Computational topology: Image classification using Vietoris-Rips complex

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Project description

As the title implies, the idea behind the project is to use the Vietoris-Rips (in future abreviated VR-cx) complex for image classification. We took pictures of three generic objects and preprocessed them so we obtained vector representations of pictures. The vector representations of images can then be looked upon as points in some n-dimensional space $\mathbb{R}^n$. Over this points we build the VR-cx for two different parameters. We use the complexes to build a classification model for the images and classify them. We also perform several interesting tests on the generated VR-cx.

Obtaining and preprocessing data

TODO: Show the images

For our dataset we used grayscale photographs of 3 different objects: a paper cup, crumpled up paper and a pen. Each of the objects was photographed 10 times from slightly different angles and under different illumination. The sizes of the images were 1080 pixels in width and 810 pixels in height.

We can think of images as matrices of size $(n \times m)$ where each entry represents the intensity of the corresponding pixel (meaning in our case we had 30 matrices of size 1080×810). With images in grayscale color space, each of the values has an integer value between 0 (black) and 255 (white). In order to then prepare the dataset for evaluation with our classification model, we flattened each matrix into one long vector of size nm (first row of the matrix being first n elements, second row the next n and so on m times). We then stacked all individual vectors vertically to form a large matrix with 30 rows, one for each individual image, and nm columns, one for each individual pixel.

With this we are left with a very large matrix, and in order to reduce processing time and decrease amount of noise, we apply principal component analysis, reducing number of columns from $n \times m$ to just a few

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 $x_1, x_2, ..., x_m \in X$, add a $(m-1)$-simplex with vertices $x_1, x_2, ..., x_m$ 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 $VR_r(X)$.

Definition 2. *We say that disjoint subsets $A_1 ... A_k$ 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 $i \in 1...k$.*
2. *The sets of vertices $A_1, ..., A_k$ are disconnected i.e. there isn't an edges $e(a, b)$ between a pair of two points (a, b) such that $a \in A_i, b \in A_j, i \neq j$.*

The classification model continued on next page...

Given the input of n m-dimensional points $X \in \mathbb{R}^m$ and a metric d (in our case the eulidian distance) we build a VR-cx for parameter $r = r_2$, where r_2 is the biggest r such that the VR-cx has three connected components. We find the parameter r_2 using a binary search on a set of all possible values of r. We then perform the classification, simply by saying that all the objects in some connected component belong to the same class. Seeing as we have three connected components in our VR-cx we will get three distinct classes.

It does not take much thought to see, that our classification model will produce the exact same results if we only use simplices of dimension 1, as it would, if we use all the simplices up to dimension h, where h is an arbitrary number in the range $h \in 1...m$. This follows from Definition 1.

Relation to single linkage clustering algorithm

Our intuition tells us, that the model we build using the VR-cx 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.
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 algortihms then constructs a graph with points X as the vertices (V) and edges E. The k connected components in the constructed graph corespond to the classes of samples.

Single linkage algorithm. The algorithm starts with n connected components (no edges in the graph). n 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 $A_1...A_k$. The graph $G_{vr}(V, E_{vr})$ induced by the Vietoris-Rips complex $VR_{d_{max}}(V)$ has the same connected components $A_1...A_k$.*

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^j_{sl} constructed by the algorithm up to that point, has the exact same conected components as G^j_{vr}, 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^0_{sl} and G^0_{vr} 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^1_{sl}. Edge e_1 has length d_1. It is obvious that $VR_{d_1}(V)$ will induce a graph G^1_{vr} 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 algortihm finds the edge e_{j+1} with length d_{j+1} and adds it to the graph. By the definition of the algortihm e_{j+1} is the smallest such edge that connects (joins) two seperate 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 two vertices, that are both allready in the same connected component. From the definition of the Vietoris-Rips complex we can see that in the graph G^{j+1}_{vr} there will only be one new edge that will join two seperate connected components, and that will be exactly edge e_{j+1}. All the other extra edges that will be added in G^{j+1}_{vr}, but do not appear in G^{j+1}_{sl} have length less than d_{j+1} and will therefore only connect vertices inside of allready existing connected components of the graph G^j_{vr}. Since by our induction hypothesis graphs G^j_{sl} and G^j_{vr} had the same connected components and we joined two of the same connected components in both graphs, this means that the graphs G^{j+1}_{sl} and G^{j+1}_{vr} also have the same connected components.

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

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 Vietrois-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 allready have k connected components in G_{vr}. To join any two together would mean a violation of a fundemental rule of the algorithm.

Computational complexity

Let us now consider the computational complexity of our model. Since we are only interested in Vietoris-Rips complexes VR_r with simplices of dimension 1, the simplest approach to construct such complex requires us to check the distance between every pair of vertices $(x_1, x_2) \in X \times X$, adding such pair to the final complex if the distance $d(x_1, x_2) \leq r$. In worst case the algorithm would have to return all distinct pairs of vertices, meaning construction of $VR_r(X)$ requires $O(n^2)$ time and consumes $O(n^2)$ space, where n is the number of vertices in X.

The problem is that we don't know the appropriate value for the parameter r. Recall that we are interested in finding biggest r, such that the Vietoris-Rips complex VR_r has as many connected components as there are distinct classes of images. Let r_{max} denote the largest distance between two vertices from X. Note that r we are looking for will always be bounded on the interval $[0, r_{max}]$, and it will furthermore be exactly one of the distances between some pair of vertices. Thus we only have n^2 different possible values of r to check, and if we sort them by size and use binary search to find the right one, we can do it in $O(n \log n)$ time and $O(n^2)$ space. To count the number of connected components obtained with each of different VR complexes, we can use a `union-find` algorithm, which roughly adds a $O(n^2)$ time to each run.

With this the final time complexity of our approach is $O((n^2 + n^2) \log n^2) = O(n^2 \log n)$ using $O(n^2)$ space.

TODO: Double check the time complexity of union-find

Contrast this with the computational complexity of single-linkage clustering, which with a clever implementation can in optimal case produce solution in $O(n^2)$ time and $O(n)$ space [1].

Results

TODO: Explain we get same results as with S-L clustering, and with that the same problems as S-L clustering.
TODO: Present MDS graph of our dataset after applying preprocessing, and emphasize different classes/recognized clusters.
TODO: Explain that simplices of larger dimension are just about useless
TODO: Explain what datasets our solution actually works with (e.g. determining position of objects on image)
TODO: Extra tests: images from midpoints of edges, barycenters of simplices, ...

Summary

TODO: Brief summary
TODO: Further work (if there even is any), what we didn't explore.

References

[1] John C Gower and GJS Ross. Minimum spanning trees and single linkage cluster analysis. *Applied statistics*, pages 54–64, 1969.