

# Data and homotopy types

J.F. Jardine

August 17, 2019

## Abstract

This paper presents explicit assumptions for the existence of interleaving homotopy equivalences of both Vietoris-Rips and Lesnick complexes associated to an inclusion of data sets. Consequences of these assumptions are investigated on the space level, and for corresponding hierarchies of clusters and their sub-posets of branch points. Hierarchy posets and branch point posets admit a calculus of least upper bounds, which is used to show that the map of branch points associated to the inclusion of data sets is a controlled homotopy equivalence.

## Introduction

This paper is a discussion of homotopy theoretic phenomena that arise in connection with inclusions  $X \subset Y \subset \mathbb{R}^n$  of data sets in topological data analysis. The manuscript is not in final form, and comments are welcome.

Suppose that  $r > 0$ , and say that  $X$  is  $r$ -dense in  $Y$  if for every point  $y$  in  $Y$  there is an  $x$  in  $X$  such that the distance  $d(y, x) < r$  in the ambient metric space.

The first result in this direction (Corollary 2 below) implies that, under the  $r$ -density assumption, the induced map  $V_s(X) \rightarrow V_s(Y)$  of Vietoris-Rips complexes is a homotopy equivalence if  $2r < t - s$ , where  $t$  is the smallest number such that  $V_t(X) \neq V_s(X)$ .

This result can be extended to the assertion that the inclusion  $L_{s,k}(X) \rightarrow L_{s,k}(Y)$  of Lesnick complexes (with fixed density parameter  $k$ ) is a homotopy equivalence if every point  $y$  in the “configuration space”  $Y_{dis}^{k+1}$  of  $k + 1$  distinct elements of  $Y$  has an element  $x \in X_{dis}^{k+1}$  such that  $d(y, x) < r$  in  $\mathbb{R}^{n(k+1)}$ . This result appears as Corollary 4 in this paper.

Corollary 2 and Corollary 4 follow from Theorem 1 and Theorem 3, respectively. Both theorems are “interleaving” homotopy type results (see also [1]) that follow from the respective  $r$ -density assumptions, by methods that amount to manipulation of barycentric subdivisions. Theorem 1 is a special case of Theorem 3 (it is the case  $k = 0$ ), but Theorem 1 was found initially, and its proof has a certain clarity in isolation.

For a fixed  $k$ , the sets  $\pi_0 L_{s,k}(X)$  of path components, as  $s$  varies, define a tree  $\Gamma_k(X)$  with elements  $(s, [x])$ ,  $[x] \in \pi_0 L_{s,k}(X)$ . The inclusion  $X \subset Y$  defines a poset morphism  $\Gamma_k(X) \rightarrow \Gamma_k(Y)$ .

The tree  $\Gamma_k(X)$  is the object studied by the HDBSCAN clustering algorithm, while the individual sets of clusters  $\pi_0 L_{s,k}(X)$  are the objects of interest for the DBSCAN algorithm.

The poset  $\Gamma_k(X)$  has a subobject  $\text{Br}_k(X)$  whose elements are the branch points of  $\Gamma_k(X)$ , suitably defined — see Section 2. The branch points of  $\Gamma_k(X)$  are in one to one correspondence with the stable components for  $\Gamma_k(X)$  that are defined in [3], in the sense that every such stable component starts at a unique branch point. Thus, we can (and do) replace the stable component discussion of [3] with the branch point poset  $\text{Br}_k(X)$ , and make particular use of its ordering.

The tree  $\Gamma_k(X)$  has least upper bounds, and these restrict to least upper bounds for the subobject  $\text{Br}_k(X)$  of branch points. This notion of least upper bounds is an extension of and a potential replacement for the distance function that is introduced by Carlsson and Mémoli [2] in their description of the ultrametric structure on a data set  $X$  that arises from the single linkage cluster hierarchy. The Carlsson-Mémoli theory does not apply in general to the tree  $\Gamma_k(X)$ , because the vertex sets of the Lesnick complexes  $L_{k,s}(X)$  vary with changes of the parameter  $s$ .

The calculus of least upper bounds and its relation with branch points is described in Lemmas 7–12 below.

The branch point tree  $\text{Br}_k(X)$  can be thought of as a highly compressed version of the hierarchy  $\Gamma_k(X)$  that is produced by the HDBSCAN algorithm.

The inclusion  $\text{Br}_k(X) \subset \Gamma_k(X)$  is a homotopy equivalence of posets, where the homotopy inverse is defined by taking the maximal branch point  $(s_0, [x_0]) \leq (s, [x])$  below  $(s, [x])$  for each object of  $\Gamma_k(X)$ . The existence of the maximal branch point below an object  $(s, [x])$  is a consequence of Lemma 12.

