Elder-Rule-Staircodes for Augmented Metric Spaces

Chen Cai
Department of Computer Science and Engineering, The Ohio State University, Columbus, OH, USA
cai.507@osu.edu

Woojin Kim
Department of Mathematics, The Ohio State University, Columbus, OH, USA
kim.5235@osu.edu

Facundo Mémoli
Department of Mathematics and Department of Computer Science and Engineering,
The Ohio State University, Columbus, OH, USA
memoli@math.osu.edu

Yusu Wang
Department of Computer Science and Engineering, The Ohio State University, Columbus, OH, USA
yusu@cse.ohio-state.edu

Abstract

An augmented metric space (X, d_X, f_X) is a metric space (X, d_X) equipped with a function $f_X : X \to \mathbb{R}$. It 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. Such an augmented metric space naturally gives rise to a 2-parameter filtration. However, the resulting 2-parameter persistence module 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 a 1-parameter filtration, 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 (X, d_X, f_X), its elder-rule-staircode consists of $n = |X|$ number of staircase-like blocks in the plane. We show that the fibered barcode, the fibered merge tree, and the graded Betti numbers associated to the zeroth homology of the 2-parameter filtration induced by (X, d_X, f_X) can all be efficiently computed once the elder-rule-staircode is given. Furthermore, for certain special cases, this staircode corresponds exactly to the set of indecomposables of the zeroth homology of the 2-parameter filtration. 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.

2012 ACM Subject Classification Mathematics of computing → Topology; Theory of computation → Computational geometry

Keywords and phrases Persistent homology, Multiparameter persistence, Barcodes, Elder rule, Hierarchical clustering, Graded Betti numbers

Digital Object Identifier 10.4230/LIPIcs.SoCG.2020.26

Related Version A full version of this paper is available at https://arxiv.org/abs/2003.04523.

Funding This work is supported by NSF grants DMS-1723003, CCF-1740761, DMS-1547357, and IIS-1815697.

Acknowledgements The authors thank to the anonymous reviewers who made a number of helpful comments to improve the paper. Also, CC and WK thank Cheng Xin for helpful discussions.

1 Introduction

An augmented metric space (X, d_X, f_X) is a metric space (X, d_X) equipped with a function $f_X : X \to \mathbb{R}$. It 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 the hierarchical clustering induced in this setting has attracted much attention recently [2, 8]. Another example is where $X = V$ equals to the vertex set of a graph $G = (V, E)$, d_X represents 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 node attributes. Given that persistence-based summaries from only the edge weights or from only node attributes have already shown promise in graph classification (e.g, [5, 9, 18, 30]), 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 4). However, while a standard (1-parameter) filtration and its induced persistence module has persistence diagram as a complete discrete invariant, multi-parameter persistence modules do not have such complete discrete invariant [6, 13]. The 2-parameter persistence module induced from an augmented metric space may still be of wild representation type, and may not have simple indecomposables [2]. Several recent work instead consider informative (but not necessarily complete) invariants for multiparameter persistence modules [15, 19, 24, 26]. In particular, RIVET [24] provides an interactive visualization of the barcodes of 1-dimensional slices of an input 2-parameter persistence module M, called the *fibered barcode*. This interactivity uses the *graded Betti numbers* of M, another invariant for the 2-parameter persistence module.

New work. 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 (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 [16]. For the 1-parameter case, *barcodes* [31] 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 topological information of the 2-parameter filtration induced by (X, d_X, f_X). In particular, the fibered barcodes, the fibered treegrams, and the graded Betti numbers associated to the zeroth homology of the 2-parameter filtration induced by (X, d_X, f_X) can all be efficiently computed from the elder-rule-staircodes (see Theorems 8, 19 and 23). Furthermore, for certain special cases, these staircodes **correspond exactly** to the set of indecomposables of the zeroth order 2-parameter persistence module induced by (X, d_X, f_X); see Theorem 17.

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 $O(n^2\alpha(n))$ 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 at `https://github.com/Chen-Cai-OSU/ER-staircode`.

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 [16, Chapter 7]. Recently this rule has come into the spotlight again for generalizing persistence diagrams [19, 26, 27] and for addressing inverse problems in TDA [14].

The software RIVET and work of [25] can also be used to recover fibered barcodes and bigraded 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 [25] computes the zeroth bigraded Betti numbers in $\Omega(n^3)$ time, while it takes $O(n^2 \log n)$ time using elder-rule-staircode via Theorem 24. For zeroth fibered barcodes, RIVET takes $O(n^8)$ time to compute a data structure of size $O(n^6)$ so as to support efficient query time of $O(\log n + |B^L|)$ where $|B^L|$ is the size of the fibered barcode B^L for a query line L of positive slope. Our algorithm computes 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 the full version of this paper [4] for more detailed comparison. However, it is important to note that RIVET allows much broader inputs and can work beyond zeroth homology.

2 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 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 the notations from [3].

▶ **Definition 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: (1) $\mathcal{J}$ is non-empty. (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 $\mathbf{a} = \mathbf{a}_0, \mathbf{a}_1, \cdots, \mathbf{a}_l = \mathbf{b}$ 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 in which elements may occur more than once.

▶ **Definition 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 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 [1], 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.

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** (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 *(abbrev.* 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 [2, 8].

▶ **Definition 4** (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* $(\varepsilon, \sigma) \mapsto \mathcal{R}_\varepsilon(X_\sigma, d_X)$.

Applying the k-th homology functor to the Rips bifiltration $\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})$, we have 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 lines of 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 *k-th fibered barcode* of $\mathcal{X}$ is the $\mathcal{L}$-parametrized collection $\{\mathbf{barc}(M|_L)\}_{L \in \mathcal{L}}$ [10, 22, 24].

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 $d_X(x_i, x_{i+1}) \leq \varepsilon$ for $i = 1, \ldots, \ell - 1$. Now given $\mathcal{X} = (X, d_X, f_X)$ and $\sigma \in \mathbb{R}_{\geq 0}$, consider a point $x \in X_\sigma$. Then for any $\varepsilon \geq 0$, 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: Given $x, x' \in X$, we say that x is *older than* x' if and only if $f_X(x) < f_X(x')$.

