed from the elder-rule-staircodes (see Theorems 3.7, 4.13, and 5.4). Furthermore, if $\mathrm{H}_0(\mathcal{K})$ is interval decomposable, then the interval indecomposables appearing in its decomposition correspond exactly to its staircode (see Theorem 4.16). This implies that testing the interval decomposability of $\mathrm{H}_0(\mathcal{K})$ is reduced to testing isomorphism of two given persistence modules [7] (see Remark 4.17). We also provide sufficient conditions on $\mathcal{X}$ which ensure the interval decomposability of $\mathrm{H}_0(\mathcal{K})$ (see Theorem 4.10 and Corollary 4.11). Therefore, to explore exotic isomorphism types of indecomposable summands of $\mathrm{H}_0(\mathcal{K})$ (a question of interest considered in [5]), it suffices to restrict our attention to augmented metric spaces which do not satisfy these conditions.

Finally, in section 6, we show that the elder-rule-staircode can be computed in $O(n^2 \log n)$ time for a finite augmented metric space (X, d_X, f_X) where $n = |X|$, and in $O(n^2\alpha(n))$ time if X is from a fixed dimensional Euclidean space and d_X is Euclidean distance. We have software to compute elder-rule-staircodes and to explore/retrieve information such as fibered barcodes interactively, which is available online from https://github.com/Chen-Cai-OSU/ER-staircode. See Figure 1 for an example of pairs of inputs and outputs of the software.

More on related work. The *elder-rule* is an underlying principle for extracting the persistence diagram from a persistence module induced by a nested family of simplicial complexes [26, Chapter 7]. Recently, this principle has come into the spotlight again for generalizing persistence diagrams [33, 42, 45] and for addressing inverse problems in TDA [22]. An algorithm for testing interval decomposability of multiparameter persistence modules has been studied [1]. A method to approximate 2-parameter persistence modules by interval-decomposable persistence modules has been proposed in [2]. A multiparameter hierarchical clustering method has been utilized for identifying dominant metastable states of molecular dynamics [16]. A consistent approach to density-based clustering has been proposed in [48].

The software RIVET and work of [40] can also be used to recover fibered barcodes and graded Betti numbers. However, for the special case of zeroth 2-parameter persistence modules induced from augmented metric spaces, our elder-rule-staircodes are simpler and more efficient to achieve these goals: In particular, given an augmented metric space containing n points, the algorithm of [40] computes the graded Betti numbers in $\Omega(n^3)$ time, while it takes $O(n^2 \log n)$ time using the elder-rule-staircode via Theorem 6.1. For zeroth fibered barcodes, RIVET takes $O(n^8)$ time to compute a data structure of size $O(n^6)$ so as to support the efficient query time of $O(\log n + |B^L|)$, where $|B^L|$ is the size of the fibered barcode B^L for a particular line L of positive slope. Our algorithm computes an elder-rule-staircode of size $O(n^2)$ in $O(n^2 \log n)$ time, after which B^L can be computed in $O(|B^L| \log n)$ time for any query line L. See section 6.2 for a more detailed comparison. However, it is important to note that RIVET allows much broader inputs and can work beyond zeroth homology.

Outline. In section 2, we review the definitions of persistence modules, barcodes, and graded Betti numbers. In section 3, we introduce a 2-parameter filtration $\mathcal{K}$ induced by an augmented metric space $\mathcal{X}$ and define the elder-rule-staircode of $\mathcal{X}$. In section 4, we show that the elder-rule-staircode recovers the fibered barcode of $\mathrm{H}_0(\mathcal{K})$. We also prove that if $\mathrm{H}_0(\mathcal{K})$ is interval decomposable, then the set of indecomposables corresponds exactly to the staircode. In section 5, we show that the elder-rule-staircode recovers the graded Betti numbers of $\mathrm{H}_0(\mathcal{K})$. In section 6, we develop and implement an efficient algorithm to compute the elder-rule-staircode. In section 7, we discuss open problems. For readability, we have relegated some proofs to some appendices.

2. Preliminaries.

In section 2.1, we review the definitions of persistence modules and their barcodes. In section 2.2, we review the notion of graded Betti number of a persistence module.

2.1. Persistence modules and their decompositions.

First, we briefly review the definition of persistence modules. Let $\mathbb{P}$ be a poset. We regard $\mathbb{P}$ as the category that has elements of $\mathbb{P}$ as objects. Also, for any $\mathbf{a}, \mathbf{b} \in \mathbb{P}$, there exists a unique morphism $\mathbf{a} \to \mathbf{b}$ if and only if $\mathbf{a} \leq \mathbf{b}$. For $d \in \mathbb{N}$, let $\mathbb{Z}^d$ be the set of d-tuples of integers equipped with the partial order

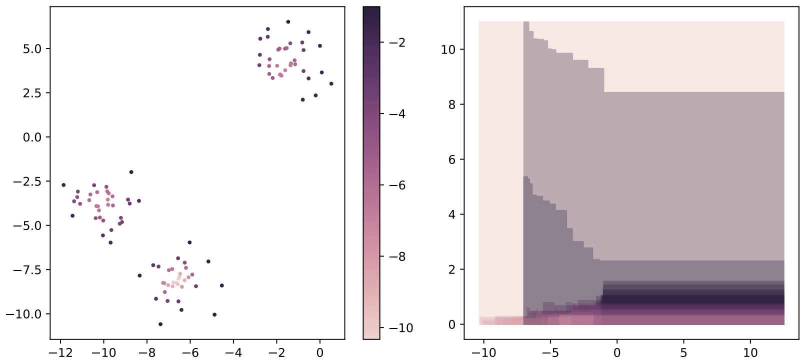


Figure 1. *Left: A finite set $X \in \mathbb{R}^2$ equipped with the Euclidean metric d_X and a codensity function $f_X : X \to \mathbb{R}$; i.e., the denser the neighborhood of $x \in X$, the smaller the $f_X(x)$. More precisely, given N points $x_1, x_2, \ldots, x_N \in \mathbb{R}^2$ and a bandwidth $h > 0$, the (unnormalized) density estimate for any $y \in \mathbb{R}^2$ is $\rho_K(x) := \sum_{i=1}^{N} K_h(||x - x_i||_2)$, where $K_h(x) := \exp(-\frac{x^2}{2h})$. We define f_X as the negative of the density estimate ρ_X. In all experiments, we used the bandwidth $h = 0.2$. Right: The elder-rule staircode of the augmented metric space (X, d_X, f_X). The largest block, depicted in a light color, is the quadrant with the left-bottom point $(\min f_X, 0)$. The existence of three notably tall blocks suggests the existence of three clusters in (X, d_X, f_X). See Figure 19 for an expanded example.*

defined as $(a_1, a_2, \ldots, a_d) \leq (b_1, b_2, \ldots, b_d)$ if and only if $a_i \leq b_i$ for each $i = 1, 2, \ldots, d$. The poset structure on $\mathbb{R}^d$ is defined in the same way.

We fix a certain field $\mathbb{F}$, and every vector space in this paper is over $\mathbb{F}$. Let **Vec** denote the category of *finite dimensional* vector spaces over $\mathbb{F}$.

A ($\mathbb{P}$-indexed) *persistence module* is a functor $M : \mathbb{P} \to \mathbf{Vec}$. In other words, to each $\mathbf{a} \in \mathbb{P}$ a vector space $M(\mathbf{a})$ is associated and to each pair $\mathbf{a} \leq \mathbf{b}$ in $\mathbb{P}$ a linear map $\varphi_M(\mathbf{a}, \mathbf{b}) : M(\mathbf{a}) \to M(\mathbf{b})$ is associated. When $\mathbb{P} = \mathbb{R}^d$ or $\mathbb{Z}^d$, M is said to be a *d-parameter persistence module*. A *morphism* between $M, N : \mathbb{P} \to \mathbf{Vec}$ is a natural transformation $f : M \to N$ between M and N. That is, f is a collection $\{f_\mathbf{a}\}_{\mathbf{a} \in \mathbb{P}}$ of linear maps such that for every pair $\mathbf{a} \leq \mathbf{b}$ in $\mathbb{P}$, the following diagram commutes:

$$\begin{array}{ccc} M(\mathbf{a}) & \xrightarrow{\varphi_M(\mathbf{a},\mathbf{b})} & M(\mathbf{b}) \\ \downarrow f_\mathbf{a} & & \downarrow f_\mathbf{b} \\ N(\mathbf{a}) & \xrightarrow{\varphi_N(\mathbf{a},\mathbf{b})} & N(\mathbf{b}). \end{array}$$

Two persistence modules M and N are *isomorphic*, denoted by $M \cong N$, if there exists a natural transformation $\{f_\mathbf{a}\}_{\mathbf{a} \in \mathbb{P}}$ from M to N where each $f_\mathbf{a}$ is an isomorphism.

We now review the standard definition of barcodes, following notation from [6].

Definition 2.1 (intervals). *Let $\mathbb{P}$ be a poset. An* interval *$\mathcal{J}$ of $\mathbb{P}$ is a subset $\mathcal{J} \subset \mathbb{P}$ such that the following hold:* (1) *$\mathcal{J}$ is nonempty.* (2) *If $\mathbf{a}, \mathbf{b} \in \mathcal{J}$ and $\mathbf{a} \leq \mathbf{c} \leq \mathbf{b}$, then $\mathbf{c} \in \mathcal{J}$.* (3) *For any $\mathbf{a}, \mathbf{b} \in \mathcal{J}$, there is a sequence $\mathbf{a} = \mathbf{a}_0, \mathbf{a}_1, \ldots, \mathbf{a}_l = \mathbf{b}$ of elements of $\mathcal{J}$ with $\mathbf{a}_i$ and $\mathbf{a}_{i+1}$ comparable for $0 \leq i \leq l - 1$.*

For $\mathcal{J}$ an interval of $\mathbb{P}$, the *interval module* $I^{\mathcal{J}} : \mathbb{P} \to \mathbf{Vec}$ is defined as

$$I^{\mathcal{J}}(\mathbf{a}) = \begin{cases} \mathbb{F} & \text{if } \mathbf{a} \in \mathcal{J}, \\ 0 & \text{otherwise,} \end{cases} \qquad \varphi_{I^{\mathcal{J}}}(\mathbf{a}, \mathbf{b}) = \begin{cases} \mathrm{id}_{\mathbb{F}} & \text{if } \mathbf{a}, \mathbf{b} \in \mathcal{J}, \ \mathbf{a} \leq \mathbf{b}, \\ 0 & \text{otherwise.} \end{cases}$$

Recall that *a multiset* is a collection of objects (called elements) in which elements may occur more than once, and the number of instances of an element is its *multiplicity*.

Definition 2.2 (interval decomposability and barcodes). *A functor $M : \mathbb{P} \to \mathbf{Vec}$ is* interval decomposable *if there exists a multiset $\mathbf{barc}(M)$ of intervals (Definition 2.1) of $\mathbb{P}$ such that $M \cong \bigoplus_{\mathcal{J} \in \mathbf{barc}(M)} I^{\mathcal{J}}$. We call $\mathbf{barc}(M)$ the* barcode *of M.*

By the theorem of Azumaya–Krull–Remak–Schmidt [3], such a decomposition is unique up to a permutation of the terms in the direct sum. Therefore, the multiset $\mathbf{barc}(M)$ is unique if M is interval decomposable. For $d = 1$, any $M : \mathbb{R}^d$ (or $\mathbb{Z}^d$) $\to \mathbf{Vec}$ is interval decomposable, and thus $\mathbf{barc}(M)$ exists. However, for $d \geq 2$, M may not be interval decomposable.

2.2. Graded Betti numbers.

Persistence module as a module over a polynomial ring. In section 2.1, we defined d-parameter persistence modules as $\mathbf{Vec}$-valued functors over the posets $\mathbb{Z}^d$ or $\mathbb{R}^d$ and morphisms between them as natural transformations. The definitions below are equivalent to those definitions [12, Theorem 1] and allow us to define the graded Betti numbers of persistence modules. We mostly adopt notation in [25, 40].

Let $\mathbb{F}[t_1, t_2, \ldots, t_d]$ be the polynomial ring in the d-variables $t_1, t_2, \ldots, t_d$. To ease notation, for $\mathbf{n} := (n_1, n_2, \ldots, n_d) \in \mathbb{Z}^d_{\geq 0}$, the monomial $t_1^{n_1} t_2^{n_2} \ldots t_d^{n_d} \in \mathbb{F}[t_1, t_2, \ldots, t_d]$ will be written as $\mathbf{x}^{\mathbf{n}}$. A d-parameter persistence module $M : \mathbb{Z}^d \to \mathbf{Vec}$ is an $\mathbb{F}[t_1, t_2, \ldots, t_d]$-module M with a direct sum decomposition as an $\mathbb{F}$-vector space $M \cong \bigoplus_{\mathbf{a} \in \mathbb{Z}^d} M_{\mathbf{a}}$ such that the action of $\mathbb{F}[t_1, t_2, \ldots, t_d]$ on M is uniquely specified as follows: for all $\mathbf{a} = (a_1, a_2, \ldots, a_d) \in \mathbb{Z}^d$ and $v \in M_{\mathbf{a}}$, and for all $\mathbf{n} = (n_1, n_2, \ldots, n_d) \in \mathbb{Z}^d_{\geq 0}$, and for all $c \in \mathbb{F}$,

$$(c \cdot \mathbf{x}^{\mathbf{n}}) \cdot v := c \cdot \varphi_M(\mathbf{a}, \mathbf{a} + \mathbf{n})(v).$$

Let M and N be any two persistence modules. A morphism $f : M \to N$ is a module homomorphism such that $f(M_{\mathbf{a}}) \subseteq N_{\mathbf{a}}$ for all $\mathbf{a} \in \mathbb{Z}^d$. The kernel, image, and cokernel of f are analogously defined to those of a linear map between vector spaces. The *kernel* of f is defined as the submodule $\ker(f) := \bigoplus_{\mathbf{a} \in \mathbb{Z}^d} \ker(f_{\mathbf{a}})$ of M. The image of f is defined as the submodule $\mathrm{im}(f) := \bigoplus_{\mathbf{a} \in \mathbb{Z}^d} \mathrm{im}(f_{\mathbf{a}})$ of N. The *cokernel* of f is defined as $\mathrm{coker}(f) := \bigoplus_{\mathbf{a} \in \mathbb{Z}^d} (N_{\mathbf{a}}/\mathrm{im}(f_{\mathbf{a}}))$.

Graded Betti numbers. We briefly review the concept of *graded Betti numbers* [12, 35, 39, 40, 46, 53]. Since our interests are in studying finite augmented metric spaces, we restrict ourselves to *finite* persistence modules—the kth homology of a filtration of a finite simplicial complex for some $k \in \mathbb{Z}_{\geq 0}$ [12].

Fix $\mathbf{a} \in \mathbb{Z}^d$. By $Q^{\mathbf{a}} : \mathbb{Z}^d \to \mathbf{Vec}$, we denote the persistence module defined as

$$Q^{\mathbf{a}}_{\mathbf{x}} = \begin{cases} \mathbb{F} & \text{if } \mathbf{a} \leq \mathbf{x}, \\ 0 & \text{otherwise,} \end{cases} \qquad \varphi_{Q^{\mathbf{a}}}(\mathbf{x}, \mathbf{y}) = \begin{cases} \mathrm{id}_{\mathbb{F}} & \text{if } \mathbf{a} \leq \mathbf{x}, \\ 0 & \text{otherwise.} \end{cases}$$

Any $F : \mathbb{Z}^d \to \mathbf{Vec}$ is said to be *free* if there exists a multiset $\mathcal{A}$ of elements of $\mathbb{Z}^2$ such that $F \cong \bigoplus_{\mathbf{a} \in \mathcal{A}} Q^{\mathbf{a}}$. For simplicity, we will refer to free persistence modules as free modules. Let

M be a persistence module. An element $m \in M_{\mathbf{a}}$ for some $\mathbf{a} \in \mathbb{Z}^d$ is called a homogeneous element of M. In this case, we write $\mathrm{gr}(m) = \mathbf{a}$. Let F be a free module. A *basis* B of F is defined as a minimal homogeneous set of generators of F. There can exist two bases B and B' of F (analogous to the fact that a vector space can have multiple bases). However, the number of elements at each grade $\mathbf{a} \in \mathbb{Z}^d$ in a basis of F is an isomorphism invariant.

For a finite M, let IM denote the submodule of M generated by the images of all linear maps $\varphi_M(\mathbf{a}, \mathbf{b})$, with $\mathbf{a} < \mathbf{b}$ in $\mathbb{Z}^2$. Assume that there is a chain of modules

$$F^\bullet : \cdots \xrightarrow{\partial_3} F^2 \xrightarrow{\partial_2} F^1 \xrightarrow{\partial_1} F^0 \xrightarrow{\partial_0} M \xrightarrow{0(=:\partial_{-1})} 0 \tag{2.1}$$

such that (1) each F^i is a free module, and (2) $\mathrm{im}(\partial^i) = \ker(\partial^{i-1})$, $i = 0, 1, 2, \ldots$. Then we call $F^\bullet$ a *resolution* of M. The condition (2) is referred to as *exactness* of $F^\bullet$. We call the resolution $F^\bullet$ *minimal* if $\mathrm{im}(\partial^i) \subseteq IF^{i-1}$ for $i = 1, 2, \ldots$. It is a standard fact that a minimal resolution of M always exists and is unique up to isomorphism [46, Chapter I].

Definition 2.3 (graded Betti numbers). *Let $M : \mathbb{Z}^d \to \mathbf{Vec}$ be finite. Assume that a minimal free resolution of M is $F^\bullet$ in (2.1). For $i \in \mathbb{Z}_{\geq 0}$, the ith graded Betti number $\beta_i^M : \mathbb{Z}^d \to \mathbb{Z}_{\geq 0}$ is defined as $\beta_i^M(\mathbf{a}) =$ (number of elements at grade $\mathbf{a}$ in any basis of F^i).*

Remark 2.4.

(i) Note that if $M \cong N_1 \bigoplus N_2$, then $\beta_i^M = \beta_i^{N_1} + \beta_i^{N_2}$. This is a key fact to define the *persistent graded Betti numbers* introduced in [25].

(ii) $\beta_i^M : \mathbb{Z}^d \to \mathbb{Z}_{\geq 0}$ is the zero function for every integer $i > d$ [28, Theorem 1.13].

(iii) Definition 2.3 is not in the exact same form as those in the literature, such as [12, 35, 39]. However, by Nakayama's lemma [46, Lemma 2.11] all those are equivalent, as already noted in [40, section 2.3].

For any $M : \mathbb{Z}^d \to \mathbf{Vec}$, the *dimension function* $\dim(M) : \mathbb{Z}^d \to \mathbb{Z}_{\geq 0}$ of M is defined as $\mathbf{a} \mapsto \dim M_{\mathbf{a}}$. The graded Betti numbers of M recover $\dim(M)$.

Theorem 2.5 (see [40, Proposition 2.3]). *Let $M : \mathbb{Z}^d \to \mathbf{Vec}$ be a finite persistence module. For all $\mathbf{a} \in \mathbb{Z}^d$,*

$$\dim(M)(\mathbf{a}) = \sum_{\mathbf{x} \leq \mathbf{a}} \sum_{i=0}^{d} (-1)^i \beta_i^M(\mathbf{x}).$$

3. Elder-rule-staircodes for augmented metric spaces.

Rips bifiltration for an aug-MS. Let (X, d_X) be a metric space. For $\varepsilon \in \mathbb{R}$, the *Rips complex* $\mathcal{R}_\varepsilon(X, d_X)$ is the abstract simplicial complex defined as

$$\mathcal{R}_\varepsilon(X, d_X) = \{A \subseteq X : \text{for all } x, x' \in A,\ d_X(x, x') \leq \varepsilon\}.$$

Let **Simp** be the category of abstract simplicial complexes and simplicial maps. The *Rips filtration* is the functor $\mathcal{R}_\bullet(X, d_X) : \mathbb{R} \to \mathbf{Simp}$ defined as

$$\varepsilon \mapsto \mathcal{R}_\varepsilon(X, d_X) \text{ and } \varepsilon \leq \varepsilon' \mapsto \mathcal{R}_\varepsilon(X, d_X) \hookrightarrow \mathcal{R}_{\varepsilon'}(X, d_X).$$

Definition 3.1 (augmented metric spaces). *Let (X, d_X) be a metric space and $f_X : X \to \mathbb{R}$ a function. We call the triple $\mathcal{X} = (X, d_X, f_X)$ an* augmented metric space *(abbreviated* aug-MS*).*

We say that $\mathcal{X}$ is injective *if $f_X : X \to \mathbb{R}$ is an injective function.*

Throughout this paper, every (augmented) metric space will be assumed to be finite. Let $\mathcal{X} = (X, d_X, f_X)$ be an aug-MS. For $\sigma \in \mathbb{R}$, let X_σ denote the sublevel set $f_X^{-1}(-\infty, \sigma] \subseteq X$. Let (X_σ, d_X) denote the restriction of the metric space (X, d_X) to the subset $X_\sigma \subseteq X$. Similarly, (X_σ, d_X, f_X) is the aug-MS obtained by restricting d_X to $X_\sigma \times X_\sigma$ and f_X to X_σ. The following 2-parameter filtration is considered in [5, 11, 12] in the context of *filtered* single linkage hierarchical clustering or *filtered* persistent homology.