The poset map  $\Gamma_k(X) \rightarrow \Gamma_k(Y)$  defines a poset map  $i_* : \text{Br}_k(X) \rightarrow \text{Br}_k(Y)$ , via the homotopy equivalences for the data sets  $X$  and  $Y$  of the last paragraph.

The configuration space  $r$ -density assumption for Theorem 3 implies that there is a poset morphism  $\theta_* : \text{Br}_k(Y) \rightarrow \text{Br}_k(X)$  that is induced by a morphism  $(s, [x]) \rightarrow (s+2r, [\theta(x)])$ , and that there are homotopies of poset maps  $i_* \cdot \theta_* \simeq s_*$  and  $\theta_* \cdot i_* \simeq s_*$ , where  $s_*$  is defined by the shift operator  $(s, [x]) \mapsto (s+2r, [x])$  on  $Y$  and  $X$ , respectively. These homotopies are “bounded” (or controlled) by the number  $2r$ .

In good circumstances, a branch point  $(s, [x])$  is the maximal branch point below the shift  $(s+2r, [x])$ , and the inequalities defining the homotopies of the last paragraph become equalities in that case.

In summary, the poset morphism  $\text{Br}_k(X) \rightarrow \text{Br}_k(Y)$  that is induced by an inclusion of data sets  $X \subset Y$  has a homotopy theoretic character, and is measurably close to a homotopy equivalence if every sufficiently large group of distinct points of  $Y$  is close to a corresponding group of distinct points for the smaller data set  $X$ . Such a statement amounts to a stability result for hierarchies of branch points, albeit not in traditional terms.

# Contents

1 Homotopy types	3
2 Branch points and upper bounds	6

## 1 Homotopy types

Suppose given (finite) data sets  $X \subset Y \subset \mathbb{R}^n$ . Suppose that  $r > 0$ .

Say that  $X$  is  $r$ -dense in  $Y$ , if for all  $y \in Y$  there is an  $x \in X$  such that  $d(y, x) < r$ .

Suppose that  $s \geq 0$ . Recall that  $V_s(X)$  is the simplicial complex with simplices  $(x_0, \dots, x_n)$  with  $x_i \in X$  and  $d(x_i, x_j) \leq s$ .

Then we have

$$X = V_0(X) \subset V_s(X) \subset V_t(X) \subset \dots \subset V_R(X) = \Delta^X$$

for  $0 \leq s < t \leq R$ , and for  $R$  sufficiently large, where  $\Delta^X := \Delta^N$  and  $N = |X| - 1$ .

The inclusion  $i : X \subset Y$  induces a map of systems of simplicial complexes  $i : V_s(X) \subset V_s(Y)$ .

The data sets  $X$  and  $Y$  are finite, so there is a finite string of parameter values

$$0 = s_0 < s_1 < \dots < s_r,$$

consisting of the distances between elements of  $Y$ . This includes the list of distances between elements of  $X$ . I say that the  $s_i$  are the **phase-change** numbers.

**Theorem 1.** *Suppose that  $X \subset Y \subset \mathbb{R}^n$ , and that  $X$  is  $r$ -dense in  $Y$ . Then there is a homotopy commutative diagram*

$$\begin{array}{ccc} V_s(X) & \xrightarrow{j} & V_{s+2r}(X) \\ \downarrow i & \nearrow \theta & \downarrow i \\ V_s(Y) & \xrightarrow{j} & V_{s+2r}(Y) \end{array}$$

in which the upper triangle commutes.

*Proof.* Define a function  $\theta : Y \rightarrow X$  by specifying  $\theta(x) = x$  for  $x \in X$ . For  $y \in Y - X$  find  $x \in X$  such that  $d(x, y) < r$  and set  $\theta(y) = x$ .

If  $(y_0, \dots, y_n)$  is a simplex of  $V_s(Y)$ ,

$$d(\theta(y_i), \theta(y_j)) \leq d(\theta(y_i), y_i) + d(y_i, y_j) + d(y_j, \theta(y_j)) \leq r + s + r.$$

It follows that  $\theta$  induces a simplicial complex map  $\theta : V_s(Y) \rightarrow V_{s+2r}(X)$ , such that the upper triangle commutes.

