Graph Similarity Using PageRank and Persistent Homology

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ABSTRACT

The PageRank of a graph is a scalar function defined on the node set of the graph which encodes nodes centrality information of the graph. In this work, we utilize the PageRank function on the lower-star filtration of the graph as input to persistent homology to study the problem of graph similarity. By representing each graph as a persistence diagram, we can then compare outputs using the bottleneck distance. We show the effectiveness of our method by utilizing it on two shape mesh datasets.

1 INTRODUCTION AND LITERATURE REVIEW

The problem of studying similarity between graphs has attracted much attention recently in the pattern recognition and machine learning domains. One of the main challenges is to construct an effective similarity measure between graphs that takes into account the complexity of the underlying structure while still being computed efficiently.

In this work, we utilize the PageRank vector [3] in conjunction with a tool available in persistent homology [4] to define a graph descriptor. More specifically, we view the PageRank as a continuous scalar function [14] defined on the vertices of the complex $K$ in any number of dimensions and on multiple scales, placing the concept of shape, as applied to data analysis, on a solid mathematical foundation. On the other hand, the PageRank function of a graph stores information regarding the centrality information of the underlying nodes.

Persistent homology provides a robust set of tools for the theoretical and practical capacity to understand the shape of data [4] in any number of dimensions and on multiple scales, placing the concept of shape, as applied to data analysis, on a solid mathematical foundation. On the other hand, the PageRank function of a graph stores information regarding the centrality information of the underlying nodes.

The PageRank vector has been studied extensively [9]. The PageRank vector has found many applications, including graph partition [1], image search [11], and citation analysis [12], among others.

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2 BACKGROUND

In this section, we give a brief review of persistent homology and the PageRank vector. While the work here is concerned with graphs, we choose here to introduce persistent homology for simplicial complexes since our work can be generalized easily to more general domains. We assume the reader is familiar with the basics of simplicial homology.

2.1 Persistent Homology

Let $K$ be a simplicial complex. We will denote the vertices of $K$ by $V(K)$. Let $S$ be an ordered sequence $\sigma_1, \ldots, \sigma_n$ of all simplicies in $K$, such that for simplex $\sigma \in K$ every face of $\sigma$ appears before $\sigma$ in $S$. Then $S$ induces a nested sequence of subcomplexes called a filtration: $\phi = \emptyset_0 \subset \emptyset_1 \subset \ldots \subset \emptyset_n = K$. A $d$-homology class $\alpha \in H_d(K_i)$ is said to be born at the time $i$ if it appears for the first time as a homology class in $H_d(K_i)$. A class $\alpha$ dies at time $j$ if it is trivial $H_d(K_j)$ but not trivial in $H_d(K_{j-1})$. The persistence of $\alpha$ is defined to be $j - i$. Persistent homology captures the birth and death events in a given filtration and summarizes them in a multi-set structure called the persistence diagram $P^d(\phi)$. Specifically, the persistence diagram of the filtration $\phi$ is a collection of pairs $(i, j)$ in the plane where each $(i, j)$ indicates a $d$-homology class that is created at time $i$ in the filtration $\phi$ and killed entering time $j$.

Persistent homology can be defined given any filtration. For the purposes of this work, the input is a piecewise linear function $f : [K] \rightarrow \mathbb{R}$ defined on the vertices of complex $K$. Furthermore, we assume the function $f$ has different values on different nodes of $K$. Any such a function induces the lower-star filtration as follows.

Let $V = v_1, \ldots, v_n$ be the set of vertices of $K$ sorted in non-decreasing order of their $f$-values, and let $K_i := \{ \sigma \in K | \max_{v \in \sigma} f(v) \leq f(v_i) \}$. The lower-star filtration is defined as:

$$\mathcal{F}_f(K) : \phi = \emptyset_0 \subset \emptyset_1 \subset \ldots \subset \emptyset_n = K. \quad (1)$$

The lower-star filtration reflects the topology of the function $f$ in the sense that the persistence homology induced by the filtration [1] is identical to the persistent homology of the sublevel sets of the function $f$. We denote by $P_f(K)$ to the persistence diagram induced by the lower-star filtration $\mathcal{F}_f(K)$. Furthermore, we will denote by $P^K_f$ to the $k^{th}$ persistence diagram induced by the lower-star filtration $\mathcal{F}_f(K)$. In this work, we will only consider the 0-dimensional persistence diagram.

Finally, given two persistence diagrams, we measure the distance between them using the bottleneck distance. Namely, given two persistence diagrams $X$ and $Y$, we let $\eta$ be a bijection between points in the diagrams. The bottleneck distance is defined as:

$$W_\infty(X,Y) = \inf_{\eta: X \rightarrow Y} \sup_{x \in X} ||x - \eta(x)||_{\infty}.$$ 

For technical reasons we usually add to the persistence diagram infinitely many points on the diagonal and each one of these points with is counted with infinite multiplicity.

2.2 PageRank

This work utilizes the lower-star filtration induced by the PageRank function [3]; more specifically, we consider a version applicable to undirected graphs [7]. The PageRank function $R : V \rightarrow \mathbb{R}$ is defined
for every vertex $v \in V$ by

$$R(v) = \frac{(1 - d)}{|V|} + d \sum_{u \in N(v)} \frac{R(u)}{|N(u)|},$$

(2)

where $N(v)$ is the set of neighbors of $v$; $0 < d < 1$ is the damping factor, typically set at 0.85. Equation (2) can be solved efficiently by the power method [10].

A high PageRank score at $v$ typically means that $v$ is connected to many nodes, which also have high PageRank scores. For our purpose, it is important to notice that the PageRank is a continuous function [14]. For example, Figure 1 illustrates the continuity of the function on the nodes of the graph on a random geometric graph.

3 Results

To validate the method proposed, we run some experiments on two publicly available datasets. We use mesh datasets to make a visual comparison between similar graphs easier.

In both experiments, we compute the persistence diagram of each mesh obtained from the lower-star filtration induced by the PageRank vector defined on that mesh. The pairwise bottleneck distance is then computed between every pair of persistence diagrams. Finally, the resulting discrete metric space is visualized using a 2d t-SNE projection.

The first dataset [12] consists of 60 meshes that are divided into 6 categories: cat, elephant, face, head, horse, and lion. Each category contains ten triangulated meshes. The result is reported in Figure 2.

The second dataset [16] consists of 30 meshes that are divided into 2 categories: kid A and kid B. The result is reported in Figure 3.

Notice how the meshes within the same category are clustered together. We also notice that meshes with similar topology tend to be closer than those with different topology. Observe for instance the clusters of horses and cats.

4 Conclusion

In this work, we have illustrated how the PageRank can be utilized in conjunction with persistent homology to study graph similarity and demonstrated our results on small datasets. In future work, we are planning to conduct a more thorough analysis with larger datasets. Moreover, the PageRank is typically defined on directed graphs. This feature of the PageRank vector can be utilized to induce a filtration that is sensitive to the directionality of the edges a directed graph. We are planning to investigate this direction in the future.

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