Definition 3.2 (Rips bifiltration of an aug-MS). *Let $\mathcal{X} = (X, d_X, f_X)$ be an aug-MS. We define the* Rips bifiltration $\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X}) : \mathbb{R}^2 \to \mathbf{Simp}$ *of $\mathcal{X}$ as $(\varepsilon, \sigma) \mapsto \mathcal{R}_\varepsilon(X_\sigma, d_X)$.*

By applying the kth simplicial homology functor to the Rips bifiltration $\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})$, we obtain the persistence module $M := \mathrm{H}_k(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})) : \mathbb{R}^2 \to \mathbf{Vec}$. Let $\mathcal{L}$ denote the set of all lines of (strictly) positive slopes in $\mathbb{R}^2$. Given $L \in \mathcal{L}$, the restriction $M|_L : L \to \mathbf{Vec}$ can be decomposed into the unique direct sum of interval modules over L, and thus we have the barcode $\mathbf{barc}(M|_L)$ of $M|_L$. The *kth fibered barcode* of $\mathcal{X}$ refers to the $\mathcal{L}$-parametrized collection $\{\mathbf{barc}(M|_L)\}_{L\in\mathcal{L}}$ [14, 36, 39].

Elder-rule-staircode for an aug-MS. Let (X, d_X) be a finite metric space. For $\varepsilon \in [0, \infty)$, an *$\varepsilon$-chain* between $x, x' \in X$ stands for a sequence $x = x_1, x_2, \ldots, x_\ell = x'$ of points in X such that $d_X(x_i, x_{i+1}) \le \varepsilon$ for $i = 1, \ldots, \ell - 1$. Now given $\mathcal{X} = (X, d_X, f_X)$ and $\sigma \in \mathbb{R}_{\ge 0}$, consider a point $x \in X_\sigma$. Then for any $\varepsilon \ge 0$, set $[x]_{(\sigma,\varepsilon)}$ as the collection of all points $x' \in X_\sigma$ that can be connected to x through an ε-chain in X_σ.

The function $f_X : X \to \mathbb{R}$ induces an order on X: consider any two $x, x' \in X$. If $f_X(x) < f_X(x')$, then we say that x is *older than* x'.

Definition 3.3 (elder-rule-staircode for an aug-MS). *Let $\mathcal{X} = (X, d_X, f_X)$ be an* injective *aug-MS. For each $x \in X$, we define* its staircode *as*

$$I_x := \{(\sigma, \varepsilon) \in \mathbb{R}^2 : x \in X_\sigma \text{ and } x \text{ is the oldest in } [x]_{(\sigma,\varepsilon)}\}. \tag{3.1}$$

The collection $\mathcal{I}_\mathcal{X} := \{I_x\}_{x\in X}$ is called the elder-rule-staircode (ER-staircode for short) *of $\mathcal{X}$.*

See Figure 2 for an example. The relationship between the ER-staircode and the classic elder-rule will become clear in section 4.1.

Definition 3.4. *An interval I of $\mathbb{R}^2$ (Definition 2.1) is a* staircase interval (or simply a staircase) *if there exists $(\sigma_0, \varepsilon_0) \in I$ such that $(\sigma_0, \varepsilon_0) \le (\sigma, \varepsilon)$ for all $(\sigma, \varepsilon) \in I$, and I is not bounded in the direction of the σ-axis (see Figure 5).*

It turns out that each $I_x \in \mathcal{I}_\mathcal{X}$ is a staircase interval.

Proposition 3.5. *Each I_x in Definition 3.3 is a staircase interval (proof in Appendix A).*

Staircodes for noninjective case. Even if f_X is not injective, we still have the concept of the ER-staircode. Consider an aug-MS $\mathcal{X} = (X, d_X, f_X)$ such that f_X is not injective. To induce the ER-staircode of $\mathcal{X}$, we pick any order on X which is *compatible* with f_X: An order $<$ on

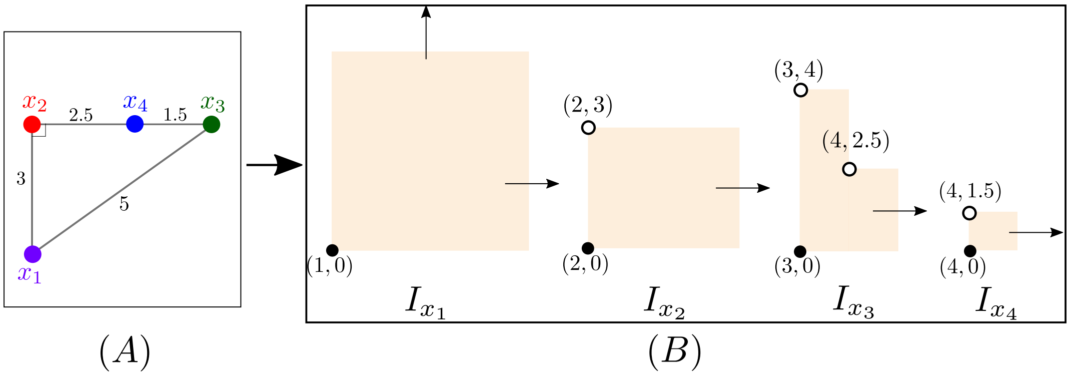


Figure 2. (A) *Consider the triangle with edge lengths* 3, 4, *and* 5. *Consider the aug-MS* $\mathcal{X} = (X, d_X, f_X)$, *where* $X := \{x_1, x_2, x_3, x_4\}$, d_X *is the Euclidean metric on the plane, and* f_X *is given as* $f_X(x_i) = i$ *for* $i = 1, 2, 3, 4$. (B) *The ER-staircode of* $\mathcal{X}$.

X is compatible with f_X if $f_X(x) < f_X(x')$ implies $x < x'$ for all $x, x' \in X$. Now we define $\mathcal{I}_{\mathcal{X}}^{<} = \{\!\{I_x^< : x \in X\}\!\}$, where

$$I_x^< := \{(\sigma, \varepsilon) \in \mathbb{R}^2 : x \in X_\sigma \text{ and } x = \min([x]_{(\sigma,\varepsilon)}, <)\} \tag{3.2}$$

(we use double curly braces $\{\!\{-\}\!\}$ to denote multisets). Regardless of the choice of $<$, the collection $\mathcal{I}_{\mathcal{X}}^{<} = \{\!\{I_x^< : x \in X\}\!\}$ satisfies all properties and theorems we prove later. Hence, for any possible compatible order $<$ we will refer to $\mathcal{I}_{\mathcal{X}}^{<}$ as an *ER-staircode* of $\mathcal{X}$.

Example 3.6 (constant function case). *Let* (X, d_X) *be a metric space of* n *points. Then the barcode of* $\mathrm{H}_0(\mathcal{R}_\bullet(X, d_X)) : \mathbb{R} \to \mathbf{Vec}$ *consists of* n *intervals* J_i, $i = 1, \dots, n$. *Let* $\mathcal{X} = (X, d_X, f_X)$ *be the aug-MS where* f_X *is constant at* $c \in \mathbb{R}$. *Then all possible total orders on* X *are compatible with* f_X *and all induce the same ER-staircode* $\mathcal{I}_{\mathcal{X}} = \{\!\{[c, \infty) \times J_i : i = 1, \dots, n\}\!\}$.

In contrast to Example 3.6, different orders on X in general induce different ER-staircodes of $\mathcal{X} = (X, d_X, f_X)$; see Example 3.8. Therefore, a single ER-staircode of $\mathcal{X}$ is not necessarily an *invariant* of $\mathcal{X}$, whereas the collection of all possible ER-staircodes of $\mathcal{X}$ can be seen so (see item 4 in section 7). This collection, however, is *not a complete invariant of* $\mathcal{X}$ for the following reasoning: It is not difficult to find two nonisometric metric spaces (X, d_X) and (Y, d_Y) such that $\mathrm{H}_0(\mathcal{R}_\bullet(X, d_X))$ and $\mathrm{H}_0(\mathcal{R}_\bullet(Y, d_Y))$ have the same barcode. Let $f_X : X \to \mathbb{R}$ and $f_Y : Y \to \mathbb{R}$ be constant at $c \in \mathbb{R}$. Then, by Example 3.6, all the ER-staircodes of (X, d_X, f_X) and (Y, d_Y, f_Y) (induced by all possible total orders on X and Y) are the same (see item 5 in section 7).

We can recover the zeroth fibered barcode of an aug-MS $\mathcal{X}$ from its ER-staircode: Computation of an ER-staircode and query time for a fibered barcode are given in Theorem 6.1.

Theorem 3.7. *Let* $\mathcal{X}$ *be an aug-MS, and let* $M := \mathrm{H}_0(\mathcal{R}_\bullet^{\mathrm{bi}}(\mathcal{X}))$. *Let* $\mathcal{I}_{\mathcal{X}} = \{\!\{I_x : x \in X\}\!\}$ *be an ER-staircode of* $\mathcal{X}$. *For each* $L \in \mathcal{L}$, *the barcode* $\mathbf{barc}(M|_L)$ *coincides with the multiset* $\{\!\{L \cap I_x : x \in X\}\!\}$ *(up to removal of empty sets; see Figure 3). The proof is after Theorem* 4.4.

Example 3.8. *If an aug-MS is not injective, then there can be different ER-staircodes with respect to different compatible orders. However, each of them will still be valid to produce*

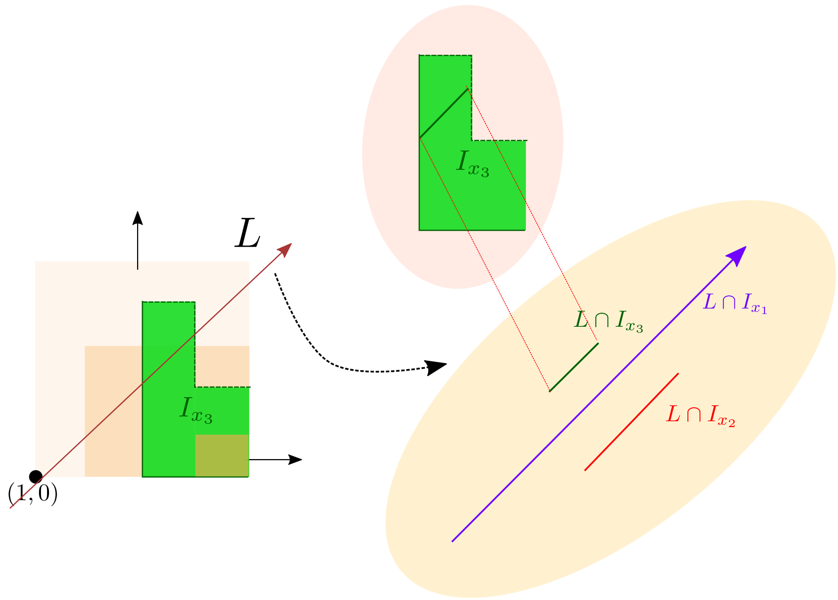


Figure 3. *Left: The stack of I_{x_i}, $i = 1, 2, 3, 4$, from Figure 2 and a line $L \in \mathcal{L}$. Right: The barcode of $M|_L$. Since L does not intersect I_{x_4}, only three intervals of $L \subset \mathbb{R}^2$ appear in the barcode.*

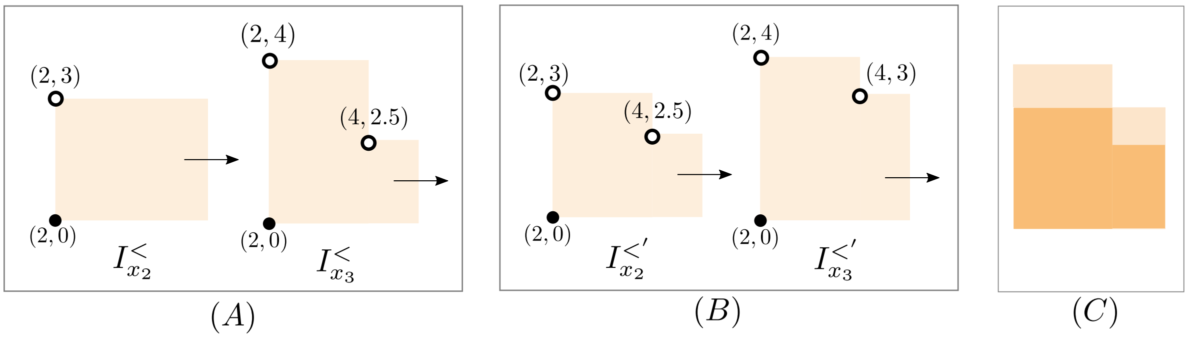


Figure 4. *Illustration for Example 3.8:* (A) $I^{<}_{x_2}$ *and* $I^{<}_{x_3}$. (B) $I^{<'}_{x_2}$ *and* $I^{<'}_{x_3}$. (C) *Stack of* $I^{<}_{x_2}$ *and* $I^{<}_{x_3}$. *Stack of* $I^{<'}_{x_2}$ *and* $I^{<'}_{x_3}$ *look the same. Observe that for any* $L \in \mathcal{L}$, $\left\{\!\!\left\{ L \cap I^{<}_{x_2}, L \cap I^{<}_{x_3} \right\}\!\!\right\} = \left\{\!\!\left\{ L \cap I^{<'}_{x_2}, L \cap I^{<'}_{x_3} \right\}\!\!\right\}$.

the fibered barcodes. For example, let (X, d_X) be the metric space in Figure 2(A). Define $g_X : X \to \mathbb{R}$ by sending x_1, x_2, x_3, x_4 to $1, 2, 2, 4$, respectively. Two orders $(x_1 < x_2 < x_3 < x_4)$ and $(x_1 <' x_3 <' x_2 <' x_4)$ are compatible with g_X. Consider the two ER-staircodes $\mathcal{I}^{<}_{\mathcal{X}} = \left\{\!\!\left\{ I^{<}_{x_i} : i = 1, 2, 3, 4 \right\}\!\!\right\}$ and $\mathcal{I}^{<'}_{\mathcal{X}} = \left\{\!\!\left\{ I^{<'}_{x_i} : i = 1, 2, 3, 4 \right\}\!\!\right\}$. While $I^{<}_{x_i} = I^{<'}_{x_i}$ for $i = 1, 4$, the equality does not hold for $i = 2, 3$. However, both $\mathcal{I}^{<}_{\mathcal{X}}$ and $\mathcal{I}^{<'}_{\mathcal{X}}$ satisfy the statement in Theorem 3.7. See Figure 4.

We will close this section with some definitions which will be helpful later. It will be useful to consider three different types of corner points of staircase intervals of $\mathbb{R}^2$. See Figure 5 for an illustration. In that figure, roughly speaking, for each staircase interval, the type-0 corner

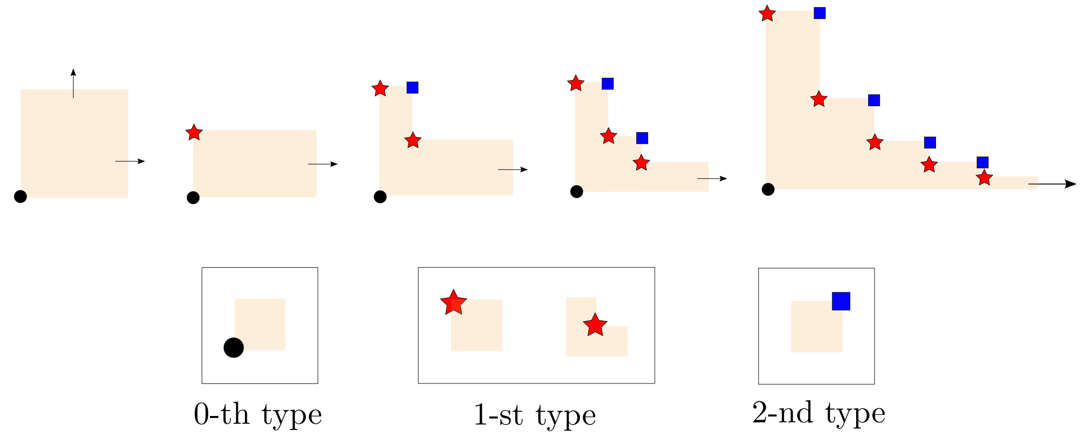


Figure 5. *Every corner point of a staircase interval falls into three different types depending on its neighborhood information, as the pictures above illustrate. Staircase intervals in the first row are decorated by their corner points (a precise description is in Definition* A.1 *of Appendix* A*).*

point corresponds to the left-bottom point; type-1 corner points are those where the boundary transitions from a vertical segment to a horizontal one, while type-2 corner points are those where the boundary transitions from a horizontal one to vertical one (precise descriptions are given in Definition A.1 of Appendix A).

Given a staircase interval I, for each $j = 0, 1, 2$ we define the function $\gamma_j(I) : \mathbb{R}^2 \to \mathbb{Z}_{\geq 0}$ as

$$\gamma_j(I)(\mathbf{a}) = \begin{cases} 1, & \mathbf{a} \text{ is a } j\text{th-type corner point of } I, \\ 0 & \text{otherwise.} \end{cases} \tag{3.3}$$

Elder-rule feature functions defined below will be useful in later sections.

Definition 3.9 (elder-rule feature functions). *Let $\mathcal{X}$ be an aug-MS and $I_{\mathcal{X}} = \{\!\{I_x : x \in X\}\!\}$ be an ER-staircode of $\mathcal{X}$. For $j = 0, 1, 2$, we define the j*th elder-rule feature function *as the sum $\gamma_j^{\mathcal{X}} = \sum_{x \in X} \gamma_j(I_x)$.*

Remark 3.10. It is not hard to check that $\gamma_j(I)$ in (3.3) is equal to the jth graded Betti number of the interval module $\mathbb{R}^2 \to \mathbf{Vec}$ supported by I (Definition 2.3). Thus, $\gamma_j^{\mathcal{X}} = \sum_{x \in X} \beta_j^{I_{I_x}}$.

4. Decorated elder-rule-staircodes and treegrams. In section 4.1, we prove Theorem 3.7 and introduce *bipersistence treegrams* to encode multiscale clustering information of aug-MSs. In section 4.2, we show that an "enriched" ER-staircode of an aug-MS $\mathcal{X}$ can recover the so-called *fibered treegram* of $\mathcal{X}$, i.e., 1-dimensional slices of the aforementioned bipersistence treegram. Also, we identify a sufficient condition on $\mathcal{X}$ for its ER-staircode to be the barcode of the 2-parameter persistence module $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{X}))$. In section 4.3, we show that if $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{X}))$ is interval decomposable, then its barcode is equal to the ER-staircode of $\mathcal{X}$. Also, we stratify the collection of aug-MSs $\mathcal{X}$ according to the complexity of the indecomposable summands of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{X}))$.