For the simplex  $(y_0, \dots, y_n)$  of  $V_s(Y)$ , the string of elements

$$(y_0, \dots, y_n, \theta(y_0), \dots, \theta(y_n))$$

defines a simplex of  $V_{s+2r}(Y)$ , since

$$d(y_i, \theta(y_j)) \leq d(y_i, y_j) + d(y_j, \theta(y_j)) \leq s + r.$$

Set

$$\gamma(y_0, \dots, y_n) = (y_0, \dots, y_n, \theta(y_0), \dots, \theta(y_n)).$$

This assignment defines a morphism  $\gamma : NV_s(Y) \rightarrow NV_{s+2r}(Y)$  of posets of non-degenerate simplices, and there are homotopies (natural transformations)

$$j \rightarrow \gamma \leftarrow i \cdot \theta$$

which are defined by face inclusions.  $\square$

**Corollary 2.** *Suppose that  $X \subset Y \subset \mathbb{R}^n$ , and that  $X$  is  $r$ -dense in  $Y$ . Suppose that  $2r < s_{i+1} - s_i$ . Then the map*

$$i : V_{s_i}(X) \rightarrow V_{s_i}(Y)$$

*is a weak homotopy equivalence.*

*Proof.* In the homotopy commutative diagram

$$\begin{array}{ccc} V_{s_i}(X) & \xrightarrow{j} & V_{s_i+2r}(X) \\ i \downarrow & \nearrow \theta & \downarrow i \\ V_{s_i}(Y) & \xrightarrow{j} & V_{s_i+2r}(Y) \end{array}$$

the horizontal morphisms  $j$  are isomorphisms (identities), and so  $V_{s_i}(X)$  is a deformation retract of  $V_{s_i}(Y)$ .  $\square$

Corollary 2 has consequences for both persistent homology and clustering.

Suppose that  $k$  is a non-negative integer. The Lesnick subcomplex  $L_{s,k}(X)$  is the full subcomplex of  $V_s(X)$  on those vertices  $x$  for which there are at least  $k$  distinct vertices  $x_i \neq x$  such that  $d(x, x_i) \leq s$  [5], [3], [4].

A simplex  $\sigma = (y_0, \dots, y_n)$  of  $V_s(X)$  is in  $L_{s,k}(X)$  if and only if each vertex  $y_i$  has at least  $k$  distinct neighbours in  $V_s(X)$  — this is the meaning of the assertion that  $L_{s,k}(X)$  is a full subcomplex of  $V_s(X)$ .

There is an array of subcomplexes

$$\begin{array}{ccc} V_s(X) & \longrightarrow & V_t(X) \\ \uparrow & & \uparrow \\ L_{s,k}(X) & \longrightarrow & L_{t,k}(X) \\ \uparrow & & \uparrow \\ L_{s,k+1}(X) & \longrightarrow & L_{t,k+1}(X) \end{array}$$

We have the following observations:

- 1)  $L_{s,0}(X) = V_s(X)$ .
- 2)  $L_{s,k}(X)$  could be empty for small  $s$  and large  $k$ . In general, for  $s \leq t$ ,  $L_{s,k}(X)$  and  $L_{t,k}(X)$  may not have the same vertices.
- 3) Every inclusion  $i : X \subset Y \subset \mathbb{R}^n$  induces maps  $i : L_{s,k}(X) \rightarrow L_{s,k}(Y)$  which are natural in  $s$  and  $k$ .

I say that  $s$  is a **spatial parameter** and that  $k$  is a **density parameter** (also a **valence**, or degree). Lesnick says [4] that  $\{L_{s,k}(X)\}$  is the **degree Rips filtration** of the system  $\{V_s(X)\}$ .

Write  $X_{dis}^{k+1}$  for the set of  $k+1$  distinct points of  $X$ , and think of it as a subobject of  $(\mathbb{R}^n)^{k+1}$ .

**Theorem 3.** *Suppose that  $X \subset Y \subset \mathbb{R}^n$  and that  $X_{dis}^{k+1}$  is  $r$ -dense in  $Y_{dis}^{k+1}$  and that  $L_{s,k}(Y) \neq \emptyset$ . Then there is a homotopy commutative diagram*

$$\begin{array}{ccc} L_{s,k}(X) & \xrightarrow{j} & L_{s+2r,k}(X) \\ i \downarrow & \nearrow \theta & \downarrow i \\ L_{s,k}(Y) & \xrightarrow{j} & L_{s+2r,k}(Y) \end{array}$$

in which the upper triangle commutes in the usual sense.

