

# Computational topology: Image classification using Vietoris-Rips complex

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## Contents

<b>Project description</b>	<b>3</b>
<b>Obtaining and preprocessing data</b>	<b>3</b>
<b>The classification model</b>	<b>3</b>
Relation to single linkage clustering algorithm . . . . .	4
<b>Testing</b>	<b>5</b>

## Project description

As the title implies, the idea behind the project is to use the Vietoris-Rips complex for image classification.

## Obtaining and preprocessing data

```

5  class Scaler(BaseEstimator, TransformerMixin):
    """ Class used for scaling the dataset x.
        Removes the mean and than scales to values from [-1, 1].
        Implements inverse_transform method.

    Args:
        axis: if 1, standardize samples (rows)
              if 0, standardize features (columns)
    """
10
    def __init__(self, axis=1):
        assert axis in [0,1]
        self.axis = axis

15
    def fit(self, x):
        shape = (len(x), 1) if self.axis == 1 else (1, len(x[0]))
        self.means = np.mean(x, self.axis).reshape(shape)
        self.maxs = np.max(np.abs(x - self.means), self.axis).reshape(shape)

20
    def transform(self, x):
        return np.nan_to_num((x - self.means)/self.maxs)

    def fit_transform(self, x):
        self.fit(x)
25
        return self.transform(x)

    def inverse_transform(self, x):
        return (x*self.maxs) + self.means

```

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## The classification model

**Definition 1** (Vietoris-Rips complex). *Let  $X$  be a set of  $m$ -dimensional points  $X \in \mathbb{R}^m$  and let  $d$  be a metric. Pick a parameter  $r > 0$ . Construct a simplicial complex as follows:*

- Add a 0-simplex for each point in  $X$ .
- For  $x_1, x_2 \in X$  add a 1-simplex between  $x_1, x_2$  if  $d(x_1, x_2) \leq r$ .
- For  $x_1, x_2, x_3 \in X$  add a 2-simplex with vertices  $x_1, x_2, x_3$  if  $d(x_1, x_2), d(x_1, x_3), d(x_2, x_3) \leq r$ .
- ...
- For  $x_1, x_2, \dots, x_m \in X$ , add a  $(m-1)$ -simplex with vertices  $x_1, x_2, \dots, x_m$  if  $d(x_i, x_j) \leq r$  for  $0 \leq i, j \leq m$ ; that is, if all the points are within a distance of  $r$  from each other.

The simplicial complex is called the Vietoris-Rips complex and is denoted  $VR_r(X)$ .

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## Relation to single linkage clustering algorithm

Our intuition tells us, that the model we build using the Vietoris-Rips complex to classify the images, produces the same results as the well known single linkage clustering algorithm. In this section we aim to prove or at least give a strong intuition that this is indeed the case.

**Definition 2.** We say that disjoint subsets  $A_1 \dots A_k$  of vertices  $V$  in graph  $G(V, E)$  are  $k$  connected components of the graph  $G$  if the following is true:

1. The vertices inside  $A_i$  are connected i.e. there exists a path between arbitrary two vertices  $a, b \in A_i$ , for every  $i \in 1 \dots k$ .
2. The sets of vertices  $A_1, \dots, A_k$  are disconnected i.e. there isn't an edges  $e(a, b)$  between a pair of two points  $(a, b)$  such that  $a \in A_i, b \in A_j, i \neq j$ .

Both algorithms take a set  $X$  of  $n$  samples with  $m$  features as input. We can think of a sample  $x$  in the set  $X$  as a point in the  $m$ -dimensional space  $x \in \mathbb{R}^m$ . The algorithms then constructs a graph with points  $X$  as the vertices ( $V$ ) and edges  $E$ . The  $k$  connected components in the constructed graph correspond to the classes of samples.

**Single linkage algorithm.** The algorithm starts with  $n$  connected components (no edges in the graph). In each step the algorithm chooses the two connected components that are closest to each according to some distance metric  $d$  (in our case the euclidean distance) and joins them into one by adding an edge between their closest two vertices.

**Definition 3.** The distance  $D$  between two connected components  $A$  and  $B$  is defined as the distance of the pair of vertices (one from  $A$  and one from  $B$ ) that are closest to each other. More formally

$$D(A, B) = \min_{a \in A, b \in B} d(a, b).$$

The algorithm stops when there are only  $k$  connected components left.