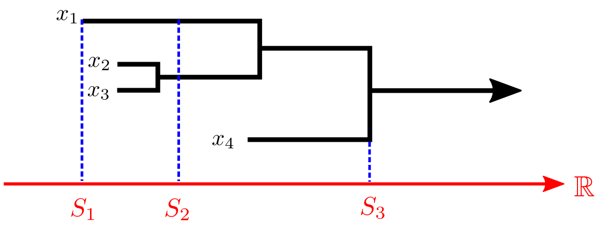


Figure 6. *A (1-dimensional) treegram θ_X over the set $X := \{x_1, x_2, x_3, x_4\}$. Notice that $\theta_X(t) = \emptyset$ for $t \in (-\infty, S_1)$. Also, $\theta_X(S_1) = \{\{x_1\}\}$, $\theta_X(S_2) = \{\{x_1\}, \{x_2, x_3\}\}$, and $\theta_X(t) = \{X\}$ for all $t \in [S_3, \infty)$.*

4.1. Bipersistence treegrams.

Partitions and subpartitions. Let X be a nonempty finite set. We will call any partition P of a subset X' of X a *subpartition* of X. In this case, we call X' the *underlying set of P*. A partition of the empty set is defined as the empty set. By $\mathbf{Subpart}(X)$, we denote the set of *all subpartitions of X*, i.e., $\mathbf{Subpart}(X) := \{P : \exists X' \subseteq X,\ P \text{ is a partition of } X'\}$. We refer to elements of a subpartition of X as *blocks*.

Let $P, Q \in \mathbf{Subpart}(X)$. By $P \leq Q$, we mean P refines Q; i.e., for all $B \in P$, there exists $C \in Q$ such that $B \subseteq C$. For example, let $X = \{x_1, x_2, x_3\}$ and consider the subpartitions $P := \{\{x_1\}, \{x_2\}\}$ and $Q := \{\{x_1, x_2\}, \{x_3\}\}$ of X. Then it is easy to see that $P \leq Q$.

Treegrams are a generalized notion of dendrograms [50], which are useful for visualizing the evolution of clustering information of 1-parameter simplicial filtrations.

Definition 4.1 (treegrams [50]). *A* treegram *over a finite set X is any order-preserving map $\theta_X : \mathbb{R} \to \mathbf{Subpart}(X)$; i.e., if $t_1 \leq t_2$, then $\theta_X(t_1) \leq \theta_X(t_2)$, satisfying the following: (1) There exists $T > 0$ such that $\theta_X(t) = \{X\}$ for $t \geq T$ and $\theta_X(t)$ is empty for $t \leq -T$, and (2) for all t there exists $\epsilon > 0$ such that $\theta_X(s) = \theta_X(t)$ for $s \in [t, t+\epsilon]$. See Figure 6 for an example. Also, even when the domain $\mathbb{R}$ is replaced by any totally ordered set L isomorphic to $\mathbb{R}$, θ_X is said to be a (1-parameter) treegram.*

Given a simplicial complex K, let $K^{(0)}$ be the vertex set of K. Let $\pi_0(K)$ be the partition of the vertex set $K^{(0)}$ according to the connected components of K. A functor $\mathcal{K} : \mathbb{P} \to \mathbf{Simp}$ is said to be a *filtration of K* if $\mathcal{K}(\mathbf{a}) \subseteq K$ for all $\mathbf{a} \in \mathbb{P}$, every internal map is an inclusion, and there exists $\mathbf{a}_0 \in \mathbb{P}$ such that for all $\mathbf{a} \in \mathbb{P}$ with $\mathbf{a}_0 \leq \mathbf{a}$, $\mathcal{K}(\mathbf{a}) = K$.

Example 4.2 (treegrams induced by simplicial filtrations). *Let K be a simplicial complex on the vertex set $X = \{x_1, x_2, \ldots, x_n\}$, and let $\mathcal{K} : \mathbb{R} \to \mathbf{Simp}$ be a filtration of K. Assume that K consists solely of one connected component, i.e., $\pi_0(K) = \{X\}$. Then the function $\pi_0(\mathcal{K}) : \mathbb{R} \to \mathbf{Subpart}(X)$ defined as $\varepsilon \mapsto \pi_0(\mathcal{K}(\varepsilon))$ is a treegram over X.*

The zeroth elder rule for a 1-parameter filtration. Let θ_X be a treegram over X. We define the *birth time* of x as $b(x) := \min\{\varepsilon \in \mathbb{R} : x \text{ is in the underlying set of } \theta_X(\varepsilon)\}$ (by (1) and (2) of Definition 4.1, every $x \in X$ has the birth time $b(x)$). Pick any order $<$ on X such that $b(x) < b(x')$ implies $x < x'$ for all $x, x' \in X$.[1] For $\varepsilon \in [b(x), \infty)$, we denote the block to which x belong in the subpartition $\theta_X(\varepsilon)$ by $[x]_\varepsilon$. We define the *death time* of x as $d^<(x) = \sup\{\varepsilon \in [b(x), \infty] : x = \min([x]_\varepsilon, <)\}$. As long as $<$ is compatible with the birth

[1]This order $<$ is uniquely specified if all $x \in X$ have different birth times.

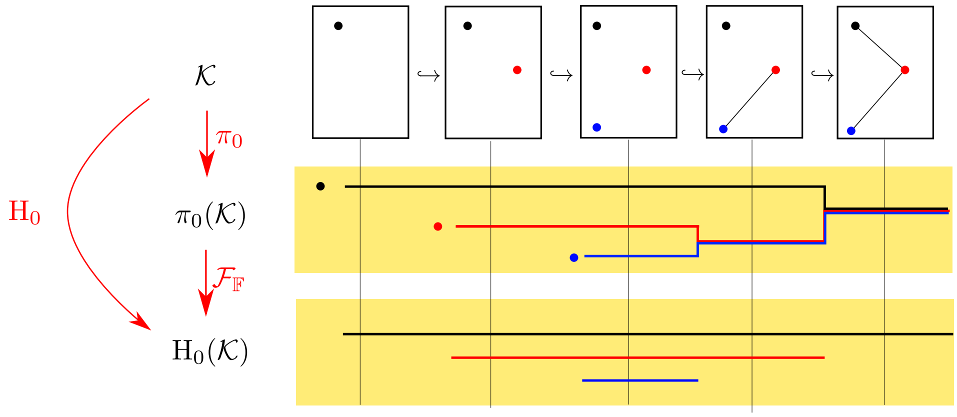


Figure 7. *The first row represents a simplicial filtration $\mathcal{K}$. The second row stands for the treegram $\pi_0(\mathcal{K})$ which encodes the evolution of clusters in $\mathcal{K}$ (Example 4.2). The third row is the barcode of $\mathrm{H}_0(\mathcal{K})$. The persistence module $\mathrm{H}_0(\mathcal{K})$ can be obtained by applying the linearization functor (Definition 4.14) to $\pi_0(\mathcal{K})$. Alternatively, the barcode of $\mathrm{H}_0(\mathcal{K})$ can also be obtained by applying the elder rule to $\pi_0(\mathcal{K})$ (Definition 4.3).*

times, the *elder-rule-barcode* is uniquely defined (which will be proved in Appendix B).

Definition 4.3 (elder-rule-barcode of a treegram). *Let $\theta_X : \mathbb{R} \to \mathbf{Subpart}(X)$ be a treegram over X. For any order $<$ on X compatible with the birth times, let $J_x := [b(x), d^<(x))$. The elder-rule-barcode of θ_X is defined as the multiset $\mathbf{barc}(\theta_X) := \{\!\{J_x : x \in X\}\!\}$.*

For the 1-parameter case, the elder-rule-barcode of a treegram can be obtained by dismantling the treegram into linear pieces with respect to the elder rule; see the theorem below. Even though this result is well known (see, e.g., [22]), we include a proof at the end of this section.

Theorem 4.4 (compatibility between the elder-rule and algebraic decomposition). *Let $\mathcal{K}$ and θ_X be the filtration and the treegram in Example 4.2, respectively. Let $\mathbf{barc}(\theta_X) = \{\!\{J_x : x \in X\}\!\}$ be the elder-rule-barcode of θ_X. Then $\mathrm{H}_0(\mathcal{K}) \cong \bigoplus_{x\in X} \mathcal{I}^{J_x}$ (see Figure 7).*

We are now ready to prove Theorem 3.7.

Proof of Theorem 3.7. Fix $L \in \mathcal{L}$. Since L is isomorphic to $\mathbb{R}$ as a totally ordered set, $\mathcal{K} = \mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})|_L : L \to \mathbf{Simp}$ can be viewed as a 1-parameter filtration. Consider the treegram $\theta_X := \pi_0(\mathcal{K}) : L \to \mathbf{Subpart}(X)$. By the definition of I_xs, it is clear that $\{\!\{L \cap I_x : x \in X\}\!\}$ is the elder-rule-barcode of the treegram θ_X (Definition 4.3). Hence, by Theorem 4.4, the multiset $\{\!\{L \cap I_x : x \in X\}\!\}$ is equal to the barcode of $\mathrm{H}_0(\mathcal{K})$. Since $\mathrm{H}_0(\mathcal{K}) = M|_L$, we have $\{\!\{L \cap I_x : x \in X\}\!\} = \mathbf{barc}(M|_L)$. ■

Bipersistence treegrams. We now extend the notion of treegrams to encode the evolution of clusters of a 2-parameter filtration (similar ideas appear in [34]). A *bipersistence treegram* over a finite set X is any order-preserving map $\theta^{\mathrm{bi}}_X : \mathbb{R}^2 \to \mathbf{Subpart}(X)$; i.e., if $\mathbf{a} \leq \mathbf{b}$ in $\mathbb{R}^2$, then $\theta^{\mathrm{bi}}_X(\mathbf{a}) \leq \theta^{\mathrm{bi}}_X(\mathbf{b})$.

We induce a bipersistence treegram over X from an aug-MS $\mathcal{X}$.

Definition 4.5 (Rips bipersistence treegrams). *Let $\mathcal{X} = (X, d_X, f_X)$ be an aug-MS. We*

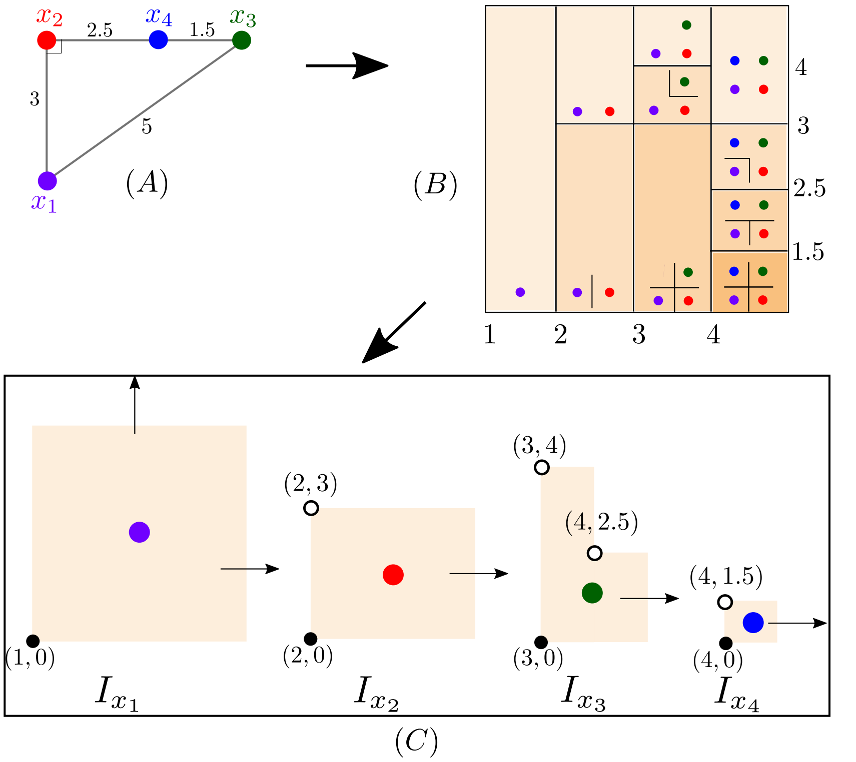


Figure 8. *Consider the aug-MS $\mathcal{X}$ defined in Figure 2. Figures* (A) *and* (C) *above are identical to Figures* 2(A) *and* (B)*, respectively.* (B) *The Rips bipersistence treegram of $\mathcal{X}$ (Definition 4.5). The summarization processes* (A)→(B)→(C) *are analogous to the processes depicted in Figure 7. Figures are best viewed in color.*

*define $\theta^{\mathrm{bi}}_{\mathcal{X}} : \mathbb{R}^2 \to$ **Subpart**(X) as $(\sigma, \varepsilon) \mapsto \pi_0\left(\mathcal{R}_\varepsilon(X_\sigma, d_X)\right)$. This $\theta^{\mathrm{bi}}_{\mathcal{X}}$ is said to be the* Rips bipersistence treegram *of $\mathcal{X}$.*

Observe that $x \in X$ belongs to the underlying set of $\theta^{\mathrm{bi}}_{\mathcal{X}}(\mathbf{a})$ if and only if $(f_X(x), 0) \leq \mathbf{a}$, i.e., $(f_X(x), 0)$ is the *birth grade* of x in $\theta^{\mathrm{bi}}_{\mathcal{X}}$. Assume that f_X is injective. Then the set of birth grades of elements in X is totally ordered. Note that the ER-staircode of $\mathcal{X}$ can be extracted from $\theta^{\mathrm{bi}}_{\mathcal{X}}$: Indeed, I_x in (3.1) can be rephrased as $I_x = \{(\sigma, \varepsilon) \in \mathbb{R}^2 : x$ is in the underlying set of $\theta^{\mathrm{bi}}_{\mathcal{X}}(\sigma, \varepsilon)$ and x has the smallest birth grade in its block of $\theta^{\mathrm{bi}}_{\mathcal{X}}(\sigma, \varepsilon)\}$. See Figure 8.

Definition 4.6 (fibered treegrams). *Let $\theta^{\mathrm{bi}}_{\mathcal{X}}$ be a Rips bipersistence treegram of an aug-MS $\mathcal{X}$. The* fibered treegram *of $\theta^{\mathrm{bi}}_{\mathcal{X}}$ refers to the collection $\{\theta^{\mathrm{bi}}_{\mathcal{X}}|_L\}_{L \in \mathcal{L}}$ of treegrams obtained by restricting $\theta^{\mathrm{bi}}_{\mathcal{X}}$ to positive-slope lines (see Figure 9 for an example).*

A combinatorial analogue of Theorem 2.5*.* Recall the elder-rule feature functions of an aug-MS $\mathcal{X}$ (Definition 3.9). We will show that they can be used to retrieve the *cardinality function* of $\theta^{\mathrm{bi}}_{\mathcal{X}}$.

Definition 4.7 (cardinality function). *Let θ^{bi}_X be a bipersistence treegram over a set X. We call the function $\left|\theta^{\mathrm{bi}}_X\right| : \mathbb{R}^2 \to \mathbb{Z}_{\geq 0}$ defined as $\mathbf{a} \mapsto \left|\theta^{\mathrm{bi}}_X(\mathbf{a})\right|$ the* cardinality function *of θ^{bi}_X.*

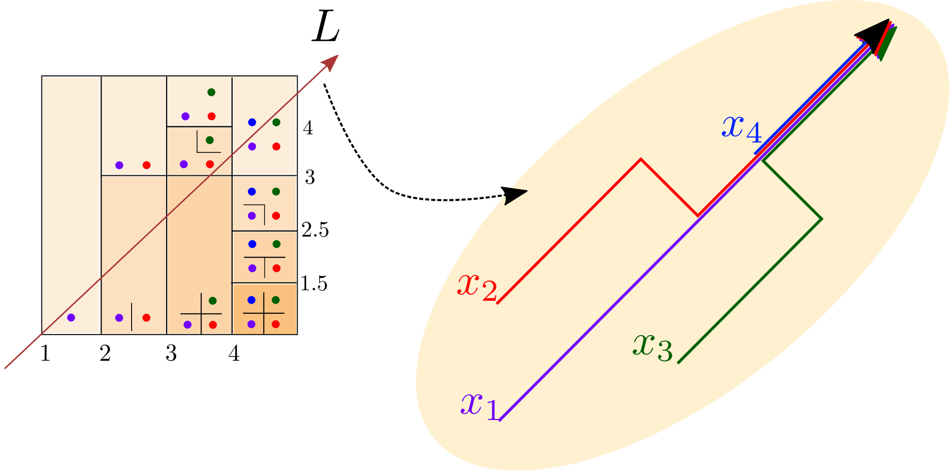


Figure 9. *Consider the bipersistence treegram in Figure 8(B), and pick a line L of positive slope. Then we obtain a treegram over L.*

For $A \subseteq \mathbb{R}^2$, we define the indicator function $\mathbb{1}_A : \mathbb{R}^2 \to \mathbb{Z}_{\geq 0}$ of A as

$$\mathbb{1}_A(\mathbf{a}) := \begin{cases} 1, & \mathbf{a} \in A, \\ 0 & \text{otherwise.} \end{cases}$$

The following proposition directly follows [24, Proposition 32].

Proposition 4.8. *Let I be a staircase interval. Then $\mathbb{1}_I(\mathbf{a}) = \sum_{\mathbf{x} \leq \mathbf{a}} \sum_{j=0}^{2} (-1)^j \gamma_j(I)(\mathbf{x})$.*

The ER-staircode and elder-rule feature functions of an aug-MS $\mathcal{X}$ recover the cardinality function of $\theta_{\mathcal{X}}^{\mathrm{bi}}$, which is analogous to Theorem 2.5.

Theorem 4.9. *Let $\mathcal{X}$ be an aug-MS, and let $I_{\mathcal{X}} = \{\!\{ I_x : x \in X \}\!\}$ be an ER-staircode of $\mathcal{X}$. For each $\mathbf{a} \in \mathbb{R}^2$,*

$$\left|\theta_{\mathcal{X}}^{\mathrm{bi}}(\mathbf{a})\right| = \sum_{x \in X}^{n} \mathbb{1}_{I_x}(\mathbf{a}) \text{ (i.e., the number of intervals } I_x \in \mathcal{I}_{\mathcal{X}} \text{ containing } \mathbf{a}) \tag{4.1}$$

$$= \sum_{\mathbf{x} \leq \mathbf{a}} \sum_{j=0}^{2} (-1)^j \gamma_j^{\mathcal{X}}(\mathbf{x}). \tag{4.2}$$

Proof. For simplicity, we assume the injectivity of $\mathcal{X}$. We prove the equality in (4.1). Let $(\sigma, \varepsilon) \in \mathbb{R}^2$. Since each block in $\theta_{\mathcal{X}}^{\mathrm{bi}}(\sigma, \varepsilon)$ contains its unique oldest element, $\left|\theta_{\mathcal{X}}^{\mathrm{bi}}(\sigma, \varepsilon)\right|$ is equal to the cardinality of the set

$$A(\sigma, \varepsilon) := \{x \in X_\sigma : x \text{ is the oldest in the block containing } x \text{ in } \theta_X(\sigma, \varepsilon)\}.$$

By (3.1), $\mathbf{a}$ belongs to I_x if and only if $x \in A(\sigma, \varepsilon)$, implying the equality

$$|A(\sigma, \varepsilon)| = (\text{the number of intervals } I_x \in \mathcal{I}_{\mathcal{X}} \text{ containing } (\sigma, \varepsilon)),$$

as desired. The equality in (4.2) directly follows from Proposition 4.8 and Definition 3.9. ■

4.2. Elder-rule-staircodes and fibered treegrams. In this section, we identify a sufficient condition on an aug-MS $\mathcal{X}$ for its ER-staircode to coincide with the barcode of the 2-parameter persistence module $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X}))$ (Theorem 4.10). Also, in general, all fibered treegrams can be recovered from ER-staircodes (Theorem 4.13).

Let (X, d_X) be a metric space, and fix $x, x' \in X$. Recall that an *ε-chain* between x and x' is a finite sequence $x = x_1, x_2, \ldots, x_\ell = x'$ in X where each consecutive pair x_i, x_{i+1} is within distance ε. Define (in fact an ultrametric) $u_X : X \times X \to \mathbb{R}_{\geq 0}$ as

$$u_X(x, x') := \min\{\varepsilon \in [0, \infty) : \text{there exists an } \varepsilon\text{-chain between } x \text{ and } x'\} \text{ (see [10])}. \tag{4.3}$$

For a metric space (X, d_X), pick any total order $<$ on X. Let $x \in X$ be a nonminimal element of $(X, <)$. A *$<$-conqueror* of x is an element $x' \in X$ such that (1) $x' < x$, and (2) for any $x'' \in X$ with $x'' < x$, it holds that $u_X(x, x') \leq u_X(x, x'')$.