▶ **Definition 5** (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:*

$$I_x := \{(\sigma, \varepsilon) \in \mathbb{R}^2 : x \in X_\sigma \text{ and } x \text{ is the oldest in } [x]_{(\sigma,\varepsilon)}\ \} \tag{1}$$

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 1 for an example. The relationship between the ER-staircode and the classic elder-rule will become clear in Section 4.1. An interval I of $\mathbb{R}^2$ (Definition 1) is a *staircase interval (or simply staircase)* if there exists $(\sigma_0, \varepsilon_0) \in \mathbb{R}^2$ such that either $I = \{(\sigma, \varepsilon) \in \mathbb{R}^2 : (\sigma_0, \varepsilon_0) \leq (\sigma, \varepsilon)\}$ (i.e. a quadrant) or there is also a stair-like upper boundary – there exists a non-increasing piecewise constant function $u : \mathbb{R} \to (\varepsilon_0, \infty)$ such that $I = \{(\sigma, \varepsilon) \in \mathbb{R}^2 : \sigma \in [\sigma_0, \infty) \text{ and } \varepsilon \in [\varepsilon_0, u(\sigma))\}$ (see Figure 4). It turns out that each $I_x \in \mathcal{I}_\mathcal{X}$ is in the form of a staircase interval (proof in the full version of this paper [4]):

▶ **Proposition 6.** *Each I_x in Definition 5 is a staircase interval of $\mathbb{R}^2$.*

Staircodes for non-injective 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 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

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

(we use double-curly-brackets $\{\!\{-\}\!\}$ to denote multisets). Regardless of the choice of $<$, the collection $\mathcal{I}_\mathcal{X}^< = \{\!\{I_x^< : x \in X\}\!\}$ satisfies all properties / 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 7** (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, $i = 1, \ldots, n$. 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 $\mathcal{I}_\mathcal{X} = \{\!\{[c, \infty) \times J_i : i = 1, \ldots, n\}\!\}$.

In contrast to Example 7, different orders on X in general induce different ER-staircodes of $\mathcal{X} = (X, d_X, f_X)$; see Example 9. 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* $\mathcal{X}$ by the following reasoning: It is not difficult to find two non-isometric 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 7, 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.

We can recover the zeroth fibered barcode of an aug-MS $\mathcal{X}$ from its ER-staircode: The proof of the following theorem will be given in Section 4.1.

▶ **Theorem 8.** *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 2).*

▶ **Example 9.** If an aug-MS is not injective, then there can be different ER-staircodes w.r.t. different compatible orders. However, each of them will still be valid to produce the fibered barcodes. For example, let (X, d_X) be the metric space in Figure 1 (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, giving 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 8. See Figure 3.

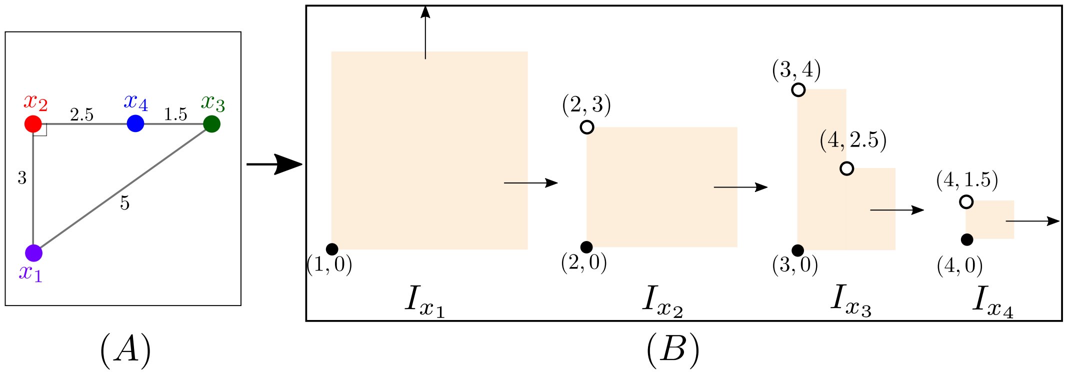

Figure 1 (A) Consider the triangle with edge lengths 3,4 and 5. Consider the aug-MS $\mathcal{X} = (X, d_X, f_X)$ where $X := \{x_1, x_2, x_3, x_4\}$, d_X is the Euclidean metric on the plane, and f_X is given as $f_X(x_i) = i$ for $i = 1, 2, 3, 4$. (B) The ER-staircode of $\mathcal{X}$.

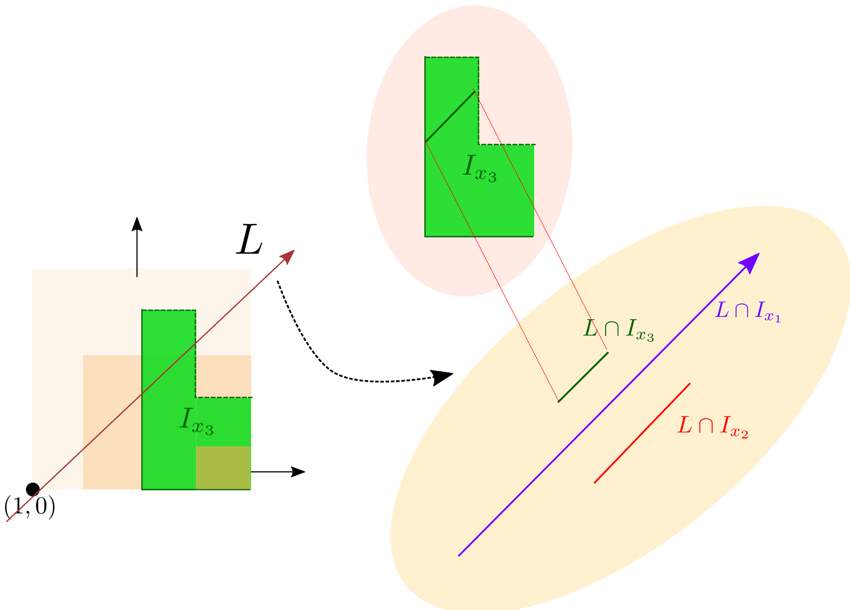

Figure 2 Left: The stack of I_{x_i}, $i = 1, 2, 3, 4$ from Figure 1 and a line $L \in \mathcal{L}$. Right: The barcode of $M|_L$. Since L does not intersect I_{x_4}, only three intervals of $L \subset \mathbb{R}^2$ appear in the barcode.