*Proof.* Suppose that  $y \in L_{s,k}(X)_0 - L_{s,k}(X)_0$ . Then there are  $k$  points  $y_1, \dots, y_k$  of  $Y$ , distinct from  $y$  such that  $d(y, y_i) < s$ . There is a  $(k+1)$ -tuple  $(x_0, x_1, \dots, x_k)$  such that

$$d((x_0, \dots, x_k), (y, y_1, \dots, y_k)) < r,$$

by assumption. Then  $d(y, x_0) < r$ ,  $d(y_i, x_i) < r$ , and so  $d(x_0, x_i) < s + 2r$ , so that  $x_0 \in L_{s+2r,k}(X)$ . Set  $\theta(y) = x_0$ , and observe that  $d(y, \theta(y)) < r$ .

If  $(y_0, \dots, y_p)$  is a simplex of  $L_{s,k}(Y)$  then  $(\theta(y_0), \dots, \theta(y_p))$  is a simplex of  $L_{s+2r,k}(X)$ , as is the string

$$(y_0, \dots, y_p, \theta(y_0), \dots, \theta(y_p)).$$

Finish according to the method of proof for Theorem 1. □

**Corollary 4.** *Suppose that  $X \subset Y \subset \mathbb{R}^n$  and that  $X_{dis}^{k+1}$  is  $r$ -dense in  $Y_{dis}^{k+1}$ . Suppose that  $2r < s_{i+1} - s_i$ . Then the inclusion  $i : L_{s_i,k}(X) \rightarrow L_{s_i,k}(Y)$  is a weak homotopy equivalence.*

**Lemma 5.** *Suppose that  $X_{dis}^{k+1}$  is  $r$ -dense in  $Y_{dis}^{k+1}$ , and that  $Y_{dis}^{k+1} \neq \emptyset$ . Then  $X_{dis}^k$  is  $r$ -dense in  $Y_{dis}^k$ .*

*Proof.* Suppose that  $\{y_0, \dots, y_{k-1}\}$  is a set of  $k$  distinct points of  $Y$ . Then there is a  $y_k \in Y$  which is distinct from the  $y_i$ , so that  $(y_0, y_1, \dots, y_k)$  is a  $(k+1)$ -tuple of distinct points of  $Y$ . There is a  $(k+1)$ -tuple  $(x_0, \dots, x_k)$  of distinct points of  $X$  such that

$$d((y_0, \dots, y_{k-1}, y_k), (x_0, \dots, x_{k-1}, x_k)) < r.$$

It follows that

$$d((y_0, \dots, y_{k-1}), (x_0, \dots, x_{k-1})) < r.$$

□

**Corollary 6.** *Suppose that  $X \subset Y \subset \mathbb{R}^n$  and that  $X_{dis}^{k+1}$  is  $r$ -dense in  $Y_{dis}^{k+1}$ . Suppose that  $2r < s_{i+1} - s_i$ . Then the inclusion  $i : L_{s_i, p}(X) \rightarrow L_{s_i, p}(Y)$  is a weak homotopy equivalence for  $0 \leq p \leq k$ .*

## 2 Branch points and upper bounds

Fix the density  $k$  and suppose that  $L_{s, k}(X) \neq \emptyset$  for  $s$  sufficiently large. Apply the path component functor to the  $L_{s, k}(X)$ , to get a diagram of functions

$$\dots \rightarrow \pi_0 L_{s, k}(X) \rightarrow \pi_0 L_{t, k} \rightarrow \dots$$

There is a graph  $\Gamma_k(X) := \Gamma(\pi_0 L_{*, k}(X))$  with vertices  $(s, [x])$  with  $[x] \in \pi_0 L_{s, k}(X)$ , and edges  $(s, [x]) \rightarrow (t, [x])$  with  $s \leq t$ . This graph underlies a contractible poset, and is therefore a tree (or hierarchy).

To reflect the poset structure of  $\Gamma_k(X)$ , I write the morphisms of  $\Gamma_k(X)$  as relations  $(s, [x]) \leq (t, [y])$ . The existence of such a relation means that  $[x] = [y] \in \pi_0 L_{t, k}(X)$ , or that the image of  $[x] \in \pi_0 L_{s, k}(X)$  under the induced function  $\pi_0 L_{s, k}(X) \rightarrow \pi_0 L_{t, k}(X)$  is  $[y]$ .

**Remarks:** 1) Partitions of  $X$  given by the set  $\pi_0 V_s(X)$  are standard **clusters**. The tree  $\Gamma_0(X) = \Gamma(V_*(X))$  defines a **hierarchical clustering** (similar to, but not the same as single linkage clustering).