Now consider an aug-MS $\mathcal{X} = (X, d_X, f_X)$. A *$<$-conqueror* function $c_x : [f_X(x), \infty) \to X$ of a nonminimal $x \in X$ sends $\sigma \in [f_X(x), \infty)$ to a conqueror of x in (X_σ, d_X). For the minimum $x' \in (X, <)$, define $c_{x'} : [f_X(x'), \infty) \to X$ to be the constant function at x'.

We generalize Theorem 4.4 and at the same time strengthen Theorem 3.7 for 2-parameter persistence modules induced by a special type of aug-MSs.

Theorem 4.10 (compatibility between the ER-staircodes and algebraic decomposition). *Let $\mathcal{X} = (X, d_X, f_X)$ be an aug-MS, and fix any order $<$ on X compatible with f_X. Assume that there exists a* constant *$<$-conqueror function for* each *$x \in X$.*[2] *Then $\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})\right)$ is interval decomposable and its barcode coincides with the ER-staircode $\mathcal{I}^<_{\mathcal{X}}$.*

The proof of Theorem 4.10 is similar to that of Theorem 4.4. Both proofs are given at the end of this section. Consider the aug-MS $\mathcal{X}$ in Figure 2. Observe that $\mathcal{X}$ satisfies the assumption in Theorem 4.10. Therefore, $\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})\right)$ is interval decomposable. There exists a class of aug-MSs to which Theorem 4.10 applies, as shown by the following corollary.

Corollary 4.11. *Let $\mathcal{X} = (X, d_X, f_X)$ be any aug-MS where d_X is an ultrametric, i.e., $d_X(x, x'') \leq \max(d_X(x, x'), d_X(x', x''))$ for all $x, x', x'' \in X$. Then $\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})\right)$ is interval decomposable (in fact, its barcode consists solely of infinite rectangular intervals).*

Proof. Let $<$ be an order on X which is compatible with f_X. For each nonminimal $x \in (X, <)$, pick an $x' \in X$ such that (1) $x' < x$, and (2) for any $x'' \in X$ with $x'' < x$, it holds that $d_X(x, x') \leq d_X(x, x'')$. Now observe that x' is a $<$-conqueror in (X_σ, d_X) for *every* $\sigma \in [f_X(x), \infty)$, completing the proof. ∎

The converse of Theorem 4.10 is false by virtue of the following example.

Example 4.12. *Let $X := \{x_i\}_{i=1}^8$. Consider $\mathcal{X} = (X, d_X, f_X)$, where (X, d_X) is depicted in Figure 10 and $f_X(x_i) = i$ for each $i = 1, \ldots, 8$. Then $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$ is interval decomposable even though $x_6 \in X$ does not have a constant conqueror. See below for the proofs of these claims.*

Details from Example 4.12. The fact that x_6 does not have a constant conqueror can be ascertained from the following observation: For $\sigma \in [6, 7)$, x_1, x_2, and x_3 are the conquerors

[2] Observe that if this property holds for the order $<$, then the same property holds for any other order $<'$ that is compatible with f_X, and $\mathcal{I}^<_{\mathcal{X}} = \mathcal{I}^{<'}_{\mathcal{X}}$.

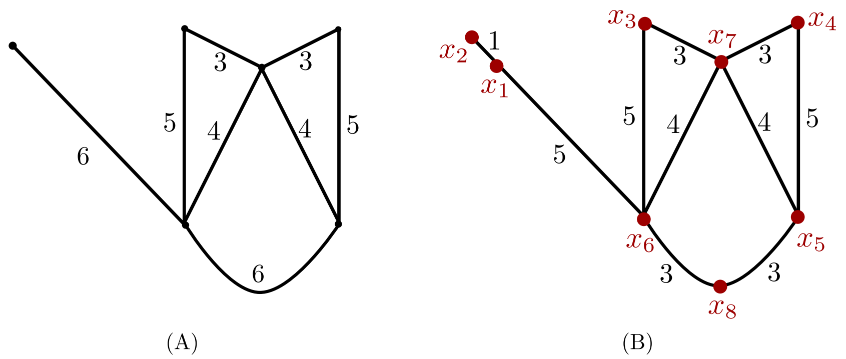


Figure 10. (A) *A metric graph G. The distance between any two points on G is the length of a shortest path connecting them.* (B) *The embedding of (X, d_X) in G.*

of x_6 in X_σ. For $\sigma \in [7, 8)$, x_3, x_4, and x_5 are the conquerors of x_6 in X_σ. For $\sigma \in [8, \infty)$, x_5 is the unique conqueror of x_6 in X_σ.

Let $\mathcal{I}_\mathcal{X} = \{I_{x_i}\}_{i=1}^8$ be the ER-staircode of $\mathcal{X}$. To prove that $M := \mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$ is interval decomposable, it suffices to construct an isomorphism f from $N := \bigoplus_{i=1}^8 I^{I_{x_i}}$ to M. For $i = 1, \ldots, 8$ and for $(\sigma, \varepsilon) \in [i, \infty) \times \mathbb{R}_+$, let $[x_i]_{(\sigma,\varepsilon)}$ be the zeroth homology class of x_i. When confusion is unlikely, we will suppress the subscript (σ, ε) in $[x_i]_{(\sigma,\varepsilon)}$.

For each i, consider $1_i := 1 \in (I^{I_{x_i}})_{(i,0)} (= \mathbb{F})$. We declare that

$$\begin{aligned}
&1_1 \overset{f_{(1,0)}}{\longmapsto} [x_1], && 1_2 \overset{f_{(2,0)}}{\longmapsto} [x_2] - [x_1],\\
&1_3 \overset{f_{(3,0)}}{\longmapsto} [x_3] - [x_1], && 1_4 \overset{f_{(4,0)}}{\longmapsto} [x_4] - [x_3],\\
&1_5 \overset{f_{(5,0)}}{\longmapsto} [x_5] - [x_4], && 1_6 \overset{f_{(6,0)}}{\longmapsto} [x_2] - [x_1] + [x_4] - [x_3] + [x_6] - [x_5],\\
&1_7 \overset{f_{(7,0)}}{\longmapsto} [x_7] - [x_3], && 1_8 \overset{f_{(8,0)}}{\longmapsto} [x_8] - [x_6].
\end{aligned}$$

Since $\{1_i : i = 1, \ldots, 8\}$ is a set of all generators of N, the above specification gives rise to a unique morphism $f : N \to M$. It is not hard to check that f is actually an *isomorphism*. ■

We enrich the ER-staircode in order to query the fibered treegram: Let $\mathcal{X} = (X, d_X, f_X)$ be an aug-MS. Let $<$ be any order on X which is compatible with f_X. For each x, we define I_x^* as the pair (I_x, c_x) of the set I_x and the $<$-conqueror function c_x. The collection $\mathcal{I}_\mathcal{X}^* := \{I_x^*\}_{x \in X}$ is said to be the *decorated ER-staircode* of $\mathcal{X}$. See Figure 11. The following result is easy to obtain with the help of decorations.

Theorem 4.13. *Given any $L \in \mathcal{L}$, the fibered treegram $\theta_\mathcal{X}^{\mathrm{bi}}|_L$ can be recovered from the decorated ER-staircode $\mathcal{I}_\mathcal{X}^*$ of the aug-MS $\mathcal{X} = (X, d_X, f_X)$.*

Proofs of Theorems 4.4 and 4.10. We first define the *linearization functor*.

Definition 4.14 (linearization functor). *Let X be a nonempty finite set. We define the linearization functor $\mathcal{F}_\mathbb{F} : \mathbf{Subpart}(X) \to \mathbf{Vec}$ as follows:*

(i) *Each $P \in \mathbf{Subpart}(X)$ is sent to the vector space $\mathcal{F}_\mathbb{F}(P)$ which consists of formal*

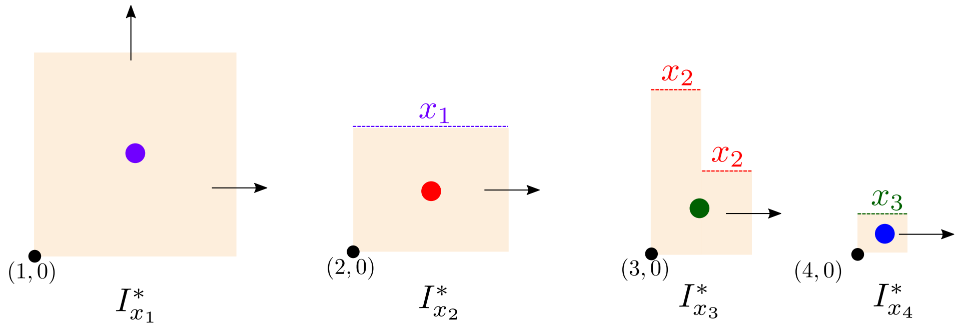


Figure 11. *Decorated intervals corresponding to the four intervals in Figure 2(B). For each $i = 2, 3, 4$, the upper boundary of I_{x_i} is decorated by the conqueror of x_i.*

linear combinations of elements of P over the field $\mathbb{F}$. In other words,

$$\mathcal{F}_{\mathbb{F}}(P) = \left\{ \sum_{B \in P} c_B B : \; c_B \in \mathbb{F} \right\}.$$

By identifying each $B \in P$ with $1 \cdot B \in \mathcal{F}_{\mathbb{F}}(P)$, the subpartition P can be viewed as a basis of $\mathcal{F}_{\mathbb{F}}(P)$.

(ii) *Each pair $P \leq Q$ in* **Subpart**(X) *is sent to the linear map $\mathcal{F}_{\mathbb{F}}(P) \to \mathcal{F}_{\mathbb{F}}(Q)$ which sends each $1 \cdot B \in \mathcal{F}_{\mathbb{F}}(P)$ to $1 \cdot B' \in \mathcal{F}_{\mathbb{F}}(Q)$ such that $B \subseteq B'$.*

The following proposition is straightforward by [44, Theorem 7.1].

Proposition 4.15.

(i) *Let $\theta_X : \mathbb{R} \to$* **Subpart**$(X)$ *be the treegram obtained by applying π_0 to a filtration $\mathcal{K} : \mathbb{R} \to$* **Simp** *(Example 4.2). The two 1-parameter persistence modules $\mathcal{F}_{\mathbb{F}} \circ \theta_X$ and $\mathrm{H}_0(\mathcal{K})$ are isomorphic.*

(ii) *Let $\mathcal{X}$ be an aug-MS. The two 2-parameter persistence modules $\mathcal{F}_{\mathbb{F}} \circ \theta^{\mathrm{bi}}_{\mathcal{X}}$ and $\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{X})\right)$ (Definitions 3.2 and 4.5) are isomorphic.*

Now we are ready to prove Theorems 4.4 and 4.10.

Proof of Theorem 4.4. Without loss of generality, let $X = \{x_1, \dots, x_n\}$. By Proposition 4.15(i), $\mathrm{H}_0(\mathcal{K})$ is isomorphic to $M := \mathcal{F}_{\mathbb{F}} \circ \theta_X$, and thus it suffices to show that $M \cong \bigoplus_{i=1}^n I^{[b(x_i), d(x_i))} =: N$. We may assume that $b(x_1) \leq b(x_2) \leq \cdots \leq b(x_n)$. For each $i \in \{2, 3, \dots, n\}$, we pick a certain $x_{q(i)}$ which merges with x_i earliest in the treegram θ_X among all the points in $\{x_1, x_2, \dots, x_{i-1}\}$. This defines a function $q : \{2, 3, \dots, n\} \to \{1, 2, \dots, n\}$ such that $q(i) < i$ for $i \in \{2, 3, \dots, n\}$ (such function q is not necessarily unique, since some two points x_{j_1}, x_{j_2} might merge with another point x_{j_3} at the same time).

For $x_i \in X$ and $\varepsilon \in [b(x_i), \infty)$, let $[x_i]_\varepsilon$ be the block containing x_i in the subpartition $\theta_X(\varepsilon)$ of X.

On the interval $(-\infty, b(x_1))$, both M and N are trivial and thus let f_ε be the zero map for $\varepsilon \in (-\infty, b(x_1))$.

Fix $\varepsilon \in [b(x_1), \infty)$. Note that the vector space $M(\varepsilon)$ is spanned by $\mathcal{A} = \{[x_i]_\varepsilon \in \theta_X(\varepsilon) : b(x_i) \leq \varepsilon\}$. Therefore, $M(\varepsilon)$ is also spanned by $\mathcal{B} = \{[x_i]_\varepsilon - [x_{q(i)}]_\varepsilon : b(x_i) \leq \varepsilon\}$, which is obtained by applying elementary linear operations on $\mathcal{A}$. Furthermore, observe that

$$\mathcal{B}' = \{[x_1]_\varepsilon\} \cup \left(\{[x_i]_\varepsilon - [x_{q(i)}]_\varepsilon : b(x_i) \leq \varepsilon\} \setminus \{0\}\right)$$

is a linearly independent set and in turn a basis of $M(\varepsilon)$. Define the linear map $f_\varepsilon : M(\varepsilon) \to N(\varepsilon)$ by defining it on the basis $\mathcal{B}'$ as follows:

(i) Send $[x_1]_\varepsilon$ to 1 in the 1st summand of $N(\varepsilon) = \bigoplus_{i=1}^n I^{[b(x_i),d(x_i))}(\varepsilon)$.

(ii) Send each basis element $[x_i]_\varepsilon - [x_{q(i)}]_\varepsilon (\neq 0)$ to 1 in the ith summand of

$$\bigoplus_{i=1}^n I^{[b(x_i),d(x_i))}(\varepsilon).$$

Then one can check that the collection $f = \{f_\varepsilon\}_{\varepsilon\in\mathbb{R}}$ is an isomorphism between M and N, as desired. ∎

We make use of the same strategy as Theorem 4.4 for proving Theorem 4.10.

Proof of Theorem 4.10. Without loss of generality, we may assume that $X = \{x_1, \ldots, x_n\}$, $f_X(x_1) \leq f_X(x_2) \leq \cdots \leq f_X(x_n)$, and let the order $<$ on X be defined as $(x_1 < x_2 < \cdots < x_n)$. Also, assume that each $<$-conqueror function $c_{x_i} : \mathbb{R} \to X$ is constant at $q(i) \in X$ (then by definition, $q(1) = x_1$). By Proposition 4.15(ii), it suffices to show that $M := \mathcal{F}_\mathbb{F} \circ \theta_\mathcal{X}^{\mathrm{bi}}$ is isomorphic to $N = \bigoplus_{i=1}^n I^{I_{x_i}^<}$.

For $x_i \in X$, and $(\sigma, \varepsilon) \in \mathbb{R}^2$ with $(\sigma, \varepsilon) \geq (f(x_i), 0)$, let $[x_i]_{(\sigma,\varepsilon)}$ be the block containing x_i in the subpartition $\theta_\mathcal{X}^{\mathrm{bi}}(\sigma, \varepsilon)$ of X.

For any $(\sigma, \varepsilon) \in \mathbb{R}^2$ such that $(\sigma, \varepsilon) \ngeq (f_X(x_1), 0)$, both $M(\sigma, \varepsilon)$ and $N(\sigma, \varepsilon)$ are trivial and thus let $f_{(\sigma,\varepsilon)}$ be the zero map for $(\sigma, \varepsilon) \ngeq (f_X(x_1), 0)$.

Fix $(\sigma, \varepsilon) \in \mathbb{R}^2$ such that $(\sigma, \varepsilon) \geq (f_X(x_1), 0)$. The vector space $M(\sigma, \varepsilon)$ is spanned by $\mathcal{A} = \{[x_i]_{(\sigma,\varepsilon)} \in \theta_\mathcal{X}^{\mathrm{bi}}(\sigma, \varepsilon) : (f_X(x_i), 0) \leq (\sigma, \varepsilon)\}$. Therefore, $M(\sigma, \varepsilon)$ is also spanned by $\mathcal{B} = \{[x_1]_{(\sigma,\varepsilon)}\} \cup \{[x_i]_{(\sigma,\varepsilon)} - [x_{q(i)}]_{(\sigma,\varepsilon)} : (f_X(x_i), 0) \leq (\sigma, \varepsilon)\}$, which is obtained by applying elementary linear operations on $\mathcal{A}$. Furthermore, note that

$$\mathcal{B}' := \{[x_1]_{(\sigma,\varepsilon)}\} \cup \left(\{[x_i]_{(\sigma,\varepsilon)} - [x_{q(i)}]_{(\sigma,\varepsilon)} : (f_X(x_i), 0) \leq (\sigma, \varepsilon)\} \setminus \{0\}\right)$$

is a linearly independent set and in turn a basis of $M(\sigma, \varepsilon)$. Let us define a linear map $f_{(\sigma,\varepsilon)} : M(\sigma, \varepsilon) \to N(\sigma, \varepsilon)$ by defining it on the basis $\mathcal{B}'$ as follows:

(i) Send $[x_1]_{(\sigma,\varepsilon)}$ to 1 in the 1st summand of $N(\sigma, \varepsilon) = \bigoplus_{i=1}^n I^{I_{x_i}}(\sigma, \varepsilon)$.

(ii) Send each basis element $[x_i]_{(\sigma,\varepsilon)} - [x_{q(i)}]_{(\sigma,\varepsilon)} (\neq 0)$ to 1 in the ith summand of $N(\sigma, \varepsilon) = \bigoplus_{i=1}^n I^{I_{x_i}}(\sigma, \varepsilon)$.

By invoking the construction of the $<$-conqueror functions c_{x_i} and the ER-staircode $\mathcal{I}_\mathcal{X}^< = \left\{\!\!\left\{ I_{x_i}^< : i = 1, \ldots, n \right\}\!\!\right\}$, one can check that the collection $f = \{f_{(\sigma,\varepsilon)}\}_{(\sigma,\varepsilon)\in\mathbb{R}^2}$ is an *isomorphism* between M and N, as desired. ∎

4.3. Elder-rule-staircodes and barcodes. The compatibility between the elder-rule and the algebraic decomposition theory (Theorem 4.10) will be enhanced to Theorem 4.16 below. For any $(\sigma_0, \varepsilon_0) \in \mathbb{R}^2$, let $U(\sigma_0, \varepsilon_0) := \{(\sigma, \varepsilon) \in \mathbb{R}^2 : (\sigma_0, \varepsilon_0) \leq (\sigma, \varepsilon)\}$, i.e., the closed quadrant whose lower-left corner point is $(\sigma_0, \varepsilon_0)$.

Theorem 4.16. *Let $\mathcal{X}$ be an injective aug-MS such that $M := \mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})\right)$ is interval decomposable. Then the barcode of M coincides with the ER-staircode $\mathcal{I}^<_\mathcal{X}$ of $\mathcal{X}$.*

The proof utilizes results in section 5 and thus is deferred to that section.

Remark 4.17. By Theorem 4.16, testing the interval decomposability of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$ is equivalent to testing whether $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X})) \cong N := \bigoplus_{i=1}^n I^{I_{x_i}}$. In [7], there exists a deterministic algorithm for testing such an isomorphism.

Classification of the collection of augmented metric spaces. Let us consider the following collections of aug-MSs:

(i) **Aug** is defined as the collection of all finite aug-MSs.

The following are subcollections of **Aug**:

(ii) **Ult** consists of all finite aug-MSs (X, d_X, f_X) where d_X is an ultrametric.

(iii) $\mathbf{Rep}(e,m)$ consists of all finite aug-MSs $\mathcal{X}$ such that the horizontal internal maps of $\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})\right)$ are injective.

(iv) **Rec** consists of all finite aug-MSs $\mathcal{X}$ such that $\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})\right)$ is rectangle decomposable, i.e., each indecomposable summand is $I^{[a,b)\times[c,d)}$ for some intervals $[a,b), [c,d)$ of $\mathbb{R}$.

(v) **ER** consists of all finite aug-MSs $\mathcal{X}$ such that the assumption of Theorem 4.10 holds (and thus is interval decomposable).

(vi) **Dec** consists of all finite aug-MSs $\mathcal{X}$ such that $\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})\right)$ is interval decomposable.

In order to clarify the relationship among these collections, we begin by recalling the following.