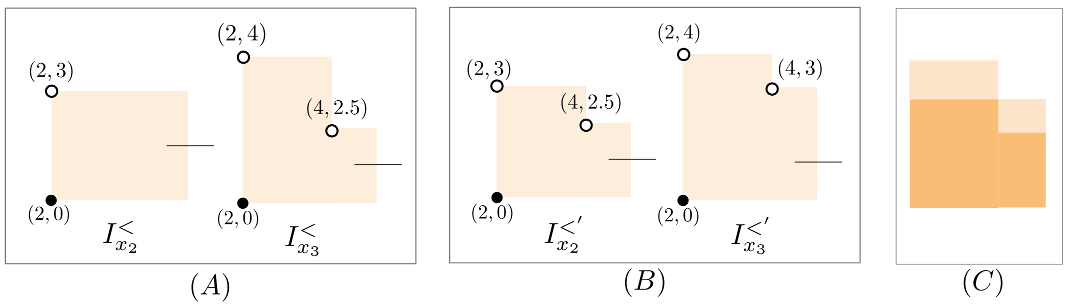

Figure 3 Example 9: (A) $I^{<}_{x_2}$ and $I^{<}_{x_3}$. (B) $I^{<'}_{x_2}$ and $I^{<'}_{x_3}$. (C) Stack of $I^{<}_{x_2}$ and $I^{<}_{x_3}$. Stack of $I^{<'}_{x_2}$ and $I^{<'}_{x_3}$ look the same. Observe that for any $L \in \mathcal{L}$, $\left\{\!\!\left\{ L \cap I^{<}_{x_2}, L \cap I^{<}_{x_3} \right\}\!\!\right\} = \left\{\!\!\left\{ L \cap I^{<'}_{x_2}, L \cap I^{<'}_{x_3} \right\}\!\!\right\}$.

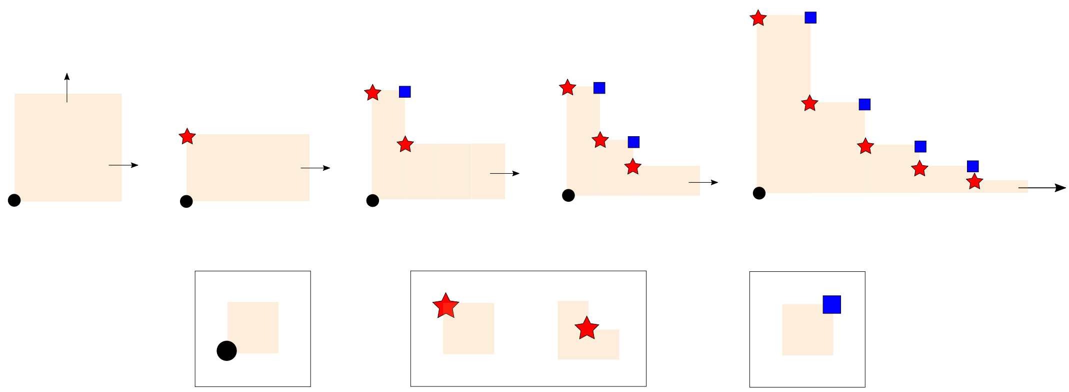

Figure 4 Every corner point of a staircase interval falls into three different types depending on its neighborhood information, as the pictures above illustrate. Staircase intervals in the first row are decorated by their corner points (a precise description is in Definition A.2 of the full version [4]).

We close this section with some definitions that will be useful later. Let I be a staircase interval of $\mathbb{R}^2$. We define the three types of corner points as in Figure 4 (rigorous definition of these corner points is in Definition A.2 in the full version [4]): Roughly speaking, for each staircase I_x, type-0 is the left-bottom point; type-1 corners are those where the boundary transitions from a vertical segment to a horizontal one, while type-2 are those transitions from a horizontal one to vertical one. For each $j = 0, 1, 2$ we define the function $\gamma_j(I) : \mathbb{R}^2 \to \mathbb{Z}_{\geq 0}$ as $\gamma_j(I)(\mathbf{a}) = \begin{cases} 1, & \mathbf{a} \text{ is a } j\text{-th type corner point of } I \\ 0, & \text{otherwise.} \end{cases}$

Elder-rule feature functions defined below will be useful in Section 5.

▶ **Definition 10.** *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 $j = 0, 1, 2$, we define the* j-th elder-rule feature function *as the sum* $\gamma_j^{\mathcal{X}} = \sum_{x \in X} \gamma_j(I_x)$.

4 Decorated elder-rule-staircodes and treegrams

In Section 4.1 we prove Theorem 8 and introduce *bipersistence treegrams* to encode multi-scale 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 $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_{\bullet}(\mathcal{X}))$.

4.1 Bipersistence treegrams

Let X be a non-empty finite set. Any partition P of a subset X' of X is a *sub-partition* of X; and we refer to X' as the *underlying set of* P. Elements of a sub-partition of X are called *blocks*. A partition of the empty set is defined as the empty set. By $\mathbf{Subpart}(X)$, we denote the set of *all sub-partitions of* X, i.e. $\mathbf{Subpart}(X) := \{P : \exists X' \subseteq X \text{ , } P \text{ is a partition of } X'\}$. Given $P, Q \in \mathbf{Subpart}(X)$, $P \leq Q$ means that P refines Q, i.e. for all $B \in P$, there exists $C \in Q$ s.t. $B \subseteq C$. For example, let $X = \{x_1, x_2, x_3\}$; then $P \leq Q$ for sub-partitions $P := \{\{x_1\}, \{x_2\}\}$ and $Q := \{\{x_1, x_2\}, \{x_3\}\}$. Treegrams are a generalized notion of dendrograms [29].

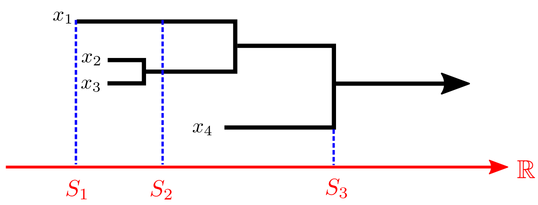

Figure 5 A (1D) treegram θ_X over the set X. Notice that $\theta_X(t) = \emptyset$ for $t \in (-\infty, S_1)$. Also, $\theta_X(S_1) = \{\{x_1\}\}$, $\theta_X(S_2) = \{\{x_1\}, \{x_2, x_3\}\}$, and $\theta_X(t) = \{X\}$ for all $t \in [S_3, \infty)$.