2) The set  $\pi_0 L_{s, k}(X)$  gives a partitioning of the set of elements of  $X$  having at least  $k$  neighbours of distance  $\leq s$ , which is the subject of the **DBSCAN** algorithm. The tree  $\Gamma_k(X) = \Gamma(\pi_0 L_{*, k}(X))$  is the basis of the **HDBSCAN** algorithm.

A *branch point* in the tree  $\Gamma_k(X)$  is a vertex  $(t, [x])$  such that either of following two conditions hold:

- 1) there is an  $s_0 < t$  such that for all  $s_0 \leq s < t$  there are distinct vertices  $(s, [x_0])$  and  $(s, [x_1])$  with  $(s, [x_0]) \leq (t, [x])$  and  $(s, [x_1]) \leq (t, [x])$ , or
- 2) there is no relation  $(s, [y]) \leq (t, [x])$  with  $s < t$ .

The second condition means that a representing vertex  $x$  is not a vertex of  $L_{s,k}(X)$  for  $s < t$ . Write  $\text{Br}_k(X)$  for the set of branch points  $(s, [x])$  in  $\Gamma_k(X)$ .

Every branch point  $(s, [x])$  of  $\Gamma_k(X)$  has  $s = s_i$ , where  $s_i$  is a phase change number for  $X$ .

The branch point poset  $\text{Br}_k(X)$  is a tree, because the element  $(s_r, [x])$  corresponding to the highest phase change number  $s_r$  is maximal.

The set of branch points  $\text{Br}_k(X)$  inherits a partial ordering from the poset  $\Gamma_k(X)$ , and the inclusion  $\text{Br}_k(X) \subset \Gamma_k(X)$  of the set of branch points defines a monomorphism of trees.

Suppose that  $(s, [x])$  and  $(t, [y])$  are vertices of the graph  $\Gamma_k(X)$ . There is a vertex  $(v, [w])$  such that  $(s, [x]) \leq (v, [w])$  and  $(t, [y]) \leq (v, [w])$ . The two relations mean, among other things, that  $[x] = [z] = [y]$  in  $\pi_0 L_{v,k}(X)$ .

It follows that there is a unique smallest vertex  $(u, [z])$  which is an upper bound for both  $(s, [x])$  and  $(t, [y])$ . The number  $u$  is the smallest parameter  $v$  such that  $[x] = [y]$  in  $\pi_0 L_{v,k}(X)$ , and so  $[z] = [x] = [y]$ .

I write

$$(s, [x]) \cup (t, [y]) = (u, [z]).$$

The vertex  $(u, [z])$  is the **least upper bound** (or join) of  $(s, [x])$  and  $(t, [y])$ .

Every finite collection of points  $(s_1, [x_1]), \dots, (s_p, [x_p])$  has a least upper bound

$$(s_1, [x_1]) \cup \dots \cup (s_p, [x_p])$$

in  $\Gamma_k(X)$ .

**Lemma 7.** *The least upper bound of branch points  $(u, [z])$  of  $(s, [x])$  and  $(t, [y])$  is a branch point.*

*Proof.* For numbers  $s, t < v < u$ ,  $(v, [x])$  and  $(v, [y])$  are distinct, because  $(u, [z])$  is a least upper bound.

Otherwise,  $s = u$  or  $t = u$ , in which case  $(u, [z]) = (s, [x])$  or  $(u, [z]) = (t, [y])$ , respectively.  $\square$

It follows from Lemma 7 that any two branch points  $(s, [x])$  and  $(t, [y])$  have a least upper bound in  $\text{Br}_k(X)$ , and that the poset inclusion  $\alpha : \text{Br}_k(X) \rightarrow \Gamma_k(X)$  preserves least upper bounds.

**Remark:** The poset  $\Gamma_k(X)$  also has greatest lower bounds (or meets). The greatest lower bound

$$(t_1, [y_1]) \cap \dots \cap (t_r, [y_r])$$

is the least upper bound of all  $(s, [x])$  such that  $(s, [x]) \leq (t_j, [y_j])$  for all  $j$ .

We have the following triviality:

**Lemma 8.** *Suppose that  $(s_1, [x_1]), (s_2, [x_2])$  and  $(s_3, [x_3])$  are vertices of  $\Gamma_k(X)$ . Then*

$$(s_1, [x_1]) \cup (s_3, [x_3]) \leq ((s_1, [x_1]) \cup (s_2, [x_2])) \cup ((s_2, [x_2]) \cup (s_3, [x_3])).$$

*Proof.* We have the identity

$$((s_1, [x_1]) \cup (s_2, [x_2])) \cup ((s_2, [x_2]) \cup (s_3, [x_3])) = (s_1, [x_1]) \cup (s_2, [x_2]) \cup (s_3, [x_3]),$$

and then

$$(s_1, [x_1]) \cup (s_3, [x_3]) \leq (s_1, [x_1]) \cup (s_2, [x_2]) \cup (s_3, [x_3]).$$

□

Carlsson and Mémoli [2] define an ultrametric  $d$  on  $X = V_0(X)$ , for which they say that  $d(x, y) = s$ , where  $s$  is the minimum parameter value such that  $[x] = [y] \in \pi_0 V_s(X)$ .