Theorem 4.18 (see [5, Corollary 3.17]). $\mathbf{Rep}(e,m) = \mathbf{Rec}$.

We enrich Theorem 4.18 as follows.

Theorem 4.19. $\mathbf{Ult} \subsetneq \mathbf{Rep}(e,m) = \mathbf{Rec} \subsetneq \mathbf{ER} \subsetneq \mathbf{Dec} \subsetneq \mathbf{Aug}$.

We in particular remark that Example 5.5 provides an aug-MS which does not belong to **Dec**. Such examples provide clues for constructing aug-MSs $\mathcal{X}$ which yield $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$ whose isomorphism type is exotic, thus complementing the results of [5].

Proof.

(i) $\mathbf{Ult} \subseteq \mathbf{Rep}(e,m)$: Consider an aug-MS $\mathcal{X} = (X, d_X, f_X)$ where d_X is an ultrametric. By Proposition 4.15(ii), it suffices to show that every horizontal internal map of $\theta^{\mathrm{bi}}_X : \mathbb{R}^2 \to \mathbf{Subpart}(X)$ is injective. Pick $(\sigma_1, \varepsilon), (\sigma_2, \varepsilon) \in \mathbb{R}^2$ with $\sigma_1 \leq \sigma_2$, and pick $x, y \in X$ with $f_X(x), f_X(y) \leq \sigma_1$. Assume that $[x]_{(\sigma_2,\varepsilon)} = [y]_{(\sigma_2,\varepsilon)}$, and let us show that $[x]_{(\sigma_1,\varepsilon)} = [y]_{(\sigma_1,\varepsilon)}$. The assumption implies that there exists a sequence $x = x_0, \ldots, x_n = y$ in X_{σ_2} such that $d_X(x_i, x_{i+1}) \leq \varepsilon$ for each i. Since d_X is an ultrametric, we have that $d_X(x,y) \leq \max_{i=0}^{n-1} d_X(x_i, x_{i+1}) \leq \varepsilon$. Invoking $f_X(x), f_X(y) \leq \sigma_1$, we have $[x]_{(\sigma_1,\varepsilon)} = [y]_{(\sigma_1,\varepsilon)}$, as desired.

(ii) $\mathbf{Ult} \neq \mathbf{Rep}(e,m)$: Let us equip the set $X := \{1,2,3\}$ with the standard metric $d(i,j) := |i-j|$, $i,j \in \{1,2,3\}$, and the map $f : X \to \mathbb{R}$ defined as $i \mapsto i$ for $i = 1,2,3$. Observe that d_X is not an ultrametric, but every horizontal internal map of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$ is injective.

(iii) $\mathbf{Rep}(e,m) \subseteq \mathbf{ER}$: Consider an aug-MS $\mathcal{X} = (X, d_X, f_X)$ in $\mathbf{Rep}(e,m)$. Pick an order $<$ on X which is compatible with f_X. Let $x \in (X,<)$ be a nonminimal element, and let $\sigma_0 := f_X(x)$. Let x' be a conqueror of x in the metric space (X_{σ_0}, d_X). It suffices to show that for each $\sigma \in [\sigma_0, \infty)$, x' is a conqueror of x in (X_σ, d_X). Fix $\sigma \in [\sigma_0, \infty)$. Let $x'' \in X_\sigma$ be a conqueror of x in (X_σ, d_X). Let $u_X^\sigma : X \times X \to \mathbb{R}$ be the (ultra)metric induced by (X_σ, d_X) as in (4.3). Let $\varepsilon := u_X^\sigma(x'', x)$. By definition of x'', we have

$$\varepsilon \leq u_X^\sigma(x', x). \tag{4.4}$$

Also, by definition of ε, we have $[x]_{(\sigma,\varepsilon)} = [x'']_{(\sigma,\varepsilon)}$. Since $\mathcal{X}$ belongs to $\mathbf{Rep}(e, m)$, it also holds that $[x]_{(\sigma_0,\varepsilon)} = [x'']_{(\sigma_0,\varepsilon)}$, implying

$$u_X^{\sigma_0}(x, x'') \leq \varepsilon. \tag{4.5}$$

Since x' is a conqueror of x in (X_{σ_0}, d_X), we have

$$u_X^{\sigma_0}(x, x') \leq u_X^{\sigma_0}(x, x''). \tag{4.6}$$

Also, since $u_X^\sigma \leq u_X^{\sigma_0}$, we have

$$u_X^\sigma(x, x') \leq u_X^{\sigma_0}(x, x'). \tag{4.7}$$

By concatenating inequalities (4.4), (4.5), (4.6), and (4.7), we obtain

$$u_X^\sigma(x, x') \leq u_X^{\sigma_0}(x, x') \leq u_X^{\sigma_0}(x, x'') \leq \varepsilon \leq u_X^\sigma(x', x).$$

The leftmost and rightmost terms are the same, implying that $\varepsilon = u_X^\sigma(x, x')$. Since $\varepsilon = u_X^\sigma(x'', x)$ and x'' is a conqueror of x in (X_σ, d_X), we conclude that x' is another conqueror of x in (X_σ, d_X), as desired.

(iv) $\mathbf{Rep}(e, m) \neq \mathbf{ER}$: It is not hard to check that the aug-MS depicted in Figure 2(A) belongs to $\mathbf{ER}$ but not $\mathbf{Rep}(e, m)$.

(v) $\mathbf{ER} \subsetneq \mathbf{Dec}$: This follows from Theorem 4.10 and Example 5.5.

(vi) $\mathbf{Dec} \subsetneq \mathbf{Aug}$: This directly follows from Example 5.5. ∎

5. Elder-rule-staircodes and graded Betti numbers. In this section, we show that given an aug-MS $\mathcal{X}$ the graded Betti numbers of $\mathrm{H}_0(\mathcal{R}_\bullet^{\mathrm{bi}}(\mathcal{X}))$ can be easily extracted from the ER-staircode of $\mathcal{X}$ (Theorem 5.4). Along the way, we obtain a characterization result for the graded Betti numbers of $\mathrm{H}_0(\mathcal{R}_\bullet^{\mathrm{bi}}(\mathcal{X}))$ (Theorem 5.2), which is of independent interest.

Computing the graded Betti numbers of $\mathrm{H}_0(\mathcal{R}_\bullet^{\mathrm{bi}}(\mathcal{X}))$ for an aug-MS $\mathcal{X}$. Given a simplicial complex K and $k \in \mathbb{Z}_{\geq 0}$, let $C_k(K)$ be the kth chain group of K, i.e., the $\mathbb{F}$-vector space freely generated by k-simplices in K. For $k \in \mathbb{Z}_{\geq 0}$, let $\partial_k : C_k(K) \to C_{k-1}(K)$ be the boundary map and $Z_k(K) := \ker(\partial_k)$ the kth cycle group of K.

Henceforth, for simplicity, every aug-MS $\mathcal{X} = (X, d_X, f_X)$ will be assumed to be *generic*: f_X is injective and $|\{d_X(x, x') \in \mathbb{R} : x, x' \in X,\ x \neq x'\}| = \binom{|X|}{2}$; i.e., all nontrivial pairwise distances are distinct. The case of nongeneric aug-MS can be easily handled; see Remark 5.6. Since $\mathcal{X}$ is finite, we consider $\mathbb{Z}^2$-indexed filtration described subsequently as a substitute of $\mathcal{R}_\bullet^{\mathrm{bi}}(\mathcal{X})$.

Definition 5.1. *Consider an aug-MS $\mathcal{X} = (X, d_X, f_X)$ with $X := \{x_1, \dots, x_n\}$, and assume that $f_X(x_1) < \cdots < f_X(x_n)$. Define $f_X^{\mathbb{Z}} : X \to \mathbb{N}$ as $x_i \mapsto i$. Define $d_X^{\mathbb{Z}} : X \times X \to \mathbb{N}$ by* *sending each nontrivial pair* (x_i, x_j) $(i \neq j)$ *to* $\ell \in \{1, \dots, \binom{n}{2}\}$*, where* $d_X(x_i, x_j)$ *is the* ℓ*th smallest distance (among nonzero distance values). The restriction of* $\mathcal{R}^{\mathrm{bi}}_\bullet(X, d^{\mathbb{Z}}_X, f^{\mathbb{Z}}_X) : \mathbb{R}^2 \to$ **Simp** *to* $\mathbb{Z}^2$ *is the* $\mathbb{Z}^2$-indexed Rips filtration[3] *of* $\mathcal{X}$*. Also, let* $\gamma^{\mathcal{X}}_j$ *denote the* j*th elder-rule feature function of* $(X, d^{\mathbb{Z}}_X, f^{\mathbb{Z}}_X)$ *for* $j = 0, 1, 2$ *in this section.*

For Theorem 5.2, we introduce relevant terminology and notation. Let $\mathcal{S}$ be the $\mathbb{Z}^2$-indexed Rips filtration of an aug-MS $\mathcal{X}$, and let $\mathcal{K}$ be the 1-*skeleton of* $\mathcal{S}$; i.e., $\mathcal{K}$ is another $\mathbb{Z}^2$-indexed filtration where $\mathcal{K}(\mathbf{a})$ is the 1-skeleton of $\mathcal{S}(\mathbf{a})$ for every $\mathbf{a} \in \mathbb{Z}^2$:

- Note that $\mathcal{K}$ is 1-*critical*: every simplex that appears in $\mathcal{K}$ has a unique birth index. Let e be an edge that appears in $\mathcal{K}$ whose birth index is $\mathbf{b}(e) = (b_1, b_2) \in \mathbb{Z}^2$. We say that the edge e is *negative* if the number of connected components in $\mathcal{K}(b_1, b_2)$ is strictly less than that of $K(b_1, b_2 - 1)$. Otherwise, the edge e is *positive*.
- For $k = 0, 1$, let $C_k(\mathcal{K}) : \mathbb{Z}^2 \to \mathbf{Vec}$ be the module defined as $C_k(\mathcal{K})(\mathbf{a}) := C_k(\mathcal{K}(\mathbf{a}))$, where the internal maps $\varphi_{\mathcal{K}}(\mathbf{a}, \mathbf{b})$ are the canonical inclusion maps $C_k(\mathcal{K}(\mathbf{a})) \hookrightarrow C_k(\mathcal{K}(\mathbf{b}))$. In particular, since $\mathcal{K}$ is 1-critical, $C_k(\mathcal{K})$ is the free module whose basis elements one-to-one correspond to all the kth simplices in $S := \mathcal{K}(n, \binom{n}{2})$. More specifically, the birth of a simplex $\sigma \in S$ in $\mathcal{K}$ at $\mathbf{a} \in \mathbb{Z}^d$ corresponds to a generator of $C_k(\mathcal{K})$ at $\mathbf{a}$.

Theorem 5.2. *Let* $\mathcal{K}$ *be the* 1*-skeleton of the* $\mathbb{Z}^2$*-indexed Rips filtration of an aug-MS. Let* $\mathcal{K}^-$ *be the filtration of* $\mathcal{K}$ *that is obtained by removing all positive edges in* $\mathcal{K}$*. Then the following hold:*

(i) *The following sequence of persistence modules is exact:*

$$0 \to Z_1(\mathcal{K}^-) \xrightarrow{i} C_1(\mathcal{K}^-) \xrightarrow{\partial_1} C_0(\mathcal{K}^-) \xrightarrow{p} \mathrm{H}_0(\mathcal{K}) \to 0, \tag{5.1}$$

where i *is the canonical inclusion,* ∂_1 *is the boundary map, and* p *is the canonical projection.*

(ii) *The sequence in* (5.1) *is a minimal free resolution of* $\mathrm{H}_0(\mathcal{K})$*.*[4]

We prove Theorem 5.2 at the end of this section. For example, consider the aug-MS $\mathcal{X}$ in Figure 2(A). We can read off the graded Betti number of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})) : \mathbb{R}^2 \to \mathbf{Vec}$ from $\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})$. See Figure 12.

The ER-staircode and the graded Betti numbers. Next, we will see that for any aug-MS $\mathcal{X}$, the graded Betti numbers of the zeroth homology of $\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})$ can be extracted from the ER-staircode of $\mathcal{X}$.

Given finite $M : \mathbb{Z}^2 \to \mathbf{Vec}$, the *support* of the ith graded Betti number β^M_i of M is defined as $\mathrm{supp}(\beta^M_i) := \{\mathbf{a} \in \mathbb{Z}^2 : \beta^M_i(\mathbf{a}) \neq 0\}$. Theorem 5.2 directly implies the following.

Lemma 5.3. *Let* $\mathcal{K}$ *be the* $\mathbb{Z}^2$*-indexed Rips filtration of an aug-MS, and let* $M := \mathrm{H}_0(\mathcal{K})$*. For each* $i = 0, 1, 2$*,* $\beta^M_i(\mathbf{a}) \leq 1$*,* $\mathbf{a} \in \mathbb{Z}^2$ *and for every pair* $i \neq j$ *in* $\{0, 1, 2\}$*, it holds that* $\mathrm{supp}(\beta^M_i) \cap \mathrm{supp}(\beta^M_j) = \emptyset$*.*

[3] $d^{\mathbb{Z}}_X$ does not necessarily satisfy the triangle inequality, but it does not prevent us from defining $\mathcal{R}^{\mathrm{bi}}_\bullet(X, d^{\mathbb{Z}}_X, f^{\mathbb{Z}}_X)$.

[4] This means that the chain obtained by setting $F^0 = C_0(\mathcal{K}^-)$, $F^1 = C_1(\mathcal{K}^-)$, $F^2 = Z_1(\mathcal{K}^-)$, and $F^i = 0$ for $i > 2$ in (2.1) satisfies the minimality condition that is described in the paragraph after (2.1).

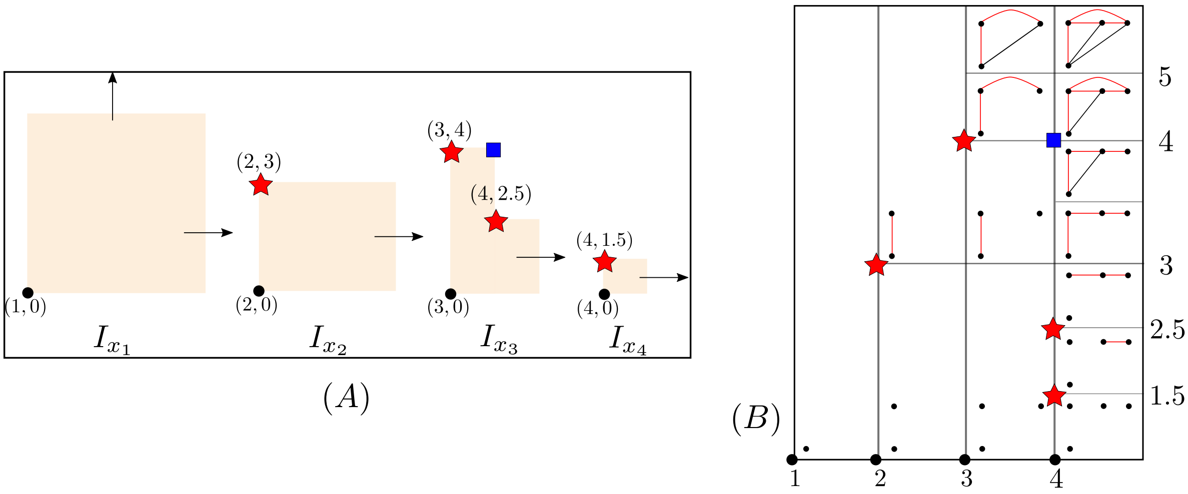


Figure 12. (A) *The ER-staircode $\mathcal{I}_{\mathcal{X}}$ of $\mathcal{X}$ in Figure 2*(A). *The types of corner points are indicated by circles (0th), stars (1st), and squares (2nd).* (B) *The* 1*-skeleton of $\mathcal{K} := \mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{X})$. Red edges and black edges are negative and positive, respectively. The four generators of $C_0(\mathcal{K})$ are located at grades* $(1,0),(2,0),(3,0),(4,0)$, *forming the support of the zeroth graded Betti number of $\mathrm{H}_0(\mathcal{K})$ (marked by circles). The birth grades of four negative edges are* $(2,3)$, $(3,4)$, $(4,1.5)$, *and* $(4,2.5)$, *forming the support of the first graded Betti number (marked by stars). The unique cycle consisting solely of negative edges is $x_2x_3+x_3x_4+x_4x_2$, which is born at* $(4,4)$, *the unique support point of the second graded Betti number.* Observe that the locations of corner points in $\mathcal{I}_{\mathcal{X}}$ one-to-one correspond to the support of graded Betti numbers of $\mathrm{H}_0(\mathcal{K})$, which illustrates that Theorem 5.4 holds.

We remind the reader that all the aug-MSs in this section are generic. In particular, when this is not the case, the lemma above will not hold in general.

Proof. Since we concern the zeroth homology of $\mathcal{K}$, let us assume that $\mathcal{K}$ itself consists solely of vertices and edges. By Theorem 5.2, it suffices to show that every generator of $Z_1(\mathcal{K}^-)$, $C_1(\mathcal{K}^-)$, and $C_0(\mathcal{K}^-)$ is born at a different grade. In $C_0(\mathcal{K}^-)$, every vertex x_i is born at $(i,0)$ for $i=1,\dots,n$. Therefore, $\beta_0^M(\mathbf{a}) \le 1$ for every $\mathbf{a}\in\mathbb{Z}^2$ and $\mathrm{supp}(\beta_0^M) \subset \mathbb{Z}\times\{0\}$. Also, by Definition 5.1, every generator of $C_1(\mathcal{K}^-)$ and $Z_1(\mathcal{K}^-)$ is born at a different grade in $\mathbb{Z}\times\mathbb{N}$, completing the proof. ■

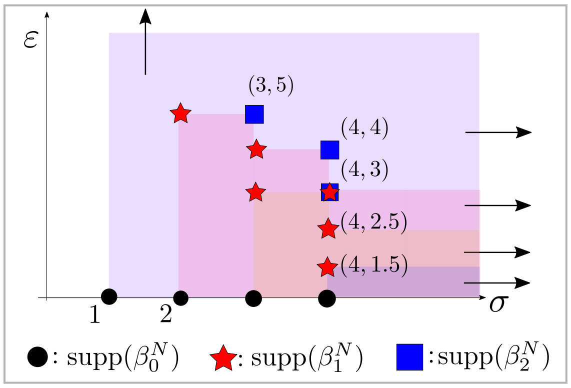
Given any two functions $\alpha,\alpha':\mathbb{Z}^2\to\mathbb{Z}_{\ge 0}$, we define $\alpha-\alpha':\mathbb{Z}^2\to\mathbb{Z}_{\ge 0}$ as

$$(\alpha-\alpha')(\mathbf{x}) = \max(\alpha(\mathbf{x})-\alpha'(\mathbf{x}),0) \text{ for } \mathbf{x}\in\mathbb{Z}^2.$$

Theorem 5.4. *Let $\mathcal{K}$ be the $\mathbb{Z}^2$-indexed Rips filtration of an aug-MS $\mathcal{X}$, and let $M := \mathrm{H}_0(\mathcal{K})$. Let β_i^M be the ith graded Betti number of M. Then*

$$\beta_0^M = \gamma_0^{\mathcal{X}}, \quad \beta_1^M = \gamma_1^{\mathcal{X}} - \gamma_2^{\mathcal{X}}, \quad \beta_2^M = \gamma_2^{\mathcal{X}} - \gamma_1^{\mathcal{X}}. \tag{5.2}$$

In particular, we note that the elder-rule feature functions $\gamma_j^{\mathcal{X}}$ are easy to compute, as one only needs to compute and aggregate the type of each corner in staircase intervals in the ER-staircode of $\mathcal{X}$. Once $\gamma_j^{\mathcal{X}}$s are known, one can easily compute the graded Betti number of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{X}))$ by Theorem 5.4. See Example 5.5 below. We also remark that *Koszul homol-*



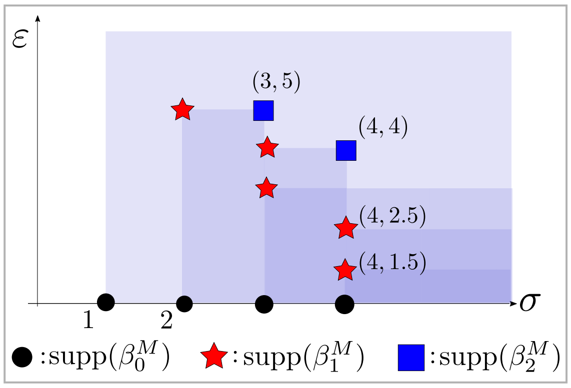


Figure 13. *The respective supports of the graded Betti numbers of N (left) and M (right) from Example 5.5. All the graded Betti numbers attain the value 1 on their supports. The graded Betti numbers of N are directly obtained by stacking the staircase intervals in the ER-staircode of $\mathcal{X}$ (Remarks 2.4(i) and 3.10). The graded Betti numbers of M are obtained by applying Theorem 5.4 to the graded Betti numbers of N; in particular, the support points of β_1^N and β_2^N at $(4,3)$ are canceled out.*

ogy formulae [40, Proposition 5.1] are in a form similar to those in (5.2). However, Koszul homology formulae do not directly imply those in (5.2) nor vice versa.