▶ **Definition 11** (Treegrams [29]). *A* treegram *over a finite set X is any function $\theta_X : \mathbb{R} \to$ $\mathbf{Subpart}(X)$ such that the following properties hold: (1) if $t_1 \leq t_2$, then $\theta_X(t_1) \leq \theta_X(t_2)$, (2) 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 (3) for all t there exists $\epsilon > 0$ s.t. $\theta_X(s) = \theta_X(t)$ for $s \in [t, t+\epsilon]$. See Figure 5 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 $\mathbf{a}_0 \leq \mathbf{a}$, $\mathcal{K}(\mathbf{a}) = K$.

▶ Remark 12 (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 Definition 11 (2), 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 $x, x' \in X$. For $\varepsilon \in [b(x), \infty)$, we denote the block to which x belongs in the sub-partition $\theta_X(\varepsilon)$ 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 times, the *elder-rule-barcode* is uniquely defined (which is proved in the full version [4]):

▶ **Definition 13** (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 w.r.t. the elder rule – see the theorem below. Even though this result is well-known (e.g, [14]), we include a proof in the full version [4].

▶ **Theorem 14** (Compatibility between the elder rule and algebraic decomposition). *Let $\mathcal{K}$ and θ_X be the filtration and the treegram in Remark 12, 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 6).*

Proof of Theorem 8. We are now ready to prove Theorem 8. 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 13). Hence, by Theorem 14, 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 $\{\!\{L \cap I_x : x \in X\}\!\} = \mathbf{barc}(M|_L)$. ◀

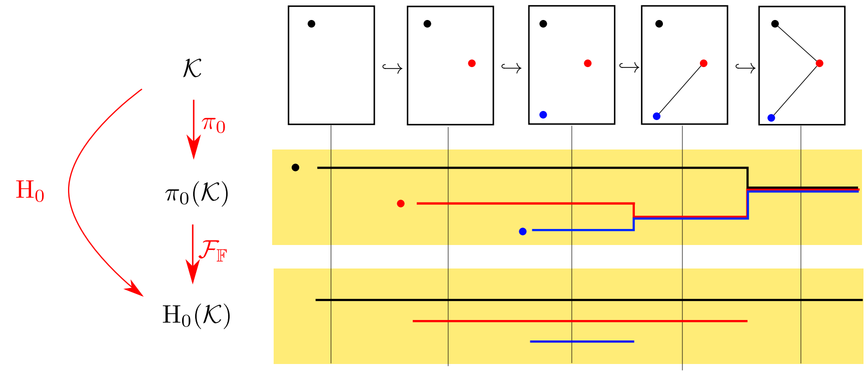

Figure 6 The first row represents a simplicial filtration $\mathcal{K}$. The second row stands for the treegram $\pi_0(\mathcal{K})$ which encodes the evolution of clusters in $\mathcal{K}$ (Remark 12). The third row is the barcode of $\mathrm{H}_0(\mathcal{K})$. The persistence module $\mathrm{H}_0(\mathcal{K})$ can be obtained by applying the linearization functor (Definition B.2 in the full version [4]) 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 13).

Bipersistence treegrams. We now extend the notion of treegrams to encode the evolution of clusters of a 2-parameter filtration (similar ideas appear in [20]). A *bipersistence treegram* over a finite set X is any function $\theta_X^{\mathrm{bi}} : \mathbb{R}^2 \to \mathbf{Subpart}(X)$ such that if $\mathbf{a} \leq \mathbf{b}$ in $\mathbb{R}^2$, then $\theta_X^{\mathrm{bi}}(\mathbf{a}) \leq \theta_X^{\mathrm{bi}}(\mathbf{b})$.

▶ **Definition 15** (Rips bipersistence treegrams)**.** *Given an aug-MS $\mathcal{X} = (X, d_X, f_X)$, the* Rips bipersistence treegram *of $\mathcal{X}$ is $\theta_{\mathcal{X}}^{\mathrm{bi}} : \mathbb{R}^2 \to \mathbf{Subpart}(X)$ such that $(\sigma, \varepsilon) \mapsto \pi_0\left(\mathcal{R}_\varepsilon(X_\sigma, d_X)\right)$.*

Observe that $x \in X$ belongs to the underlying set of $\theta_{\mathcal{X}}^{\mathrm{bi}}(\mathbf{a})$ if and only if $(f_X(x), 0) \leq \mathbf{a}$, i.e. $(f_X(x), 0)$ is the *birth grade* of x in $\theta_{\mathcal{X}}^{\mathrm{bi}}$. Assume that $\mathcal{X}$ is injective. Then the birth grades of elements in X is totally ordered. The ER-staircode of $\mathcal{X}$ can be extracted from $\theta_{\mathcal{X}}^{\mathrm{bi}}$: Indeed, I_x in equation (1) can be rephrased as $I_x = \{(\sigma, \varepsilon) \in \mathbb{R}^2 : x$ is in the underlying set of $\theta_{\mathcal{X}}^{\mathrm{bi}}(\sigma, \varepsilon)$ and x has the smallest birth grade in its block of $\theta_{\mathcal{X}}^{\mathrm{bi}}(\sigma, \varepsilon)\}$. See Figure 7.

▶ **Definition 16** (Fibered treegrams)**.** *Let $\theta_{\mathcal{X}}^{\mathrm{bi}}$ be a Rips bipersistence treegram of an aug-MS $\mathcal{X}$. The* fibered treegram *of $\theta_{\mathcal{X}}^{\mathrm{bi}}$ refers to the collection $\{\theta_{\mathcal{X}}^{\mathrm{bi}}|_L\}_{L \in \mathcal{L}}$ of treegrams obtained by restricting $\theta_{\mathcal{X}}^{\mathrm{bi}}$ to positive-slope lines (see Figure 8 for an example).*

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 $\mathrm{H}_0(\mathcal{R}_\bullet^{\mathrm{bi}}(\mathcal{X}))$ (Theorem 17). Also, in general, all fibered treegrams can be recovered from ER-staircodes (Theorem 19).

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

$$u_X(x, x') := \min\{\varepsilon \in [0, \infty) : \text{there exists an } \varepsilon\text{-chain between } x \text{ and } x'\} \text{ (see [7]).}$$

For a metric space (X, d_X) and pick any total order $<$ on X. Let $x \in X$ be a non-minimal 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 $u_X(x, x') \leq u_X(x, x'')$.