Suppose given  $[x]$  and  $[y]$  in  $\pi_0 L_{s,k}(X)$  (equivalently, points  $(s, [x])$  and  $(s, [y])$  in  $\Gamma_k(X)$ ). Write  $d([x], [y]) = u - s$ , where  $(s, [x]) \cup (s, [y]) = (u, [w])$ .

**Lemma 9.** *Given  $[x], [y]$  and  $[z]$  in  $\pi_0 L_{s,k}(X)$ , we have a relation*

$$d([x], [z]) \leq \max\{d([x], [y]), d([y], [z])\}.$$

*Proof.* Suppose that  $(s, [x]) \cup (s, [y]) \cup (s, [z]) = (v, [w])$ . Then

$$v - s = \max\{d([x], [y]), d([y], [z])\}$$

and

$$d([x], [z]) \leq v - s$$

by Lemma 8. □

**Corollary 10.** *The function*

$$d : \pi_0 L_{s,k}(X) \times \pi_0 L_{s,k}(X) \rightarrow \mathbb{R}_{\geq 0}$$

*of Lemma 9 gives the set  $\pi_0 L_{s,k}(X)$  the structure of an ultrametric space.*

**Remark:** One could define a “distance” function  $d$  on the full set of points of  $\Gamma_k(X)$  by setting

$$d((s, [x]), (t, [y])) = \max\{u - s, u - t\},$$

where  $(s, [x]) \cup (t, [y]) = (u, [z])$ .

The ultrametric property of Lemma 9 fails for the points  $(s, [x]), (t, [x])$  and  $(u, [x])$  where  $s < t < u$ , since it is not the case that  $u - s \leq \max\{t - s, u - t\}$ .

**Lemma 11.** *Every vertex  $(s, [x])$  of  $\Gamma_k(X)$  has a unique largest branch point  $(s_0, [x_0])$  such that  $(s_0, [x_0]) \leq (s, [x])$ .*

*Proof.* The least upper bound of the finite list of the branch points  $(t, [y])$  such that  $(t, [y]) \leq (s, [x])$  is a branch point, by Lemma 7. □

In the situation described by Lemma 11, I say that  $(s_0, [x_0])$  is the **maximal branch point below**  $(s, [x])$ .

**Lemma 12.** *Suppose that  $(s_0, [x_0])$  and  $(t_0, [y_0])$  are maximal branch points below the points  $(s, [x])$  and  $(t, [y])$ , respectively.*

*Then  $(s_0, [x_0]) \cup (t_0, [y_0])$  is the maximal branch point below  $(s, [x]) \cup (t, [y])$ .*

*Proof.* Suppose that  $s \leq t$ .

We have

$$(s_0, [x_0]) \cup (t_0, [y_0]) \leq (s, [x]) \cup (t, [y]).$$

and  $(s_0, [x_0]) \cup (t_0, [y_0])$  is a branch point by Lemma 7. Write

$$(v, [z]) = (s_0, [x_0]) \cup (t_0, [y_0]).$$

Suppose that  $v \leq t$ . Then  $(t_0, [y_0]) \leq (t, [y])$  and  $(t_0, [y_0]) \leq (v, [z])$ , so that  $(v, [z]) \leq (t, [y])$  since  $v \leq t$ . Also,  $(s_0, [x_0]) \leq (s, [x])$  and  $(s_0, [x_0]) \leq (v, [z]) \leq (t, [y])$  so that  $(s, [x]) \leq (t, [y])$ . Then  $(s_0, [x_0]) \leq (t_0, [y_0])$  by maximality, and it follows that

$$(s_0, [x_0]) \cup (t_0, [y_0]) = (t_0, [y_0])$$

is the maximal branch point of

$$(s, [x]) \cup (t, [y]) = (t, [y])$$

Suppose that  $v > t$ . Then  $(s, [x]) = (s, [x_0]) \leq (v, [z])$  and  $(t, [y]) = (t, [y_0]) \leq (v, [z])$  because  $s \leq t < v$ , so that

$$(s, [x]) \cup (t, [y]) \leq (s_0, [x_0]) \cup (t_0, [y_0]),$$

Thus,  $(s_0, [x_0]) \cup (t_0, [y_0]) = (s, [x]) \cup (t, [y])$  is a branch point, by Lemma 7.  $\square$

The poset inclusion  $\alpha : \text{Br}_k(X) \rightarrow \Gamma_k(X)$  has an inverse

$$\text{max} : \Gamma_k(X) \rightarrow \text{Br}_k(X),$$

up to homotopy.

