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Research Project Report on the Topic:

Geometrical and Topological Deep Learning

(interim, the first stage)

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Abstract

The primary objective of this research is to seamlessly integrate topological data analysis methodologies into deep learning pipelines. Leveraging topological features facilitates the extraction of intricate shape-based information, thereby proving pivotal in various tasks, such as fingerprint classification, and beyond.

Абстракт

Основная цель данной работы заключается в интеграции методов топологического анализа данных в пайплайны глубокого обучения. Использование топологических особенностей облегчает извлечение сложной формообразующей информации, что является ключевым в различных задачах, таких как классификация отпечатков пальцев и других.

Keywords

Topology, DL, Classification, Shapes, Images, Feature extracting

1 Introduction

1.1 Subject area

In this study, we aim to integrate the methodologies of topological data analysis (TDA) and deep learning (DL). TDA offers insights into the shape of multidimensional data, making it particularly suitable for incorporation into deep learning pipelines. One significant advantage of this approach is its capability to extract features from diverse domains, such as images, graphs, and 3D meshes. However, our focus will be specifically on images. Key topological processors include persistent homology transform and Euler characteristic transform. Following data processing, the resultant output can be conceptualized as a multi-set of embeddings. Subsequently, deep learning pipelines can be applied to address the original task using these multi-set embeddings.

1.2 Problem statement

It has been demonstrated that the Persistent Homology Transform (PHT) is injective. However, after following discretization, this advantage is lost. Therefore, our research will investigate how increasing the number of utilized directions impacts prediction quality. Additionally, PHT is using height fitraion, but we will try other, including convolutional filters, where the convolutional layer processes the image and the brightness of the grayscale image is considered as the moment of component birth.

The output of the Persistent Homology Transform yields k multi-sets, which can be represented as a multi-set of 3D vectors. Furthermore, we add additional dimensions after applying multiple filters to incorporate filter parameters, resulting in a multi-set of 4D+ vectors after applying PHT.

Numerous Deep Learning models are capable of classifying sets. In this study, we will examine Deep Sets [7] and Transformer-based [6] models.

At this moment, the pipeline involves statically filtering images using different directions and calculating Persistence Diagrams for each direction. Subsequently, a DL model (e.g., Transformers or Deep Sets) is trained on these sets.

Once this static pipeline is implemented, the filters can be trained. Since both the PHT and Euler Characteristic Transform (ECT) are differentiable, we can train not only the DL model but also the directions for height filters or convolutional layers for convolutional filters.

Currently there was researches with several amount of static filters [4] and with one trainable [1], in this work we will research how increasing of filters change quality of pipeline while using it trainable.

2 Related Work

2.1 Simplicial Complex and Homology of Simplicial Complex

The base object that we will work with is Simplicial Complex. Formally, K is a **simplicial complex** on the finite set of vertices M, if $K \subset 2^M$ and (i) $T \subset P \wedge P \in K \Rightarrow T \in K$ and (ii) $\emptyset \in K$. In practice, we can consider simplicial complex as combination of tetraeders (0-dimensional is point, then line, triangle etc.). For $I \in K$, $\dim I := |I| - 1$. And $\dim K = \max_{I \in K} \dim I$
Given simplicial complex K, **simplicial k-chain** of K is a linear combination of k-simplicies (I elements of K such that $\dim I = k$) in K. We will consider chains only over $\mathbb{Z}_2$ (though here can be any field). The k-chains is a vector space, denote it as $C_k(K, \mathbb{Z}_2)$. Function $\delta_k : C_k(K, \mathbb{Z}_2) \to C_{k-1}(K, \mathbb{Z}_2)$

$$\delta_k((v_1, v_2, \cdots, v_k)) = \sum_{i=0}^{k} (-1)^i (v_1, \cdots, \hat{v_j}, \cdots, v_k)$$

is called called differential. For $\mathbb{Z}_2$ it simplifies to

$$\delta_k((v_1, v_2, \cdots, v_k)) = \sum_{i=0}^{k} (v_1, \cdots, \hat{v_j}, \cdots, v_k)$$

Denote $Z_k(K) := \mathrm{Ker}\delta_k$ is the vector subspace of k-dimensional "cycles". $B_k(K) := \mathrm{Im}\delta_{k+1}$ is the vector subspace of k-dimensional "cycles" that are borders of some bigger component. Check shows, that $\delta_{k-1} \circ \delta_k = 0 \Rightarrow B_k(K) \subset Z_k(K) \subset C_k(K, \mathbb{Z}_2)$, so we can denote k-th homology of K: $H_k(K) := Z_k(K)/B_k(K)$. In practice $H_k(K)$ is factor-space of k dimensional holes.