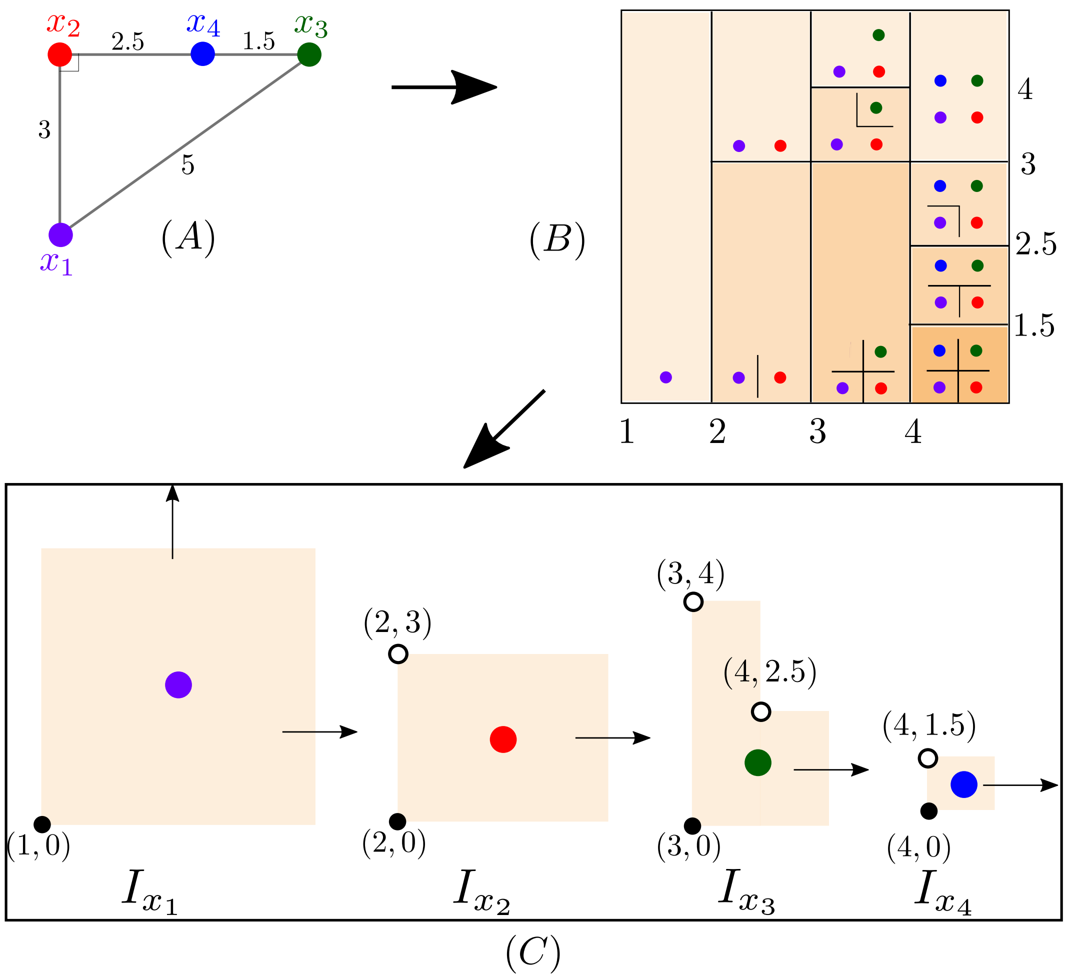

Figure 7 Consider the aug-MS $\mathcal{X}$ defined in Figure 1. Figure (A) and (C) above are identical to Figure 1 (A) and (B), respectively. (B) The Rips bipersistence treegram of $\mathcal{X}$ (Definition 15). The summarization processes (A)→(B)→(C) are analogous to the processes depicted in Figure 6.

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 non-minimal $x \in X$ 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 14 and at the same time strengthen Theorem 8 for 2-parameter persistence modules induced by a special type of aug-MSs:

▶ **Theorem 17** (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 *$x \in X$.*[1] *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 17 is similar to that of Theorem 14, and is in the full version [4]. Consider the aug-MS $\mathcal{X}$ in Figure 1, which satisfies the assumption in Theorem 17. Therefore, $\mathrm{H}_0\left(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})\right)$ is interval decomposable. The following corollary (proof in the full version [4]) gives an example of a class of aug-MSs to which Theorem 17 applies.

[1] 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 $\mathcal{I}^<_{\mathcal{X}} = \mathcal{I}^{<'}_{\mathcal{X}}$.

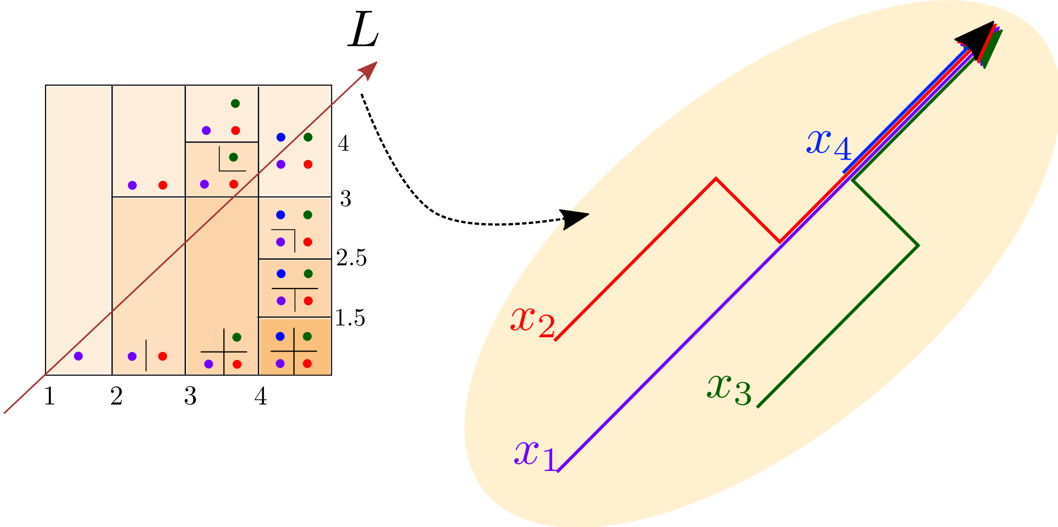

Figure 8 Consider the bipersistence treegram in Figure 7 (B) and pick a line L of positive slope. Then, we obtain a treegram over L.

▶ **Corollary 18.** *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, $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X}))$ is interval decomposable (in fact, its barcode consists solely of infinite rectangular intervals).*

We enrich the ER-staircode in order to query the fibered treegram: Given an aug-MS $\mathcal{X} = (X, d_X, f_X)$, let $<$ be any order on X compatible with f_X. For each x, 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 9. The following result holds for general aug-MSs.