In effect, Lemma 11 implies that every vertex  $(s, [x])$  of  $\Gamma_k(X)$  has a unique maximal branch point  $(s_0, [x_0])$  such that  $(s_0, [x_0]) \leq (s, [x])$ . Set

$$\text{max}(s, [x]) = (s_0, [x_0]).$$

The maximality condition implies that  $\text{max}$  preserves the ordering. The composite  $\text{max} \cdot \alpha$  is the identity on  $\text{Br}_k(X)$ , and the relations  $(s_0, [x_0]) \leq (s, x)$  define a homotopy  $\text{max} \cdot \alpha \leq 1$ .

Return to the inclusion  $i : X \subset Y \subset \mathbb{R}^n$  of finite data sets. Suppose that  $X_{dis}^{k+1}$  is  $r$ -dense in  $Y_{dis}^{k+1}$  and that  $L_{s,k}(Y)$  is non-empty, as in the statement of Theorem 3.

Write  $i_* : \text{Br}_k(X) \rightarrow \text{Br}_k(Y)$  for the composite

$$\text{Br}_k(X) \xrightarrow{\alpha} \Gamma_k(X) \xrightarrow{i_*} \Gamma_k(Y) \xrightarrow{\text{max}} \text{Br}_k(Y)$$

This map takes a branch point  $(s, [x])$  to the maximal branch point below  $(s, [i(x)])$ . The map  $i_*$  preserves least upper bounds by Lemma 7.

Poset morphisms  $\theta_* : \text{Br}_k(Y) \rightarrow \text{Br}_k(X)$  and  $s_* : \text{Br}_k(X) \rightarrow \text{Br}_k(X)$  are similarly defined, by the poset morphism  $\theta : \Gamma_k(Y) \rightarrow \Gamma_k(X)$  with  $(t, [y]) \mapsto (t + 2r, [\theta(y)])$ , and the shift morphism  $s : \Gamma_k(X) \rightarrow \Gamma_k(X)$  with  $(s, [x]) \mapsto (s + 2r, [x])$ .

The construction of the poset map  $i_* : \text{Br}_k(X) \rightarrow \text{Br}_k(Y)$  is not functorial in maps of the form  $X \rightarrow Y$ , but it is functorial up to coherent homotopy.

Similarly, the map  $i_* : \text{Br}_k(X) \rightarrow \text{Br}_k(Y)$  only preserves least upper bounds up to homotopy. Suppose that  $(s, [x])$  and  $(t, [y])$  are branch points of  $X$ , and let  $(s_0, [x_0]) \leq (s, [i(x)])$  and  $(t_0, [y_0]) \leq (t, [i(y)])$  be maximal branch points below the images of  $(s, [x])$  and  $(t, [y])$  in  $\Gamma_k(Y)$ . Then

$$(s_0, [x_0]) \cup (t_0, [y_0]) \leq (s, [i(x)]) \cup (t, [i(y)]),$$

so that

$$i_*(s, [x]) \cup i_*(t, [y]) \leq i_*((s, [x]) \cup (t, [y])).$$

Similar inequalities hold for least upper bounds with respect to the other maps that one encounters, namely  $\theta_* : \text{Br}_k(Y) \rightarrow \text{Br}_k(X)$  and the shift map  $s_* : \text{Br}_k(X) \rightarrow \text{Br}_k(X)$ .

1) Consider the poset maps

$$\text{Br}_k(X) \xrightarrow{i_*} \text{Br}_k(Y) \xrightarrow{\theta_*} \text{Br}_k(X).$$

If  $(s, [x])$  is a branch point for  $X$ , choose maximal branch points  $(s_0, [x_0]) \leq (s, [i(x)])$  for  $Y$ ,  $(s_1, [x_1]) \leq (s_0 + 2r, [\theta(x_0)])$  and  $(v, [y]) \leq (s + 2r, [x])$  below the respective objects.