**Vietoris-Rips classification algorithm.** The algorithm builds a (1-dimensional) Vietoris-Rips complex  $V_r(X)$  with parameter  $r$ . We choose the biggest  $r$  such that the Vietoris-Rips complex  $V_r(X)$  has  $k$  connected components.

To prove that the two algorithms indeed produce the same connected components we will first prove the next claim.

**Claim 1.** *Let  $G_{sl}(V, E_{sl})$  be a graph produced by the single linkage algorithm for finding  $k$  clusters and let  $d_{max}$  denote the distance between vertices in graph  $G_{sl}$  that were connected in the last iteration of the algorithm. Graph  $G_{sl}$  has connected components  $A_1 \dots A_k$ . The graph  $G_{vr}(V, E_{vr})$  induced by the Vietoris-Rips complex  $VR_{d_{max}}(V)$  has the same connected components  $A_1 \dots A_k$ .*

*Proof.* We prove the Claim 1 by induction on the steps in the single linkage algorithm. We start with a set of vertices  $V$ . Let  $j$  denote the step (iteration) of the algorithm,  $e_j$  the edge added in  $j$ -th step and  $d_j$  its length. We claim that at each  $j$  the graph  $G_{sl}^j$  constructed by the algorithm up to that point, has the exact same connected components as  $G_{vr}^j$ , that is the graph induced by the Vietoris-Rips complex  $VR_{d_j}(V)$ .

**Base case.** For  $j = 0$  this is obvious, since this is the initial state of the algorithm. Both graphs  $G_{sl}^0$  and  $G_{vr}^0$  consist only of vertices  $V$ . For  $j = 1$  the algorithm adds the smallest edge  $e_1$  out of all possible candidates and builds a graph  $G_{sl}^1$ . Edge  $e_1$  has length  $d_1$ . It is obvious that  $VR_{d_1}(V)$  will induce a graph  $G_{vr}^1$  that will also only contain edge  $e_1$ , since no other pairwise distance between vertices  $V$  is smaller.

**Induction step.** Here we show that if for some  $j$  our claim holds, it will also hold after another iteration of the algorithm i.e. for  $j + 1$ . In  $(j + 1)$ -th iteration, the algorithm finds the edge  $e_{j+1}$  with length  $d_{j+1}$  and adds it to the graph. By the definition of the algorithm  $e_{j+1}$  is the smallest such edge that connects (joins) two separate connected components. This means that every other edge  $e'$  with length  $d' < d_{j+1}$  would not join connected components, but would instead just connect some vertices, that are both already in the same connected component. From the definition of the Vietoris-Rips complex we can see that in the graph  $G_{vr}^{j+1}$  there will only be one new edge that will join two separate connected components, and that will be exactly edge  $e_{j+1}$ . All the other extra edges that will be added in  $G_{vr}^{j+1}$ , but do not appear in  $G_{sl}^{j+1}$  will only connect vertices in the already existing connected components of the graph  $G_{vr}^j$ . Since by our induction hypothesis graphs  $G_{sl}^j$  and  $G_{vr}^j$  had the same connected components and we joined two of the same connected components in both graphs this means that the graphs  $G_{sl}^{j+1}$  and  $G_{vr}^{j+1}$  also have the same connected components.

We have proven that the graph  $G_{sl}^j$  constructed in  $j$ -th iteration of the single linkage algorithm indeed contains the same connected components as the graph  $G_{vr}^j$  induced by  $VR_{d_j}(V)$  for an arbitrary  $j$ . This also proves Claim 1.  $\square$

Using Claim 1 we see that the connected components in  $G_{vr}$  and  $G_{sl}$  are indeed the same. We need to take into account that the Vietoris-Rips algorithm takes the biggest such  $r$ , so that the graph has  $k$  connected components, so  $r > d_{max}$ . But we can quickly see that the extra edges in the graph induced by  $V_r(V_{sl})$  will not change the connected components. After all we already have  $k$  connected components in  $G_{vr}$ . To join any two together would mean a violation of a fundamental rule of the algorithm.

## Testing

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## References

- [1] Leslie Lamport, *L<sup>A</sup>T<sub>E</sub>X: a document preparation system*, Addison Wesley, Massachusetts, 2nd edition, 1994.