▶ **Theorem 19.** *Given any $L \in \mathcal{L}$, the fibered treegram $\theta^{\mathrm{bi}}_{\mathcal{X}}|_L$ can be recovered from the decorated ER-staircode $\mathcal{I}^*_{\mathcal{X}}$ of the aug-MS $\mathcal{X} = (X, d_X, f_X)$.*

5 Elder-rule-staircodes and graded Betti numbers

We now show that we can retrieve the graded Betti numbers of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X}))$ from the ER-staircode of an aug-MS $\mathcal{X}$ (Theorem 23). Along the way, we obtain a characterization result for the graded Betti number of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X}))$ (Theorem 22), which is of independent interest.

Graded Betti numbers. We briefly review the concept of *graded Betti numbers* [6, 21, 24, 25, 28, 31]. Since our interests are in studying finite aug-MSs, we restrict ourselves to *finite* persistence modules – the k-th homology of a filtration of a finite simplicial complex for some $k \in \mathbb{Z}_{\geq 0}$ [8].

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

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

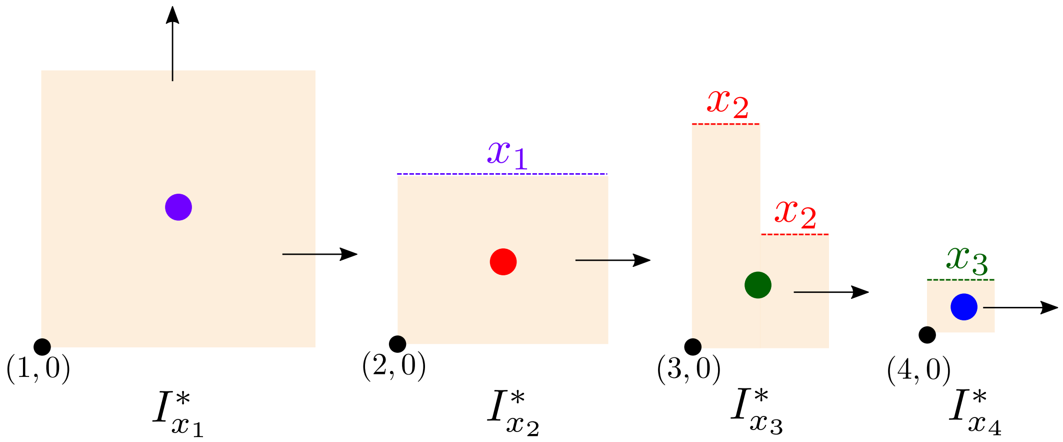

Figure 9 Decorated intervals corresponding to the four intervals in Figure 1 (C). For each $i = 2, 3, 4$, the upper boundary of I_{x_i} is decorated by the conqueror of x_i.

element of M, denoted by $\mathrm{gr}(m) = \mathbf{a}$. Let F be a free module. A *basis* B of F is a minimal homogeneous set of generators of F (see full version [4] for details). There can exist multiple bases of F, but 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 $\mathbb{Z}^d$. Assume that there is a chain of modules

$$F^\bullet : \cdots \xrightarrow{\partial_3} F^2 \xrightarrow{\partial_2} F^1 \xrightarrow{\partial_1} F^0 \xrightarrow{\partial_0} M \xrightarrow{0(=:\partial_{-1})} 0 \tag{3}$$

such that (1) each F^i is a free module, and (2) $\mathrm{im}(\partial^i) = \ker(\partial^{i-1})$, $i = 0, 1, 2, \cdots$. 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 $i = 1, 2, \cdots$. It is a standard fact that a minimal resolution of M always exists and is unique up to isomorphism [28, Chapter I].

▶ **Definition 20** (Graded Betti numbers). *Let $M : \mathbb{Z}^d \to$ **Vec** be finite. Assume that a minimal free resolution of M is $F^\bullet$ in (3). For $i \in \mathbb{Z}_{\geq 0}$, the i-th 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).*

We remark that $\beta_i^M : \mathbb{Z}^d \to \mathbb{Z}_{\geq 0}$ is the zero function for every $i > d$ [17, Theorem 1.13].

The graded Betti numbers of $\mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X}))$. Henceforth, every aug-MS $\mathcal{X} = (X, d_X, f_X)$ is assumed to be *generic*: f_X is injective and each pair of elements in X has different distance. Non-generic aug-MSs can also be easily handled; see the full version [4]. Since $\mathcal{X}$ is finite, we consider $\mathbb{Z}^2$-indexed filtration described subsequently as a substitute of $\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})$:

▶ **Definition 21.** *Consider an aug-MS $\mathcal{X} = (X, d_X, f_X)$ with $X := \{x_1, \ldots, x_n\}$ and assume that $f_X(x_1) < \ldots < f_X(x_n)$. 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 non-trivial pair (x_i, x_j) $(i \neq j)$ to $\ell \in \left\{1, \ldots, \binom{n}{2}\right\}$, where $d_X(x_i, x_j)$ is the ℓ-th smallest distance (among non-zero distance values). The restriction of $\mathcal{R}^{\mathrm{bi}}_\bullet(X, d_X^{\mathbb{Z}}, f_X^{\mathbb{Z}}) : \mathbb{R}^2 \to$ **Simp** to $\mathbb{Z}^2$ is the $\mathbb{Z}^2$-*indexed Rips filtration *of $\mathcal{X}$. Also, let $\gamma_j^{\mathcal{X}}$ denote the j-th elder-rule feature function of $(X, d_X^{\mathbb{Z}}, f_X^{\mathbb{Z}})$ for $j = 0, 1, 2$ in this section.*

For Theorem 22, 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 $\mathbf{a} \in \mathbb{P}$.