Then  $\theta_* i_*(s, [x]) = (s_1, [x_1])$ , and there is a natural relation

$$\theta_* i_*(s, [x]) = (s_1, [x_1]) \leq (v, [y]) = s_*(s, [x]) \leq (s + 2r, [x]).$$

We therefore have a homotopy of poset maps

$$\theta_* i_* \leq s_* : \text{Br}_k(X) \rightarrow \text{Br}_k(X).$$

Note that  $(s, [x]) \leq s_*(s, [x])$  since  $(s, [x])$  is a branch point and  $s_*(s, [x])$  is the maximal branch point below  $(s + 2r, [x])$ . This means that the shift morphism  $s_*$  is homotopic to the identity on  $\text{Br}_k(X)$ .

The branch point  $(s, [x])$  has a ‘‘close’’ shared upper bound  $(s + 2r, [x])$  with the element  $(s_0 + 2r, [\theta(x_0)])$ , which is the image of the branch point  $(s_0, [x_0])$  under the poset map  $\theta_* : \Gamma_k(Y) \rightarrow \Gamma_k(X)$ .

2) Similarly, if  $(t, [y])$  is a branch point of  $Y$ , then

$$i_* \theta_*(t, [y]) \leq s_*(t, [y]) \geq (t, [y])$$

while  $s_*(t, [y]) \leq (t + 2r, [y])$ .

The element  $(t + 2r, [y])$  is a close shared upper bound for  $(t, [y])$  and an element of the form  $(t_0, [i(y_0)])$ , where  $(t_0, [y_0])$  is a maximal branch point of  $X$  below  $(s + 2r, [\theta(y)])$ .

**Remark:** The subobject of  $\text{Br}_k(X)$  consisting of all branch points of the form  $(s, [x])$  as  $s$  varies has an obvious notion of distance on it: the distance between points  $(s, [x])$  and  $(t, [x])$  is  $|t - s|$ . The closeness referred to in constructions 1) and 2) above can be expressed in terms of such a distance.

Suppose that  $(s_1, [x_1])$  and  $(s_2, [x_2])$  are branch points of  $X$ , let

$$(s, [x]) = (s_1, [x_1]) \cup (s_2, [x_2]),$$

and write

$$(t, [y]) = (s_1, [i(x_1)]) \cup (s_2, [i(x_2)]).$$

Then  $(s, [i(x)])$  is an upper bound for  $(s_1, [i(x_1)])$  and  $(s_2, [i(x_2)])$ , so that  $(t, [y]) \leq (s, [i(x)])$ .

The element  $(t + 2r, [\theta(y)])$  is an upper bound for  $(s_1, [x_1])$  and  $(s_2, [x_2])$ , so that

$$(s, [x]) \leq (t + 2r, [\theta(y)]) \leq (s + 2r, [x]). \quad (1)$$

It follows that  $s - 2r \leq t \leq s$ , which gives a constraint on the parameter  $t$  corresponding to the least upper bound  $(t, [y])$  in  $\Gamma_k(Y)$ , in terms of the least upper bound  $(s, [x])$  in  $\Gamma_k(X)$ , or in  $\text{Br}_k(X)$ . The number  $2r$  is a bound on the distances between the three points in (1).

If the bound  $2r$  is sufficiently small, then  $(s, [x])$  is the largest branch point below  $(s + 2r, [x])$  and  $s_*(s, [x]) = (s, [x])$  in that case. Similarly, in  $\Gamma_k(Y)$ ,  $s_*(t, [y]) = (t, [y])$  if  $2r$  is sufficiently small.

Recall that if  $(s, [x])$  is a branch point, then  $s = s_i$  is one of the phase shift numbers. Then  $(s_i, [x])$  is the maximal branch point below  $(s_i + 2r, [x])$  if  $2r < s_{i+1} - s_i$ .

## References

- [1] Andrew J. Blumberg and Michael Lesnick. Universality of the homotopy interleaving distance. *CoRR*, abs/1705.01690, 2017.
- [2] Gunnar Carlsson and Facundo Mémoli. Characterization, stability and convergence of hierarchical clustering methods. *J. Mach. Learn. Res.*, 11:1425–1470, 2010.
- [3] J.F. Jardine. Stable components and layers. Preprint, 2019.
- [4] M. Lesnick and M. Wright. RIVET: visualization and analysis of two-dimensional persistent homology. <http://rivet.online>, 2019.
- [5] Leland McInnes and John Healy. Accelerated hierarchical density based clustering. In *2017 IEEE International Conference on Data Mining Workshops, ICDM Workshops 2017, New Orleans, LA, USA, November 18-21, 2017*, pages 33–42, 2017.