Example 5.5 (noninterval-decomposable case). *Consider the metric space $(\{x_i\}_{i=1}^4, d_X)$ in Figure 2(A). Define $h_X : \{x_i\}_{i=1}^4 \to \mathbb{R}$ as $h_X(x_1) = 1$, $h_X(x_2) = 3$, $h_X(x_3) = 2$, $h_X(x_4) = 4$. For $\mathcal{X} := (X, d_X, g_X)$, let $\mathcal{I}_{\mathcal{X}} := \{I_{x_i} : i = 1, 2, 3, 4\}$ be the ER-staircode and let $M :=$ $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$ and $N := \bigoplus_{i=1}^4 I^{I_{x_i}}$. Utilizing Theorem 5.4, it it not hard to check that $\beta_1^M \neq \beta_1^N$ and $\beta_2^M \neq \beta_2^N$ (see Figure 13). Therefore, $M \not\cong N$, and thus, by Theorem 4.16, M is* not *interval decomposable.*

Proof of Theorem 5.4. Let $\mathcal{X} := (X, d_X, f_X)$ with $X = \{x_1, \ldots, x_n\}$, and assume that $f_X(x_1) < \cdots < f_X(x_n)$. By the construction of $\mathcal{K}$ and $\gamma_i^{\mathcal{X}}$, it suffices to show the equalities in (5.2) hold on $\mathcal{A} := \{1, 2, \ldots, n\} \times \{0, 1, \ldots, \binom{n}{2}\} \subset \mathbb{Z}^2$ (β_i^M and $\gamma_i^{\mathcal{X}}$ vanish outside $\mathcal{A}$ for $i = 0, 1, 2$). By Theorem 5.2 and the construction of $\gamma_0^{\mathcal{X}}$, both of β_0^M and $\gamma_0^{\mathcal{X}}$ have values 1 on $\mathcal{A}|_{y=0} = \{(1,0), (2,0), (3,0) \ldots, (n,0)\}$ and zero outside $\mathcal{A}|_{y=0}$, implying that $\beta_0^M = \gamma_0^{\mathcal{X}}$. Note that when $i = 1, 2$, the supports of β_i^M and $\gamma_i^{\mathcal{X}}$ are contained in $\mathcal{A}|_{y>0} =$ $\{1, 2, \ldots, n\} \times \{1, \ldots, \binom{n}{2}\}$. Using induction on the x-coordinate of $\mathbb{Z}^2$, we will prove that $\beta_1^M = \gamma_1^{\mathcal{X}} - \gamma_2^{\mathcal{X}}$ and $\beta_2^M = \gamma_2^{\mathcal{X}} - \gamma_1^{\mathcal{X}}$ *on the horizontal line* $\mathcal{A}|_{y=1} = \{1, 2, \ldots, n\} \times \{1\}$. Note that $\mathcal{K}(1, b) = \{\{x_1\}\}$ for all $1 \leq b \leq \binom{n}{2}$, and thus again by Theorem 5.2 and the construction of $\gamma_i^{\mathcal{X}}$, $i = 1, 2$,

$$\text{(5.3)} \qquad \text{for } 1 \leq b \leq \binom{n}{2}, \quad \beta_1^M(1, b) = \gamma_1^{\mathcal{X}}(1, b) = 0, \text{ and } \beta_2^M(1, b) = \gamma_2^{\mathcal{X}}(1, b) = 0.$$

Specifically, we have $\beta_1^M(1,1) = \gamma_1^{\mathcal{X}}(1,1) = \gamma_1^{\mathcal{X}}(1,1) - \gamma_2^{\mathcal{X}}(1,1)$ and $\beta_2^M(1,1) = \gamma_2^{\mathcal{X}}(1,1) =$ $\gamma_2^{\mathcal{X}}(1,1) - \gamma_1^{\mathcal{X}}(1,1)$. Fix a natural number $m > 2$, and assume that $\beta_1^M(a,1) = \gamma_1^{\mathcal{X}}(a,1) -$ $\gamma_2^{\mathcal{X}}(a,1)$ and $\beta_2^M(a,1) = \gamma_2^{\mathcal{X}}(a,1) - \gamma_1^{\mathcal{X}}(a,1)$ for $1 \leq a \leq m-1$. By Theorems 4.9 and 2.5, we have $\sum_{\mathbf{x} \leq (m,1)} \sum_{i=0}^2 (-1)^i \beta_i^M(\mathbf{x}) \overset{(*)}{=} \sum_{\mathbf{x} \leq (m,1)} \sum_{i=0}^2 (-1)^i \gamma_i^{\mathcal{X}}(\mathbf{x})$. Since (1) $\beta_0^M = \gamma_0^{\mathcal{X}}$ on the entire $\mathbb{Z}^2$, and (2) $\beta_i^M, \gamma_i^{\mathcal{X}}$ vanish outside $\mathcal{A}$ for $i = 1, 2$, the induction hypothesis reduces equality (∗) to

$$-\beta_1^M(m,1)+\beta_2^M(m,1)=-\gamma_1^{\mathcal{X}}(m,1)+\gamma_2^{\mathcal{X}}(m,1).$$

By Lemma 5.3, we cannot have $\beta_1^M(m,1)=\beta_2^M(m,1)=1$. Therefore, we have (Case 1) $\beta_1^M(m,1)=1$ and $\beta_2^M(m,1)=0$, (Case 2) $\beta_1^M(m,1)=0$ and $\beta_2^M(m,1)=1$, or (Case 3) $\beta_1^M(m,1)=0$ and $\beta_2^M(m,1)=0$. Invoking that $\gamma_1^{\mathcal{X}}(m,1)$ and $\gamma_2^{\mathcal{X}}(m,1)$ are nonnegative, in all cases, we have

$$\beta_1^M(m,1)=\gamma_1^{\mathcal{X}}(m,1)-\gamma_2^{\mathcal{X}}(m,1),\quad \beta_2^M(m,1)=\gamma_2^{\mathcal{X}}(m,1)-\gamma_1^{\mathcal{X}}(m,1),$$

completing the proof of $\beta_1^M=\gamma_1^{\mathcal{X}}-\gamma_2^{\mathcal{X}}$ and $\beta_2^M=\gamma_2^{\mathcal{X}}-\gamma_1^{\mathcal{X}}$ on $\mathcal{A}|_{y=1}$. We next apply the same strategy to the horizontal lines $y=2,\ldots,\ y=\binom{n}{2}$ in order, completing the proof. ■

Remark 5.6 (Theorem 5.4 for nongeneric cases). Let $\mathcal{X}=(X,d_X,f_X)$ be an aug-MS where every pair of elements in X has a different distance. Then, even if f_X is not injective, with any choice of an order on X that is compatible with f_X, all equalities in (5.2) hold. In order to prove this, note that negative edges of the 1-skeleton $\mathcal{K}:\mathbb{R}^2\to\mathbf{Simp}$ of the filtration $\mathcal{R}^{\mathrm{bi}}(\mathcal{X}):\mathbb{R}^2\to\mathbf{Simp}$ are well-defined and that $M:=\mathrm{H}_0(\mathcal{K})$ has the minimal free resolution described in (5.1). Furthermore, based on an argument similar to the one in the proof of Lemma 5.3, the 0th, 1st, and 2nd graded Betti numbers of M have mutually disjoint supports. Then an argument similar to that in the proof of Theorem 5.4 applies.

On the other hand, if d_X is not injective, the equalities $\beta_1^M=\gamma_1^{\mathcal{X}}-\gamma_2^{\mathcal{X}}$ and $\beta_2^M=\gamma_2^{\mathcal{X}}-\gamma_1^{\mathcal{X}}$ in (5.2) do not always hold, whereas $\beta_0^M=\gamma_0^{\mathcal{X}}$ still holds without restriction: It is not difficult to construct an aug-MS $\mathcal{X}=(X,d_X,f_X)$ such that d_X is noninjective, and $\mathrm{supp}(\beta_1^M)\cap\mathrm{supp}(\beta_2^M)\neq\emptyset$. In this case, note that, regardless of the choice of order on the edges of $\mathcal{K}$, the equalities $\beta_1^M=\gamma_1^{\mathcal{X}}-\gamma_2^{\mathcal{X}}$ and $\beta_2^M=\gamma_2^{\mathcal{X}}-\gamma_1^{\mathcal{X}}$ are *not* compatible.

Below, we will make use of Theorem 5.4 in proving Theorem 4.16.

Proof of Theorem 4.16. Without loss of generality, let us assume that $X=\{x_1,x_2,\ldots,x_n\}$ with $f_X(x_i)=i$ for $i=1,2,\ldots,n$. Also, let $M\cong\bigoplus_{k\in K}I^{J_k}$ for some indexing set K. Observe that M is *upper-right continuous*, i.e., for each $(\sigma_0,\varepsilon_0)\in\mathbb{R}^2$, there exist $e_1,e_2>0$ such that if $\sigma_0\le\sigma\le\sigma_0+e_1$ and $\varepsilon_0\le\varepsilon\le\varepsilon_0+e_2$, then $M_{(\sigma_0,\varepsilon_0)}=M_{(\sigma,\varepsilon)}$. Hence, the lower-left boundary[5] of each J_k belongs to J_k. Also, note that $M_{(\sigma,\varepsilon)}\neq 0$ if and only if $(\sigma,\varepsilon)\in U(1,0)$.

Claim 1. [$\mathbf{barc}(M)$ consists of n staircase intervals (Definition 3.4), and their minimal elements are $(1,0)$,$(2,0)$,…,$(n,0)$.] First, let us show that each interval in $\mathbf{barc}(M)$ is a staircase whose minimal element lies on the σ-axis. Suppose not; i.e., there exists $k_0\in K$ such that J_{k_0} is either (not a staircase) or (a staircase whose minimum is not in the σ-axis). Either implies that J_{k_0} contains a minimal element $\mathbf{a}$ in the interior of $U(0,0)$ (see Figure 14). Then, since $M\cong\bigoplus_{k\in K}I^{J_k}$, by Remark 2.4(i), we have

$$1=\beta_0^{I^{J_{k_0}}}(\mathbf{a})\le\sum_{k\in K}\beta_0^{I^{J_k}}(\mathbf{a})=\beta_0^M(\mathbf{a}).$$

[5] $(\sigma,\varepsilon)\in\mathbb{R}^2$ is a lower-left boundary point of J_k if (σ,ε) belongs to the boundary of J_k and for any $r>0$, $(\sigma-r,\varepsilon-r)\notin J_k$. The set of lower-left boundary points of J_k is called the lower-left boundary of J_k.

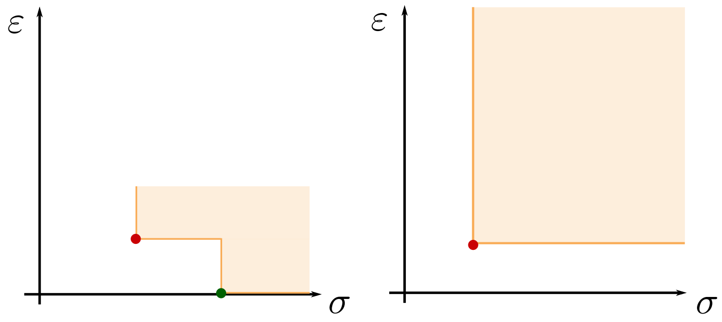


Figure 14. *If an interval J that is contained in the quadrant $U(1,0)$ is either (not a staircase) or (a staircase whose minimum is not in the σ-axis), then there exists a point $\mathbf{a}$ in the interior of $U(0,0)$ such that $\beta_0^{I^J}(\mathbf{a}) = 1$ (red points in the figure above).*

However, by Theorem 5.4, we have

$$\operatorname{supp}(\beta_0^M) = \{(i,0) : i = 1,\dots,n\} \not\ni \mathbf{a},$$

a contradiction. Therefore, (1) each J_k has its minimum element in the σ-axis, and (2) since $\beta_0^M = \sum_{k\in K} \beta_0^{I^{J_k}}$, by invoking Remark 3.10, the minimums of J_ks form the set $\{(i,0) : i = 1,\dots,n\}$. This implies that the indexing set K contains n elements, as desired. □

From now on, we denote $\mathbf{barc}(M)$ by $\{J_k\}_{k=1}^n$, where the minimum of J_k is $(k,0)$ for each k. Also, let

$$\varepsilon_1 := \max_{x_i,x_j\in X} d_X(x_i,x_j). \tag{5.4}$$

Claim 2. $[J_1 = U(1,0).]$ Observe that if $\sigma \in [n,\infty)$ and $\varepsilon \in [\varepsilon_1,\infty)$, then

$$\dim M_{(\sigma,\varepsilon)} = 1 \quad \text{and} \quad \operatorname{rank} \varphi_M((1,0),(\sigma,\varepsilon)) = 1.$$

Since $\operatorname{rank} \varphi_M((1,0),(\sigma,\varepsilon))$ is equal to the total multiplicity of elements of $\mathbf{barc}(M)$ which contain both $(1,0)$ and (σ,ε), J_1 must be $U(1,0)$. □

Now let $f : \bigoplus_{k=1}^n I^{J_k} \to M$ be any isomorphism. For each k, let $1_k := 1 \in (I^{J_k})_{(k,0)} (= \mathbb{F})$, and let $f_{(k,0)}(1_k) := v_k \in M_{(k,0)}$. For $x_k \in X$ and $(\sigma,\varepsilon) \in [k,\infty) \times \mathbb{R}_+$, let $[x_k]_{(\sigma,\varepsilon)}$ be the zeroth homology class of x_k. When confusion is unlikely, we will suppress the subscript (σ,ε) in $[x_k]_{(\sigma,\varepsilon)}$.

Note that, by the definition of $M_{(k,0)}$ for each $k = 1,\dots,n$, there exist $c_{k\ell} \in \mathbb{F}$ for $\ell = 1,\dots,k$ such that

$$\begin{aligned} v_1 &= c_{11}[x_1], \\ v_2 &= c_{21}[x_1] + c_{22}[x_2], \\ &\vdots \\ v_n &= c_{n1}[x_1] + \cdots + c_{nn}[x_n]. \end{aligned} \tag{5.5}$$

An $x_\ell \in X$ will be called a *summand of* v_k if $c_{kl} \neq 0$. Also, for each k, we define the function $\mathbf{v}_k : U(k,0) \to \coprod_{(\sigma,\varepsilon)\in U(k,0)} M_{(\sigma,\varepsilon)}$ as $(\sigma,\varepsilon) \mapsto \varphi_M((k,0),(\sigma,\varepsilon))(v_k)$. Let $\operatorname{supp}(\mathbf{v}_k)$ be the set of $(\sigma,\varepsilon)\in U(k,0)$ such that $\mathbf{v}_k(\sigma,\varepsilon)$ is nonzero in $M_{(\sigma,\varepsilon)}$. Since f is an isomorphism, we have the following:

(i) $\{\mathrm{supp}(\mathbf{v}_k)\}_{k=1}^n=\{J_k\}_{k=1}^n$.

(ii) For each $(\sigma,\varepsilon)\in U(1,0)$, $\{\mathbf{v}_k(\sigma,\varepsilon):\sigma\in[k,\infty)\}$ is a basis of $M_{(\sigma,\varepsilon)}$.

Now we investigate constraints on the coefficients $c_{k\ell}$.

Claim 3. [For each k, x_k is a summand of v_k.] By item (ii) above, the set

$$B_k:=\{\mathbf{v}_1(k,0),\mathbf{v}_2(k,0),\dots,\mathbf{v}_k(k,0)\}$$

is linearly independent in $M_{(k,0)}$. Invoking equations in (5.5) and the definition of $\mathbf{v}_k$, observe that if $c_{kk}=0$, then B_k is linearly dependent, a contradiction. □

Claim 4. [For $k\in\{2,\dots,n\}$, $\sum_{\ell=1}^k c_{k\ell}=0$ and v_k has at least two summands.] Fix $k\in\{2,\dots,n\}$, and pick any $(\sigma,\varepsilon)\in U(n,\varepsilon_1)$ (see (5.4)). Then we have $[x_{\ell_1}]_{(\sigma,\varepsilon)}=[x_{\ell_2}]_{(\sigma,\varepsilon)}$ for all $\ell_1,\ell_2\in\{1,\dots,n\}$, and thus $\mathbf{v}_k(\sigma,\varepsilon)=(\sum_{\ell=1}^k c_{k\ell})\cdot[x_k]_{(\sigma,\varepsilon)}$. Note that $1=\dim M_{(\sigma,\varepsilon)}$, which is equal to the number of intervals in $\mathbf{barc}(M)$ that includes (σ,ε). Since $U(1,0)\in\mathbf{barc}(M)$ includes (σ,ε) (Claim 2), $\mathrm{supp}(\mathbf{v}_k)$ must *not* include (σ,ε), which implies $\sum_{\ell=1}^k c_{k\ell}$ to be 0. This also forces v_k to admit at least two different summands, including x_k (Claim 3). □

Recall that, for each k, I_{x_k} denotes the elder-rule interval associated to x_k (see (3.1)).

Claim 5. [For each k, $I_{x_k}\subseteq\mathrm{supp}(\mathbf{v}_k)$.] By Claim 2, item (i) above, and Definition 3.3, we readily know $I_{x_1}=\mathrm{supp}(\mathbf{v}_1)=U(1,0)$. Let us fix any $k\in\{2,\dots,n\}$ and any $(\sigma,\varepsilon)\in I_{x_k}$. By definition of I_{x_k}, $[x_k]_{(\sigma,\varepsilon)}$ is the singleton $\{x_k\}$. Therefore, in $\mathbf{v}_k(\sigma,\varepsilon)=\sum_{\ell=1}^k c_{k\ell}[x_\ell]_{(\sigma,\varepsilon)}$, the nontrivial term $c_{kk}[x_k]_{(\sigma,\varepsilon)}$ cannot be combined with any other term (by Claim 3, $c_{kk}\neq 0$, and by Claim 4, there is another nonzero $c_{k\ell}$). This implies that $\mathbf{v}_k(\sigma,\varepsilon)\neq 0$ and in turn $(\sigma,\varepsilon)\in\mathrm{supp}(\mathbf{v}_k)$. □

By Claim 5, we have

$$\dim(M)=\sum_{k=1}^n \mathbb{1}_{I_{x_k}}\leq\sum_{k=1}^n \mathbb{1}_{\mathrm{supp}(\mathbf{v}_k)}=\dim(M).$$

This implies that for each k, $\mathbb{1}_{I_{x_k}}=\mathbb{1}_{\mathrm{supp}(\mathbf{v}_k)}$ and in turn $I_{x_k}=\mathrm{supp}(\mathbf{v}_k)=J_k$ by item (i) above. ■

Proof of Theorem 5.2. In order to prove Theorem 5.2, we need the two lemmas below.