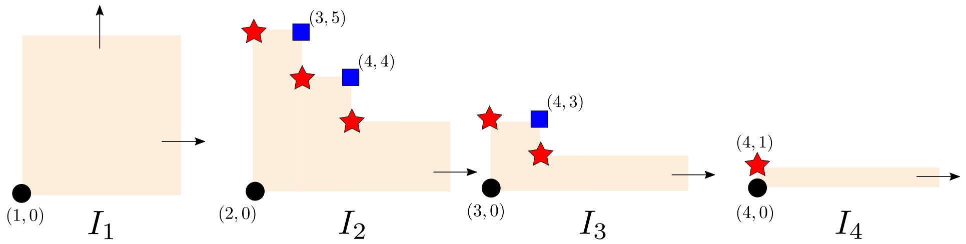

Figure 10 Assume that an aug-MS $\mathcal{X}$ consists of four staircase intervals as above with types of corners marked. From these corner types, we can obtain the graded Betti numbers of $M := \mathrm{H}_0(\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X}))$ via Theorem 23: Let $\mathrm{supp}(\beta_i^M) := \{\mathbf{a} \in \mathbb{Z}^2 : \beta_i^M(\mathbf{a}) \neq 0\}$ for $i = 0, 1, 2$ (the *support* of β_i^M). By Theorem 23, we have $\mathrm{supp}(\beta_0^M) = \{(i, 0) : i = 1, 2, 3, 4\}$, $\mathrm{supp}(\beta_1^M) = \{(2, 5), (3, 4), (4, 3), (3, 3), (4, 2), (4, 1)\} \setminus \{(3, 5), (4, 4), (4, 3)\} = \{(2, 5), (3, 4), (3, 3), (4, 2), (4, 1)\}$, and $\mathrm{supp}(\beta_2^M) = \{\{(3, 5), (4, 4), (4, 3)\}\} \setminus \{(2, 5), (3, 4), (4, 3), (3, 3), (4, 2), (4, 1)\} = \{(3, 5), (4, 4)\}$. All graded Betti numbers are 1 on their supports and 0 otherwise. In particular, note that the grade $\mathbf{a} = (4, 3)$ receives both a 1-st type mark (in I_2) and a 2-nd type mark (in I_3). Thus it contributes value 1 both to $\gamma_1^{\mathcal{X}}(\mathbf{a})$ and $\gamma_2^{\mathcal{X}}(\mathbf{a})$, and as a result, it does not appear in the support for β_1^M nor β_2^M.

- 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*.
- Given a simplicial complex K and $k \in \mathbb{Z}_{\geq 0}$, let $C_k(K)$ be the k-th chain group of 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 k-th cycle group of K.
- Let $\mathcal{K} : \mathbb{Z}^2 \to \mathbf{Simp}$ be a filtration. For each $k \in \mathbb{Z}_{\geq 0}$, 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, if $\mathcal{K}$ is 1-critical, then $C_k(\mathcal{K})$ is the free module whose basis elements one-to-one correspond to all the k-th simplices in S. 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 22.** *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,*

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

$$0 \to Z_1(\mathcal{K}^-) \xrightarrow{i} C_1(\mathcal{K}^-) \xrightarrow{\partial_1} C_0(\mathcal{K}^-) \xrightarrow{p} \mathrm{H}_0(\mathcal{K}) \to 0, \tag{4}$$

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

(ii) *The sequence in (4) is a minimal free resolution of* $\mathrm{H}_0(\mathcal{K})$.[2]

Theorem 22 is proved in the full version [4].

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

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

For any aug-MS $\mathcal{X}$, we can compute the graded Betti numbers of the zeroth homology of $\mathcal{R}^{\mathrm{bi}}_\bullet(\mathcal{X})$ from the ER-staircode of $\mathcal{X}$, as specified by the following result.

[2] This means that $F^0 = C_0(\mathcal{K}^-)$, $F^1 = C_1(\mathcal{K}^-)$, $F^2 = Z_1(\mathcal{K}^-)$ and $F^i = 0$ for $i > 2$ in the chain of (3).

▶ **Theorem 23.** *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 i-th grade Betti number of M. Then,*

$$\beta_0^M = \gamma_0^{\mathcal{X}}, \quad \beta_1^M = \gamma_1^{\mathcal{X}} - \gamma_2^{\mathcal{X}}, \quad \beta_2^M = \gamma_2^{\mathcal{X}} - \gamma_1^{\mathcal{X}}. \tag{5}$$

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 $\mathrm{H}_0(\mathcal{R}_\bullet^{\mathrm{bi}}(\mathcal{X}))$ by Theorem 23. See Figure 10 for an example. We also remark that *Koszul homology formulae* [25, Proposition 5.1] are in a similar form to those in (5). However, Koszul homology formulae do not directly imply those in (5) nor vice versa.

Sketch of proof of Theorem 23. Let $\mathcal{X} := (X, d_X, f_X)$ with $X = \{x_1, \ldots, x_n\}$, and assume that $f_X(x_1) < \ldots < f_X(x_n)$. By the construction of $\mathcal{K}$ and $\gamma_i^{\mathcal{X}}$, it suffices to show the equalities in (5) 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 22 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 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 22 and the construction of $\gamma_i^{\mathcal{X}}$, $i = 1, 2$,

$$\text{for } 1 \leq b \leq \tbinom{n}{2}, \quad \beta_1^M(1, b) = \gamma_1^{\mathcal{X}}(1, b) = 0, \text{ and } \beta_2^M(1, b) = \gamma_2^{\mathcal{X}}(1, b) = 0. \tag{6}$$

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 Theorem A.5 and Theorem C.1 in the full version [4], 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 C.4 in the full version [4], three cases are possible: (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 non-negative, 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. ◀

6 Computation and Algorithms

▶ **Theorem 24.** *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.*

Below we sketch the proof of the above theorem, with missing details in [4].

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 Remark 12). 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 folklore 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 $f_X(x_i) \le f_X(x_j)$ 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 $T_i := MST(G_i)$ is the minimum spanning tree (MST) for the weighted graph G_i. Our algorithm depends on the following lemma, the proof of which is in the full version [4].

▶ **Lemma 25.** *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 i-th iteration,

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

(Step 2): We use the approach described in the proof of Lemma 25 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 [12], one can update the minimum spanning tree 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 14 in the full version [4]). 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 $O(n^2 \log n)$.

Knowing the order of all edges in T_{i-1} does not appear to 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 the full version [4] that if $X \subset \mathbb{R}^d$ for a fixed dimension d, then each T_i will only have 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 24 (a) follows. See the full version [4] for the proofs of (b) and (c).

7 Discussion

Some open questions and conjectures are as follows:

1. **Barcodes and elder-rule-staircodes.** We conjecture that if the zeroth homology of the Rips bifiltration of an augmented metric space is interval decomposable, then the barcode must coincide with the elder-rule-staircode. Also, we suspect the sufficient condition for $\mathcal{X}$ to be interval decomposable given in Theorem 17 is actually also a necessary condition. Note that Theorem 17 and these conjectures are closely related to questions raised in [2].