2.2 Filtration

Filtration is a $K = \{K_r : r \in \mathbb{R}\}$, such that $\forall_{\alpha \in \mathbb{R}} \quad K_\alpha$ is a simplicial complex and $\forall_{\alpha < \beta} K_\alpha \subset K_\beta$. Hence $K_\alpha \subset K_\beta$, we can denote $\iota : K_\alpha \to K_\beta$ - inclusion map which induces

$$\iota : B_k(K_\alpha) \to B_k(K_\beta)$$
$$\iota : Z_k(K_\alpha) \to Z_k(K_\beta)$$
$$\iota_k^{a \to b} : H_k(K_\alpha) \to H_k(K_\beta)$$

It is worth mentioning that $H_k(K_\alpha)$ may not includes in $H_k(K_\beta)$. Denote $H_k(\alpha, \beta) := Z_k(K_\alpha)/(Z_k(K_\alpha) \cap B_k(K_\beta))$ - k-th persistence homology, it shows which classes in $H_k(K_\alpha)$ persist to $H_k(K_\beta)$.

The class $h \in H_k(K_i)$ is born at the moment a if $\exists a' < a$ such that $h \in \mathrm{coker}(\iota_k^{a' \to a})$ and die at moment b if $\exists a' < a < b' < b$ such that $\iota_k^{a \to b}(h) \in \mathrm{Im}\iota_k^{a \to b} \wedge \iota_k^{a \to b'}(h) \notin \mathrm{Im}\iota_k^{a \to b'}$. If the class never dies we call it essential. Given filtration, k-th persistence diagram of the filtration is a multi-set of points in $\{(a,b) : a \in \{-\infty\} \cup \mathbb{R} \wedge b \in \mathbb{R} \cup \{+\infty\}\}$, such that for $\forall a, b \in \mathbb{R} \quad \dim H_k(a,b)$ is equal to number of points in $[-\infty; a] \times [b; +\infty]$. Informally speaking, first coordinate show the birth moment and the second one the death moment.

2.3 Persistence Homology Transform

For $M \subset R^d$ that can be rewritten as simplicial complex, height filtration over direction $v \in S^{d-1}$ for height r is $\{m \subset M : \forall_{x \in m}\ x \cdot v \leq r\}$. For each simplex, it is ensured that it is taken only after all its components are taken, and the empty set is always included. Therefore, for every r, it forms a simplicial complex. Once an element is included, it cannot be removed by increasing the height, ensuring the correctness of the filtration. The k-th diagram of this filtration is denoted as $X_k(M, v)$.

Now we are ready to define Persistence Homology Transform, given the simplicial complex K

$$PHT(K) : \mathbb{S}^{d-1} \to D^d, \text{ where D is a persistence diagram}$$
$$v \mapsto (X_0(K, v), \cdots, X_{d-1}(K, v))$$

In [5] is showed that PHT is a injective for 2 and 3 dimensional objects, it means that $K \neq K' \Rightarrow PHT(K) \neq PHT(K')$

2.4 Euler Characteristic Transform

In [2] is described another topological characteristic of object is ECT. Given simplicial complex K, Euler Characteristic $X(K) := \sum_{k=0}^{\dim K} (-1)^k c_k$, where c_k is count of k-simplicies in K We can look at height filtration K over given direction v and compute EC for every moment, it is called Euler Characteristic Curve

$$ECC(K, v) : \mathbb{R} \to \mathbb{Z}$$

$$v \mapsto X(K_v)$$

Euler Characteristic Transform is a function that map direction to ECC with selected direction

$$ECT(K) : \mathbb{S}^{d-1} \to \mathbb{Z}^{\mathbb{R}}$$

$$v \mapsto ECC(K, v)$$

There are approaches how to differentiable compute ECT [3] and PHT [1]

3 Proposed plan

Firstly, we will use MNIST data to test pipeline.

(i) Write directional and convolutional filters to filter image statically.

(ii) Use algorithms, which build simplicial complex (in images it rather cubical complex) out of image and then run PHT over it.

(iii) On produced features train two DL models.

(iv) Compare different DL models and filters, also check the theory that increasing of filters increase total quality of pipeline.

(v) Rewrite calculating of transform, so it computes differentiable.

(vi) Test this approach with previous ones.

Then use this pipeline for real data, where the shape of objects is critical (e.g. fingerprint)

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