Lemma 5.7. *Let $\mathcal{K}:\mathbb{Z}^2\to\mathbf{Simp}$ be the 1-skeleton of the $\mathbb{Z}^2$-indexed Rips filtration of an aug-MS. Let K^- be the filtration of $\mathcal{K}$ that is obtained by removing all positive edges in $\mathcal{K}$. Then $\mathrm{H}_0(\mathcal{K})\cong\mathrm{H}_0(\mathcal{K}^-)$.*

Proof. Observe that, for each $\mathbf{a}\in\mathbb{Z}^2$, it holds that $\pi_0(\mathcal{K}(\mathbf{a}))=\pi_0(\mathcal{K}^-(\mathbf{a}))\in\mathbf{Subpart}(X)$. Therefore, the two bipersistence treegrams $\pi_0(\mathcal{K}),\pi_0(\mathcal{K}^-):\mathbb{Z}^2\to\mathbf{Subpart}(X)$ are the same. By Proposition 4.15, we have $\mathrm{H}_0(\mathcal{K})\cong\mathcal{F}_{\mathbb{F}}\circ\pi_0(\mathcal{K})\cong\mathcal{F}_{\mathbb{F}}\circ\pi_0(\mathcal{K}^-)\cong\mathrm{H}_0(\mathcal{K}^-)$. ■

Lemma 5.8. *For any simplicial 1-complex, the following sequence is exact:*

$$0\to Z_1(K)\xrightarrow{i}C_1(K)\xrightarrow{\partial_1}C_0(K)\xrightarrow{p}\mathrm{H}_0(K)\to 0,$$

where i is the canonical inclusion, ∂_1 is the boundary map, and p is the canonical quotient.

The proof is straightforward, and thus we omit it.

For a persistence module M, let IM denote the submodule of M that is generated by the images of all linear maps $\varphi_N(\mathbf{a}, \mathbf{b})$, with $\mathbf{a} < \mathbf{b}$ in $\mathbb{Z}^2$. We are now ready to prove Theorem 5.2.

Proof of Theorem 5.2. Let us prove (i). By Lemma 5.7, $\mathrm{H}_0(\mathcal{K}^-)$ is isomorphic to $\mathrm{H}_0(\mathcal{K})$, and thus it suffices to show the exactness of

$$0 \to Z_1(\mathcal{K}^-) \xrightarrow{i} C_1(\mathcal{K}^-) \xrightarrow{\partial_1} C_0(\mathcal{K}^-) \xrightarrow{p} \mathrm{H}_0(\mathcal{K}^-) \to 0.$$

At each grade $\mathbf{a} \in \mathbb{Z}^2$, we have the sequence of vector spaces and linear maps

$$0 \to Z_1(\mathcal{K}^-_{\mathbf{a}}) \xrightarrow{i_{\mathbf{a}}} C_1(\mathcal{K}^-_{\mathbf{a}}) \xrightarrow{(\partial_1)_{\mathbf{a}}} C_0(\mathcal{K}^-_{\mathbf{a}}) \xrightarrow{p_{\mathbf{a}}} \mathrm{H}_0(\mathcal{K}^-_{\mathbf{a}}) \to 0,$$

which is exact by Lemma 5.8.

Next, we prove (ii). In the following proof, we assume the ground field $\mathbb{F}$ is $\mathbb{Z}_2$ for the sake of simplicity. We need to show that (a) $C_0(\mathcal{K}^-)$, $C_1(\mathcal{K}^-)$, and $Z_1(\mathcal{K}^-)$ are free modules and that (b) the sequence in (5.1) satisfies the minimality condition. Let us prove (a). By definition, it is clear that $C_0(\mathcal{K}^-)$ and $C_1(\mathcal{K}^-)$ are free . Also, $Z_1(\mathcal{K}^-)$, the kernel of ∂_1, is free by [15, section 6].[6] Let us check (b). We show that the image of $C_1(\mathcal{K}^-)$ via ∂_1 is contained in $IC_0(\mathcal{K}^-)$. It suffices to show that every generator of $C_1(\mathcal{K}^-)$ is mapped into $IC_0(\mathcal{K}^-)$. Pick any edge x_ix_j $(i < j)$ that appears in $\mathcal{K}^-$. Then, in the filtration $\mathcal{K}^-$, x_ix_j is born at $(j, d^{\mathbb{Z}}_X(x_i, x_j)) =: \mathbf{a}$, whereas the vertices x_i and x_j are born at $(i, 0)$ and $(j, 0)$, respectively. Note that $(i, 0) < (j, 0) < \mathbf{a}$ in $\mathbb{Z}^2$. Therefore, $\partial_1|_{\mathbf{a}}(x_ix_j) = x_i + x_j \in IC_0(\mathcal{K}^-)_{\mathbf{a}}$.

Since $Z_1(\mathcal{K}^-)$ is free, the sequence (5.1) is a minimal free resolution of $\mathrm{H}_0(\mathcal{K}^-)$; this fact directly follows from a standard construction of a minimal free resolution of a finitely generated module over a graded ring [46, Theorem 7.3] (the polynomial ring $\mathbb{F}[t_1, t_2]$ is a graded ring by degree). ∎

6. Computation and algorithms.

6.1. Algorithm.

Theorem 6.1. *Let (X, d_X, f_X) be a finite aug-MS with $n = |X|$:*

(a) *We can compute the ER-staircode $I_{\mathcal{X}} = \{\!\{I_x : x \in X\}\!\}$ in $O(n^2 \log n)$ time. If $X \subset \mathbb{R}^d$ for a fixed d and d_X the Euclidean distance, the time can be improved to $O(n^2\alpha(n))$, where $\alpha(n)$ is the inverse Ackermann function.*

(b) *Each $I_x \in I_{\mathcal{X}}$ has complexity $O(n)$. Given $I_{\mathcal{X}}$, we can compute zeroth fibered barcode B^L for any line L with positive slope in $O(|B^L| \log n)$ time where $|B^L|$ is the size of B^L.*

(c) *Given $I_{\mathcal{X}}$, we can compute the zeroth graded Betti numbers in $O(n^2)$ time.*

We sketch the proof of the above theorem in the remainder of this section, with missing details in Appendix C.

Consider a function value $\sigma \in \mathbb{R}$, and recall that X_σ consists of all points in X with f_X value at most σ. Let $\mathcal{K}_\sigma = \mathcal{R}_\bullet(X_\sigma, d_X)$ denote the Rips filtration of (X_σ, d_X) (recall Example

[6] The authors of [15] observe that for any two free modules $M, N : \mathbb{Z}^2 \to \mathbf{Vec}$, the kernel of any natural transformation $f : M \to N$ is a free module.

Table 1

Complexity comparison with [39, 40] for computing the fibered barcode and graded Betti number of $\mathrm{H}_0(\mathcal{K})$, where $\mathcal{K}$ is the 1-skeleton $\mathbb{Z}^2$-indexed Rips bifiltration of an aug-MS of n points. $|B^L|$ is the cardinality of the fibered barcode for query line L of positive slope.

	Our algorithm	RIVET [39]	Graded Betti number [40]
Size of descriptor	$O(n^2)$	$O(n^6) \sim O(n^8)$	$\Omega(n^2)$
Fibered barcodes query time	$O(\lvert B^L\rvert \log n)$	$O(\log n + \lvert B^L\rvert)$	-
Computation time	$O(n^2 \log n)$	$O(n^8) \sim O(n^9)$	$\Omega(n^3)$

4.2). The corresponding 1-parameter treegram (dendrogram) is $\theta_\sigma := \pi_0(\mathcal{K}_\sigma)$. On the other hand, for any σ, we can consider the *complete weighted graph* $G_\sigma = (V_\sigma = X_\sigma, E_\sigma)$ with edge weight $w(x, x') = d_X(x, x')$ for any $x, x' \in X_\sigma$. It is well known that the treegram θ_σ can be computed from the minimum spanning tree (MST) T_σ of G_σ.

Assume all points in X are ordered $x_1, x_2, \ldots, x_n$ such that $f_X(x_i) \leq f_X(x_j)$ whenever $i < j$, and set $\sigma_i = f(x_i)$ for $i \in [1, n]$. Note that as σ varies, X_σ only changes at σ_i. For simplicity, we set $\theta_i := \theta_{\sigma_i} = \pi_0(\mathcal{K}_{\sigma_i})$, $G_i := G_{\sigma_i}$, and $T_i := MST(G_i)$ as the MST for the weighted graph G_i. Our algorithm depends on the following lemma, the proof of which is in Appendix C.2.

Lemma 6.2. *A decorated ER-staircode for the finite aug-MS (X, d_X, f_X) can be computed from the collection of treegrams $\{\theta_i, i \in [1, n]\}$ in $O(n^2)$ time.*

In light of the above result, the algorithm to compute ER-staircode is rather simple:

(Step 1): We start with T_0 = empty tree. At the ith iteration,

- **(Step 1-a)** we update T_{i-1} (already computed) to obtain T_i, and
- **(Step 1-b)** we compute θ_i from T_i and θ_{i-1}.

(Step 2): We use the approach described in the proof of Lemma 6.2 to compute the ER-staircode in $O(n^2)$ time.

For (Step 1-a), note that G_i is obtained by inserting vertex x_i, as well as all $i-1$ edges between (x_i, x_j), $j \in [1, i-1]$, into graph G_{i-1}. By [20], one can update the MST T_{i-1} of G_{i-1} to obtain the MST T_i of G_i in $O(n)$ time.

For (Step 1-b), once all $i-1$ edges spanning i vertices in T_i are sorted, then we can easily build the treegram θ_i in $O(i\alpha(i)) = O(n\alpha(n))$ time, by using union-find data structure (see Figure 17 above Appendix C.2). Sorting edges in T_i takes $O(i \log i) = O(n \log n)$ time. Hence, the total time spent on (Step 1-b) for all $i \in [1, n]$ is $O(n^2 \log n)$.

We remark that knowing the order of all edges in T_{i-1} may not help, as compared to T_{i-1}, T_i may have $\Omega(i)$ different edges newly introduced, and these new edges still need to be sorted. Nevertheless, we show in Appendix C.1 that if $X \subset \mathbb{R}^d$ for a fixed dimension d, then each T_i will only have a constant number of different edges compared to T_{i-1}, and we can sort all edges in T_i in $O(n)$ time by inserting the new edges to the sorted list of edges in T_{i-1}. Hence, θ_i can be computed in $O(n\alpha(n)) + O(n) = O(n\alpha(n))$ time for this case.

Putting everything together, Theorem 6.1(a) follows. See Appendix C.1 for the proofs of (b) and (c).

6.2. Comparison with other algorithms. Let $\mathcal{K}$ be the 1-skeleton of the $\mathbb{Z}^2$-indexed Rips filtration of an aug-MS $\mathcal{X} = (X, d_X, f_X)$, where $|X| = n$. Let $M := \mathrm{H}_0(\mathcal{K})$.

Comparison with [39]. Let $\kappa := \kappa_x\kappa_y$, where κ_x and κ_y are the number of different values of x and y coordinates in $\mathrm{supp}(\beta_0^M) \cup \mathrm{supp}(\beta_1^M)$, respectively. In our case, $\kappa_x = n$ and $\kappa_y =$ (the number of negative edges in $\mathcal{K}$), which is between $O(n)$ and $O(n^2)$. Let m be the number of simplices in $\mathcal{K}$, which is $O(n^2)$.

From the filtration $\mathcal{K}$, RIVET computes a certain data structure $\mathcal{A}^\bullet(M)$ of size $O\left(m\kappa^2\right)$ in $O\left(m^3\kappa + (m + \log\kappa)\kappa^2\right)$ time and $O\left(m^2 + m\kappa^2\right)$ memory. This $\mathcal{A}^\bullet(M)$ allows efficient query about the fibered barcode of M in $O(\log\kappa + |B^L|)$, where $|B^L|$ is the size of the fibered barcode $\mathbf{barc}(M|_L)$ for a positive slope line $L \in \mathcal{L}$. See Table 1 for the comparison of computational complexity between RIVET and our method.

Comparison with [40]. The algorithm in [40] takes as input a short chain complex of free modules $F^2 \xrightarrow{\partial^2} F^1 \xrightarrow{\partial^1} F^0$ such that $M \cong \ker\partial^1 / \operatorname{im}\partial^2$ and outputs a minimal presentation of a 2-parameter persistence module M, from which the graded Betti numbers of M are readily computed. It runs in time $O\big(\sum_i |F^i|^3\big)$ and requires $O\big(\sum_i |F^i|^2\big)$ memory, where $|F^i|$ denotes the size of a basis of F^i. In our setting, we readily have $|F^0| = 0$, $|F^1| = n$, and $|F^2| =$ (the number of negative edges in $\mathcal{K}$), which is between $O(n)$ and $O(n^2)$. Therefore, in order to obtain the graded Betti numbers via the method in [40], it takes at least $\Omega(n^3)$ time and $\Omega(n^2)$ memory.

7. Discussion.

Some open questions and conjectures follow:

1. *Barcodes and elder-rule-staircodes.* (1) Let $\mathcal{X} = (X, d_X, f_X)$ be an aug-MS. If $x \in X$ has a constant conqueror, is the interval module supported by I_x in (3.1) a summand of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$? (2) By virtue of Theorem 4.16, if $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$ is interval decomposable, then the ER-staircode is identical to the *generalized persistence diagram* of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}(\mathcal{X}))$ [33]. In general, what is the relation between the ER-staircode and the generalized persistence diagram?
2. *Extension to d-aug-MSs.* Can we generalize our results to the setting of more than two parameters? Namely, for d-aug-MSs $\mathcal{X}^d := (X, d_X, f_1, f_2, \ldots, f_d)$, $f_i : X \to \mathbb{R}$, $i = 1, \ldots, d$, can we recover the zeroth homological information of the $(d{+}1)$-parameter filtration induced by $\mathcal{X}^d$ by devising "an elder-rule-staircode" of $\mathcal{X}^d$? Note that, under the assumption that the set $\{(f_i(x))_{i=1}^d \in \mathbb{R}^d : x \in X\}$ is totally ordered in the poset $\mathbb{R}^d$, a straightforward generalization of the elder-rule staircode is conceivable. However, without this strict assumption, it is not very clear how elder-rule-staircodes should be defined.
3. *Extension to higher-order homology.* The ambiguity mentioned in the previous paragraph also arises when trying to devise an "elder-rule-staircode" for higher-order homology of a multiparameter filtration; namely, when $k \geq 1$, the birth indices of k-cycles are not necessarily totally ordered in the multiparameter setting, and thus determining which cycle is older than another is not clear in general.
4. *Metrics and stability.* Recall that the collection $E(\mathcal{X})$ of all possible ER-staircodes of an aug-MS $\mathcal{X}$ is an invariant of $\mathcal{X}$ (the paragraph after Example 3.6). One possible metric between two collections of ER-staircodes is the Hausdorff distance d_{H}^b in the metric space of barcodes over $\mathbb{R}^2$ with the generalized bottleneck distance d_b [6]. On

the other hand, there exists a metric d^1_{GH} which measures the difference between aug-MSs [11] (see also [17]). Let d_{I} be the interleaving distance between 2-parameter persistence modules [38]. Are there constants $\alpha, \beta > 0$ such that for all aug-MSs $\mathcal{X}$ and $\mathcal{Y}$, the inequalities below hold?

$$\alpha \cdot d_{\mathrm{I}}\left(\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{X})\right), \mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{Y})\right)\right) \leq d^b_{\mathrm{H}}(E(\mathcal{X}), E(\mathcal{Y})) \leq \beta \cdot d^1_{\mathrm{GH}}(\mathcal{X}, \mathcal{Y}).$$

5. *Completeness.* Recall that the collection $E(\mathcal{X})$ of all the elder-rule-staircodes of an aug-MS $\mathcal{X}$ is not a complete invariant (the paragraph after Example 3.6). How faithful is this collection in general? Is there any class of aug-MSs $\mathcal{X}$ such that $E(\mathcal{X})$ completely characterizes $\mathcal{X}$?

Appendix A. Missing details from section 3.

Proof of Proposition 3.5. Let $x \in X$ be the point which achieves the minimum of f_X. Then $I_x = \{(\sigma, \varepsilon) \in \mathbb{R}^2 : (f_X(x), 0) \leq (\sigma, \varepsilon)\}$, the closed quadrant whose lower-left corner is $(f_X(x), 0)$. Let $y \in X$ be a point which does not achieve the minimum of f_X. Define $u_y : \mathbb{R} \to \mathbb{R}_{\geq 0}$ by sending $\sigma \in \mathbb{R}$ to the minimum $\varepsilon \in \mathbb{R}_{\geq 0}$ for which there exists $z \in X$ with $f_X(z) < f_X(y)$ such that y belongs to the same block with z in the partition $\pi_0(\mathcal{R}_\varepsilon(X_\sigma, d_X))$ (see the paragraph after Definition 4.1). It is clear that u_y is nonincreasing. Also, since X is finite, u_y is piecewise constant. By observing $I_y = \{(\sigma, \varepsilon) \in \mathbb{R}^2 : \sigma \in [f_X(y), 0) \text{ and } \varepsilon \in [0, u_y(\sigma))\}$, we complete the proof. ■

We precisely define the jth-type corner points of staircase intervals depicted in Figure 5.

Definition A.1 (types of corner points). *Let I be a staircase interval of $\mathbb{R}^2$. Fix $\mathbf{a} \in \mathbb{R}^2$. This $\mathbf{a}$ is a* 0th type corner point *of I if*

$$\mathbb{1}_I(\mathbf{a}) = 1, \quad \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (\varepsilon, 0)) = \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (0, \varepsilon)) = \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (\varepsilon, \varepsilon)) = 0.$$

The point $\mathbf{a}$ is a 1st-type corner point *of I if*

$$\mathbb{1}_I(\mathbf{a}) - \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (\varepsilon, 0)) - \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (0, \varepsilon)) + \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (\varepsilon, \varepsilon)) = -1.$$

The point $\mathbf{a}$ is a 2nd-type corner point *of I if*

$$\mathbb{1}_I(\mathbf{a}) = 0, \quad \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (\varepsilon, 0)) = \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (0, \varepsilon)) = \lim_{\varepsilon \to 0+} \mathbb{1}_I(\mathbf{a} - (\varepsilon, \varepsilon)) = 1.$$

We remark that Definition A.1 is closely related to the *differential* of an interval introduced in [25].

Appendix B. Missing details from section 4.

In order to show that Definition 4.3 is well-defined, it suffices to show the following.

Proposition B.1 (elder-rule-barcode is well-defined). *Let $\theta_X : \mathbb{R} \to \mathbf{Subpart}(X)$ be a treegram over X, and suppose that there exist different $y, z \in X$ with $b(y) = b(z)$. Consider two orders $<_1, <_2$ which are the same except for the pair y, z, i.e., $y <_1 z$ and $z <_2 y$. Then $\{\!\{[b(x), d^{<_1}(x)) : x \in X\}\!\} = \{\!\{[b(x), d^{<_2}(x)) : x \in X\}\!\}$.*

Proof. For $x \in X$ different from y and z, it is clear that $[b(x), d^{<_1}(x)) = [b(x), d^{<_2}(x))$. Hence, letting $b := b(y) = b(z)$, it suffices to show that

$$\left\{\!\!\left\{ \left[b, d^{<_1}(y)\right), \left[b, d^{<_1}(z)\right) \right\}\!\!\right\} = \left\{\!\!\left\{ \left[b, d^{<_2}(y)\right), \left[b, d^{<_2}(z)\right) \right\}\!\!\right\},$$

or equivalently $\{\!\{d^{<_1}(y), d^{<_1}(z)\}\!\} = \{\!\{d^{<_2}(y), d^{<_2}(z)\}\!\}$. Assume that y and z merge at $\varepsilon = r_0$ in θ_X. Since $<_1$ and $<_2$ are the same except for the pair y, z, we use $<$ to denote both $<_1$ and $<_2$ *when we compare* y, z *with the other elements in* X. In the treegram θ_X, there are only two possible cases: (Case 1) An element $w \in X$ with $w < y, z$ merges with the block containing both y, z at $\varepsilon = r_1 \geq r_0$. Then $d^{<_1}(y) = r_1$ and $d^{<_1}(z) = r_0$, whereas $d^{<_2}(y) = r_0$ and $d^{<_2}(z) = r_1$. (Case 2) Assume that there are $w_1 < y$ and $w_2 < z$ such that w_1 and y merge at $\varepsilon = r_2 \leq r_0$ and w_2 and z merge at $\varepsilon = r_3 \leq r_0$ (it is possible that $w_1 = w_2$). Then $d^{<_1}(y) = d^{<_2}(y) = r_2$ and $d^{<_1}(z) = d^{<_2}(z) = r_3$, completing the proof. ■

Appendix C. Missing details from section 6.