2. **Extension to d-augmented metric spaces.** Can we generalize our results to the setting of more than two parameters? Namely, for d-augmented metric spaces $\mathcal{X}^d := (X, d_X, f_1, f_2, \ldots, f_d)$, $f_i : X \to \mathbb{R}$, $i = 1, \ldots, d$, 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 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. But it is not clear how to define elder-rule staircode without the assumption.
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 7). 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 [3]. On the other hand, there exists a metric d_{GH}^1 which measures the difference between aug-MSs [11] and let d_{I} be the interleaving distance between 2-parameter persistence modules [23]. Are there constants $\alpha, \beta > 0$ such that for all aug-MSs $\mathcal{X}$ and $\mathcal{Y}$, the inequalities below hold?

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

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 7). How faithful is this collection in general? Is there any class of aug-MSs $\mathcal{X}$ such that $E(\mathcal{X})$ completely characterizes $\mathcal{X}$?

References

1 Gorô Azumaya et al. Corrections and supplementaries to my paper concerning krull-remak-schmidt's theorem. *Nagoya Mathematical Journal*, 1:117–124, 1950.

2 Ulrich Bauer, Magnus B Botnan, Steffen Oppermann, and Johan Steen. Cotorsion torsion triples and the representation theory of filtered hierarchical clustering. *arXiv preprint*, 2019. `arXiv:1904.07322`.

3 Magnus Botnan and Michael Lesnick. Algebraic stability of zigzag persistence modules. *Algebraic & geometric topology*, 18(6):3133–3204, 2018.

4 Chen Cai, Woojin Kim, Mémoli Facundo, and Yusu Wang. Elder-rule-staircodes for augmented metric spaces. *arXiv preprint*, 2020. `arXiv:2003.04523`.

5 Chen Cai and Yusu Wang. Understanding the power of persistence pairing via permutation test. *arXiv preprint*, 2020. `arXiv:2001.06058`.

6 G. Carlsson and A. Zomorodian. The theory of multidimensional persistence. *Discrete & Computational Geometry*, 42(1):71–93, 2009. `doi:doi:10.1007/s00454-009-9176-0`.

7 Gunnar Carlsson and Facundo Mémoli. Characterization, stability and convergence of hierarchical clustering methods. *Journal of machine learning research*, 11(Apr):1425–1470, 2010.

8 Gunnar Carlsson and Facundo Mémoli. Multiparameter hierarchical clustering methods. In *Classification as a Tool for Research*, pages 63–70. Springer, 2010.

9 Mathieu Carriere, Frédéric Chazal, Yuichi Ike, Théo Lacombe, Martin Royer, and Yuhei Umeda. A general neural network architecture for persistence diagrams and graph classification. *arXiv preprint*, 2019. `arXiv:1904.09378`.

10 Andrea Cerri, Barbara Di Fabio, Massimo Ferri, Patrizio Frosini, and Claudia Landi. Betti numbers in multidimensional persistent homology are stable functions. *Mathematical Methods in the Applied Sciences*, 36(12):1543–1557, 2013.

11 Frédéric Chazal, David Cohen-Steiner, Leonidas J Guibas, Facundo Mémoli, and Steve Y Oudot. Gromov-Hausdorff stable signatures for shapes using persistence. In *Computer Graphics Forum*, volume 28 (5), pages 1393–1403. Wiley Online Library, 2009.

12 Francis Chin and David Houck. Algorithms for updating minimal spanning trees. *Journal of Computer and System Sciences*, 16(3):333–344, 1978.

13 David Cohen-Steiner, Herbert Edelsbrunner, and John Harer. Stability of persistence diagrams. *Discrete & Computational Geometry*, 37(1):103–120, 2007.

14 Justin Curry. The fiber of the persistence map for functions on the interval. *Journal of Applied and Computational Topology*, 2(3-4):301–321, 2018.

15 Tamal K Dey and Cheng Xin. Generalized persistence algorithm for decomposing multi-parameter persistence modules. *arXiv preprint*, 2019. `arXiv:1904.03766`.

16 Herbert Edelsbrunner and John Harer. *Computational topology: an introduction*. American Mathematical Soc., 2010.

17 David Eisenbud. *Commutative Algebra: with a view toward algebraic geometry*, volume 150. Springer Science & Business Media, 2013.

18 Christoph Hofer, Roland Kwitt, Marc Niethammer, and Andreas Uhl. Deep learning with topological signatures. In *Advances in Neural Information Processing Systems*, pages 1634–1644, 2017.

19 Woojin Kim and Facundo Mémoli. Generalized persistence diagrams for persistence modules over posets. *arXiv preprint*, 2018. `arXiv:1810.11517`.

20 Woojin Kim and Facundo Mémoli. Spatiotemporal persistent homology for dynamic metric spaces. *Discrete & Computational Geometry*, pages 1–45, 2020. `doi:10.1007/s00454-019-00168-w`.

21 Kevin P. Knudson. A refinement of multi-dimensional persistence. *Homology, Homotopy and Applications*, 10(1):259–281, 2008.

22 Claudia Landi. The rank invariant stability via interleavings. In *Research in Computational Topology*, pages 1–10. Springer, 2018.

23 Michael Lesnick. The theory of the interleaving distance on multidimensional persistence modules. *Found. Comput. Math.*, 15(3):613–650, June 2015. `doi:10.1007/s10208-015-9255-y`.

24 Michael Lesnick and Matthew Wright. Interactive visualization of 2-d persistence modules. *arXiv preprint*, 2015. `arXiv:1512.00180`.

25 Michael Lesnick and Matthew Wright. Computing minimal presentations and betti numbers of 2-parameter persistent homology. *arXiv preprint*, 2019. `arXiv:1902.05708`.

26 Alex McCleary and Amit Patel. Multiparameter persistence diagrams. *arXiv preprint*, 2019. `arXiv:1905.13220v3`.

27 Amit Patel. Generalized persistence diagrams. *Journal of Applied and Computational Topology*, 1(3-4):397–419, 2018.

28 Irena Peeva. *Graded syzygies*, volume 14. Springer Science & Business Media, 2010.

29 Zane Smith, Samir Chowdhury, and Facundo Mémoli. Hierarchical representations of network data with optimal distortion bounds. In *Signals, Systems and Computers, 2016 50th Asilomar Conference on*, pages 1834–1838. IEEE, 2016.

30 Qi Zhao and Yusu Wang. Learning metrics for persistence-based summaries and applications for graph classification. In *33rd Annu. Conf. Neural Inf. Processing Systems (NeuRIPS)*, 2019. to appear.

31 Afra Zomorodian and Gunnar Carlsson. Computing persistent homology. *Discrete & Computational Geometry*, 33(2):249–274, 2005.