C.1. Proofs of Theorem 6.1. We first present a lemma needed for the proof of Theorem 6.1(a). For simplicity, we assume that all distances between points in X (and thus edge weights in G_is) are distinct. If this is not the case, we only need to fix a total order compatible with all distances for the algorithm to work in the same way.

Lemma C.1. *Given a graph $G = (V, E)$ with distinct edge weights, if $e \in E$ is the largest edge of a cycle C in G, then e will not appear in the MST of G.*

Proof. Let us denote e as the largest edge in the cycle C of size $k+1$ where C consists of edges $e, e_1, e_2, \ldots, e_k$. Also denote the MST of G as T. From C and T, we will give a way to construct new cycle C' where all edges except e belong to T.

Since T is an MST, for any $i \in \{1, 2, \ldots, k\}$, if e_i does not belong to T, adding e_i will form a cycle C_i where e_i is the largest edge and the only non-MST edge in C_i.

Construct new cycle $C' = C + \Sigma_{i \in \{j | e_j \notin T\}} C_i$ where the addition is performed on $\mathbb{F}_2$. Every time we add C_i, it will cancel out e_i. Since we did so for all non-MST edges, the resulting cycle C' will consist of all MST edges plus e.

We argue that e is also the largest edge in C'. This holds because every time we added C_i, we knew e_i is the largest edge in C_i, and because $|w(e)| \geq |w(e_i)|$, where w is weight function on edges, we knew e is also the largest edge in C'. By the property of MST (any non-MST edge is the largest edge in the cycle created by adding itself to MST), we conclude that e is a non-MST edge. ■

The following lemma, combined with the argument in the main text, will establish the time complexity of the algorithm to compute an ER-staircode for the case when X is from a fixed dimensional Euclidean space $\mathbb{R}^d$.

Lemma C.2. *Let T_{i-1} and T_i be the MST of G_{i-1} and G_i as defined in the algorithm. For fixed dimensional $\mathbb{R}^d$ and d_X to be Euclidean distance, the number of edges in $T_i \setminus T_{i-1}$ is $O(1)$ (depending on d).*

Proof. Recall that G_i is obtained by adding a new vertex x_i and edges incident to x_i. First, note that by Lemma C.1, edges in $T_i = MST(G_i)$ are either from $T_{i-1} = MST(G_{i-1})$

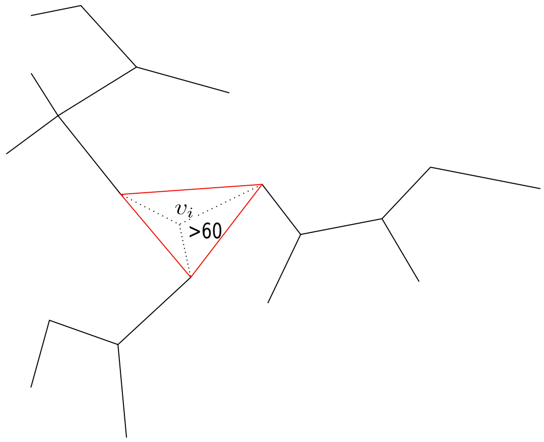


Figure 15. *Illustration of packing argument in the proof of Lemma C.2. x_i is the new vertex. Dashed edges are new edges entering T_i. Red edges are non-MST edges, and therefore by the property of non-MST edges, the angle corresponding to red edges must be at least $\frac{\pi}{3}$.*

or new edges just inserted. That is, no edge in $G_{i-1} \setminus T_{i-1}$ will contribute to T_i: Such an edge will be the largest-weight edge of some cycle in G_i.

We now prove that for the case where $X \subset \mathbb{R}^d$ only $O(1)$ (where the big-O hides terms depending on d), new edges (incident to x_i) can be in T_i.

In particular, comparing T_{i-1} and T_i, there are only two types of edges that are subject to change: (1) edges that are in T_{i-1} but will leave T_{i-1} and (2) edges incident to x_i and will enter the new T_i.

Assume there are k edges that will leave T_{i-1}. By deleting them, the original T_{i-1} is decomposed into $k+1$ small trees. There must be $k+1$ edges incident to x_i entering T_i. We denote those $k+1$ edges as $\mathcal{E}_{new,i} = \{x_i x_{i_1}, x_i x_{i_2}, \dots, x_i x_{i_{k+1}}\}$.

Pick any two nodes a, b from $\mathcal{E}_{new,i} = \{x_{i_1}, x_{i_2}, \dots, x_{i_{k+1}}\}$; they will form a triangle with x_i. By the property of MST, edge ab in triangle $\triangle_{abx_i}$ is the longest edge, as $ab \notin T_i$ while $x_i a, x_i b \in T_i$. By elementary Euclidean geometry, it can be shown that angle $\sphericalangle a x_i b$ must be no less than $\frac{\pi}{3}$, and this holds for *every pair* of nodes from $\mathcal{E}_{new,i} = \{x_{i_1}, x_{i_2}, \dots, x_{i_{k+1}}\}$. Now by a packing argument, we can show that there can be $O(C^d)$ such well-separated points around x_i in $\mathbb{R}^d$ for some constant C; see Figure 15 for an illustration.

Indeed, consider the unit sphere S around x_i in $\mathbb{R}^d$, and let y_j be the intersection of the ray starting at x_i and passing through x_{i_j} with S. The previous paragraph establishes that the angle $\sphericalangle y_j x_i y_{j'} \geq \pi/3$ for any $j \neq j' \in [1, k+1]$. It then follows that the geodesic distance between y_j and $y_{j'}$ on S is at least $\pi/3$. In other words, geodesic balls of radius $\pi/6$ centered at y_j's for $j \in [1, k+1]$ have to be all disjoint. The number of such balls (and thus $k+1$) is at most $Area(S)/B$, where $Area(S)$ stands for the surface volume of unit d-sphere in $\mathbb{R}^d$, while B is the volume of a $(d-1)$-ball of radius $sin\frac{\pi}{6} = \frac{1}{2}$. Hence, there exists some constant $C > 1$ such that $k = O(C^d)$. This proves the lemma. ∎

We now present proofs for parts (b) and (c) of Theorem 6.1.

Lemma C.3. *The size of the ER-staircode is $O(n^2)$.*

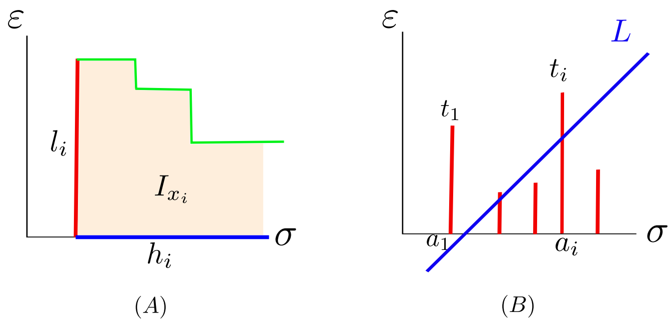


Figure 16. (A) *An illustration of I_{x_i} where its lower envelope l_i (vertical line segment) and h_i (horizontal ray) are colored red and blue.* (B) *An illustration of Case* 2 *in the proof of Lemma* C.4.

Proof. We claim that for every $x \in \mathcal{X}$, the size of I_x is $O(n)$ and the lemma will then follow. This holds because every I_x has a staircase shape, and the x-coordinates of corner points can only be one of the values $f_X(x_i)$ for some $x_i \in X$. ■

Lemma C.4. *Given $I_{\mathcal{X}}$, after $O(n^2 \log n)$ time preprocessing, we can build a data structure of size $O(n^2)$ so that, given any line L with positive slope, the zeroth fibered barcode B^L with respect to L can be computed in $O(|B^L| \log n)$ time, where $|B^L|$ is the size of the fibered barcode.*

Proof. First, given an I_x, recall that it has a staircase shape; see Figure 16. In particular, its lower envelope consists of one vertical and one horizontal segment. Its upper envelope U is the graph of a piecewise constant nondecreasing function in the plane consisting of $O(n)$ horizontal and vertical line segments. Given a line L with positive slope, its intersection with the lower envelope of I_x thus takes only $O(1)$ time. The upper envelope can only intersect with L at most one point, either within some horizontal segment of U or within a vertical segment of U. To identify this intersection point, we simply binary search twice, once among all horizontal segments and once among all vertical segments in $O(\log n)$ time.

Next, we show that we can avoid checking all n number of I_xs. Instead, we will compute only the set $\widehat{\mathcal{I}}_L$ of I_xs that will intersect L: Note that there are $k = |B^L|$ number of such staircodes. In what follows, we describe how to preprocess all staircodes so that this set $\widehat{\mathcal{I}}_L$ can be reported in $O(\log n + k)$ time.

Specifically, for any $x_i \in \mathcal{X}$, let ℓ_i and h_i be the vertical and horizontal segments of the lower envelope of I_{x_i}; see Figure 16 for an illustration. Note that each h_i is in fact a half line in the x-axis. It is easy to see that the line L intersects I_{x_i} *if and only if* L intersects either ℓ_i or h_i.

Case 1: Reporting intersection with h_is. Given the collection of all h_is, $i \in [1, n]$, in $O(n \log n)$ time, we can build a standard 1D range reporting data structure of size $O(n)$, over the collection of left endpoints a_i's of h_is , $i \in [1, n]\}$, so that given a query point b, we can report all points in $\{a_i\}$ to the left of b in $O(\log n + s)$ time, where s is the number of such points.

Now given a query line L, let b_L be the intersection between L and the x-axis. We use the data structure to compute, say, k_1 number of points from $\{a_i\}$ to the left of b_L in $O(\log n + k_1)$ time. Each such point corresponds to a ray h_i that will intersect L.

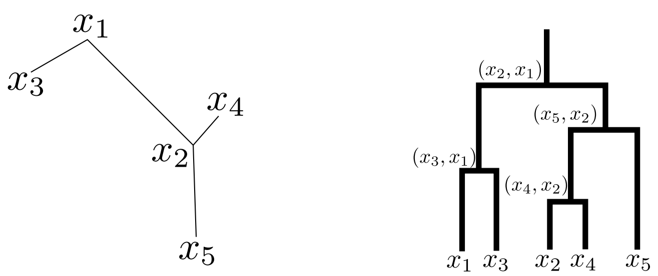


Figure 17. *The left figure shows an MST of five points where nodes with low (high) index appear early (later). The weight of each edge is the length of the edge (e.g., $w(x_1, x_3) > w(x_2, x_4)$). The right figure shows the corresponding decorated treegram. At each nonleaf node, we only need to store a tuple where the first number stands for the index of the node that is conquered while the second number stands for the index of the node that has not been conquered (eldest) in the subtree.*

Case 2: Reporting intersection with ℓ_is. What remains is to build a data structure to report the set of ℓ_is intersecting L. To this end, note that for each $i \in [1, n]$, the point a_i introduced above is also the bottom endpoint of the vertical segment ℓ_i; let t_i denote the top endpoint for ℓ_i. Given a query line L, we wish to report all i's such that t_i is above L while a_i is below L. Again, let b_L denote the intersection of L with the x-axis: As the slope of L is positive, if a vertical segment ℓ_i intersects L, then a_i must lie to the right of b_L.

Now for each $j \in [1, n]$, set

$$A_j := \{t_i \mid a_i \geq a_j\}.$$

Given L, let a_r be the closest point to b_L with $a_r \geq b_L$. Obviously, the line L intersects ℓ_i *if and only if* $t_i \in A_r$ and t_i is above L. Hence, we want to perform a half-plane range reporting query among the points in A_r. To this end, for each $i \in [1, n]$, we use the classic approach of [19] to build a data structure of size $O(|A_i|) = O(n)$ in time $O(|A_i| \log |A_i|) = O(n \log n)$, so that given a line L, the set of points from A_i above L can be reported in $O(\log n + s)$ time where s is the number of such points. Overall, the total size of all such data structures for all $i \in [1, n]$ is $O(n^2)$ and can be constructed in $O(n^2 \log n)$ time. Given L, we first identify a_r as described above, and then query for the set of t_is from A_r lying above L in $O(\log n + k_2)$ time, where k_2 is the number of such t_is.

Putting Cases 1 and 2 together, we can report all $k = k_1 + k_2$ staircodes $\widehat{\mathcal{I}}_L$ intersecting a query line L of positive slope in $O(\log n + k)$ time.

Once we have $\widehat{\mathcal{I}}_L$, for each $I_x \in \widehat{\mathcal{I}}_L$, we use the procedure described at the beginning of this proof to compute the intersection between L and I_x in $O(\log n)$ time for each I_x. In total, it takes $O(k \log n)$ to compute all intersections. The total query time is $O(\log n + k + k \log n) = O(k \log n) = O(|B^L| \log n)$, as claimed. ■

Lemma C.5. *Given $I_{\mathcal{X}}$, we can compute the zeroth graded Betti numbers in $O(n^2)$ time.*

Proof. Since the total number of segments of the ER-staircode is $O(n^2)$, so is the number of corner points. In other words, only $O(n^2)$ grades could potentially have a nonzero $\gamma_i^{\mathcal{X}}$ or β_i^M value for $i = 0, 1,$ or 2. We can therefore compute graded Betti numbers according to the formula in Theorem 5.4, by evaluating $\gamma_i^{\mathcal{X}}$ and β_i^M at each of the $O(n^2)$ possible grades. ■

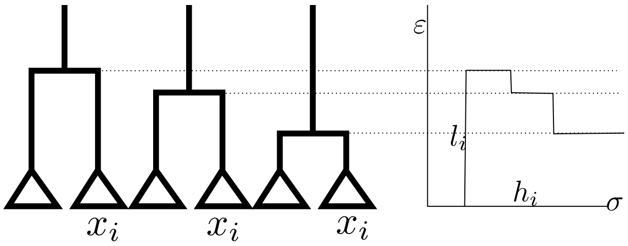


Figure 18. *Illustration of the assembling process to recover I_{x_i}. Note that we do not plot the whole treegram at each function value for simplicity. x_i here is a leaf in the right subtree of every treegram. We will first compute the decorated treegrams, illustrated in Figure 17. From these decorated treegrams, we are able to retrieve ϵ values of I_x for each of the n function values $\sigma_1, \dots, \sigma_n$ with $\sigma_i = f(x_i)$ and thus assemble I_{x_i}.*

C.2. Proof of Lemma 6.2. We now give a detailed description of the process to recover the ER-staircode from the collection of treegrams in $O(n^2)$ time. Recall that conqueror is defined in section 4.2. When x' is a conqueror of x in $G_i = G_{\sigma_i}$, we also say x is conquered by x' at *height* $u_{X_{\sigma_i}}(x, x')$. To convert treegrams at different function values to staircode, we will decorate the treegrams with some extra information. On the high level, we need to keep the information about the node index conquered at different heights in the treegram, which can be done in linear time by traversing the treegram from bottom to top.

Specifically, denote the sorted height values of treegram θ_i at function value σ_i as $\mathcal{E}_i = \{\epsilon_1 < \epsilon_2 < \cdots < \epsilon_{i-1}\}$. At each nonleaf node of height $\epsilon_j \in \mathcal{E}_i$ in the treegram θ_i, we record (a) the index of the node that is conquered at height ϵ_j and (b) the index of the single node in subtrees (rooted at height ϵ_j) who has not been conquered yet. (b) is needed to update (a) of the node at height ϵ_{j+1} in constant time. Traversing treegrams bottom-up and computing (a) and (b) for every nonrooted node takes $O(i) = O(n)$ time. An illustration of the idea of decorated treegrams is shown in Figure 17.

After computing n decorated treegrams at n function values, we can recover the ER-staircode by assembling decorated treegrams in the following way. Without loss of generality, we state the process to recover single I_x in the ER-staircode. For every function value ϵ_i, find corresponding σ (i.e., $u_{X_{\sigma_i}}(x, x')$) in $\mathcal{E}_i$ at which x is conquered. Repeating this process for all function values will recover I_x. Figure 18 illustrates the idea.

We restate Lemma 6.2 with a proof.

Lemma C.6. *A decorated ER-staircode for the finite aug-MS (X, d_X, f_X) can be computed from the collection of dendrograms $\{\theta_i, i \in [1, n]\}$ in $O(n^2)$ time.*

Proof. The decoration of every treegram takes $O(n)$ time and in total $O(n^2)$ for n treegrams. Assembling I_x for each $x \in \mathcal{X}$ takes $O(n)$ time since the complexity of every I_x is $O(n)$, and so totally recovering the ER-staircode takes $O(n^2)$ time. For correctness, we prove that our process can recover I_x for every $x \in \mathcal{X}$. This holds because for any $x \in \mathcal{X}$ and $\sigma_i \in f_X$ we can recover $u_{X_{\sigma_i}}(x, x')$, where x' is the conqueror of x. ■

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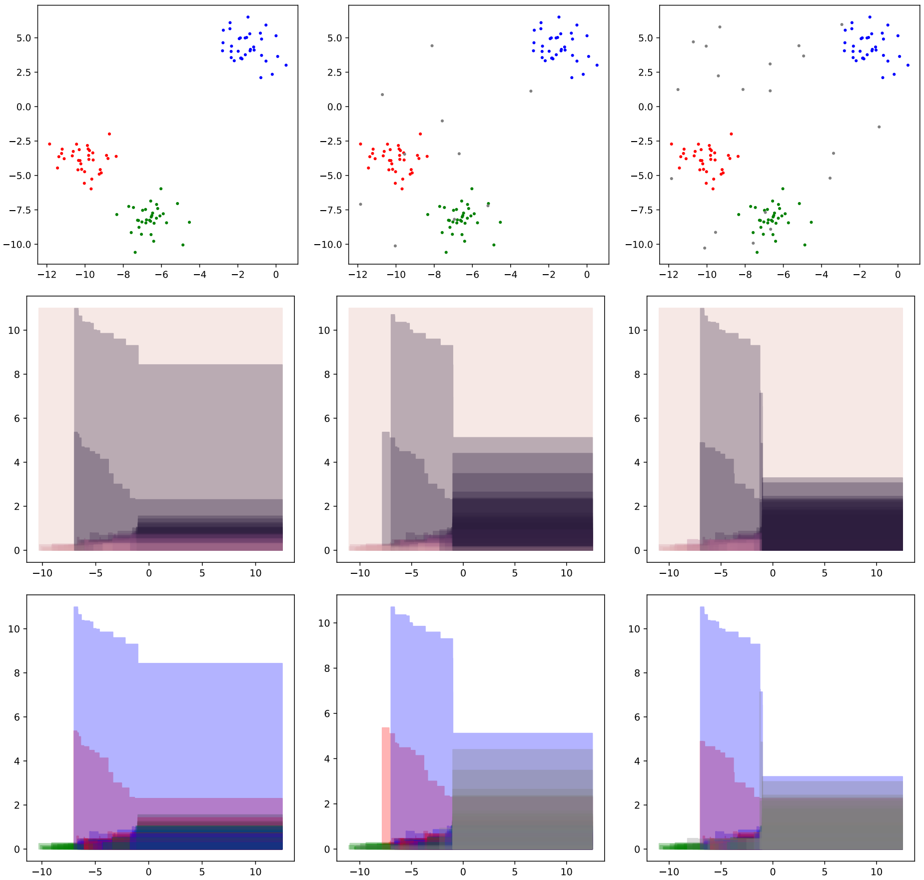

Figure 19. *A complement to Figure 1. First row: Three point clouds sampled from $\mathbb{R}^2$ at increasing noise levels: the leftmost point cloud consists of three different clusters (cluster labels are denoted by three different colors: red, blue, and green), the middle and rightmost point clouds contain increasingly more outlier points, i.e., "noise"; these points are colored in gray. By equipping these three point clouds with codensity functions (as described in Figure 1) and Euclidean distance, we obtain three aug-MSs. Second row: The ER-staircodes corresponding to these three aug-MSs. Observe that* (1) *the blocks corresponding to the outlier points (in gray) have lower density and therefore appear later (i.e., large x-coordinates of the left-bottom corners) in their corresponding ER staircodes;* (2) *for different noise levels, there are three large blocks, reflecting the presence of three well-defined clusters. Third row: The same ER staircodes without their respective largest blocks for visual clarity. Blocks are colored according to their cluster membership. See the GitHub repository https://github.com/Chen-Cai-OSU/ER-staircode for the code used for producing this example.*

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