Design of Activation Function Using Topological Framework in Deep Neural Networks

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Abstract

Success of deep neural networks in diverse tasks across domains of computer vision, speech recognition and natural language processing, has necessitated understanding the dynamics of training process and also working of trained models. For classification tasks, one of the main requirements of the layer transfer function is to transform data such that only information required for classification is preserved and all other information is discarded. Further the data should be transformed such that samples belonging to a single class should come closer in the transformed space which will help in drawing a clear decision boundary across classes. This enforces the need for topological simplification of the point cloud data set formed using samples from each class. We analyze the topological transformation of the space of training samples as it gets transformed by each successive layer during training, by changing the activation function. The impact of changing activation function on the convergence during training is reported for the task of binary classification. A novel activation function aimed at faster convergence for classification tasks is proposed. Here, Betti numbers are used to quantify topological complexity of data. Results of experiments on popular synthetic binary classification datasets with large Betti numbers (¿150) using MLPs are reported. Results show that the proposed activation function results in faster convergence requiring fewer epochs by a factor of 1.5 to 2, since Betti numbers reduce faster across layers with the proposed activation function. The proposed methodology was verified on benchmark image datasets: fashion MNIST, CIFAR-10 and cat-vs-dog images, using CNNs.

Keywords: Training Convergence; Activation function; Topological Data Analysis; Betti Numbers

1. Introduction

Deep neural networks have become the default choice for solving many complex tasks across several domains Krizhevsky et al. (2012); Redmon et al. (2016); Chen et al. (2017); Ronneberger et al. (2015). This is mainly because: 1) many tasks in domains such as computer vision, speech analysis and NLP, involve high dimensional datasets for which a complex model is required 2)for tasks performed by humans, which they acquired by birth, it is not well now how humans perform the task and what features they use. Deep neural networks, originally inspired by biological neural networks in cat's, is computing the features in a hierarchical fashion.

However, choosing the right architecture (like the selection of hyper parameters activation function, number of layers and number of units per layer) for a specific task is mostly based on 1) trial and error or 2) previous empirical results of tasks of similar complexity. The transfer function of each layer and the entire neural network is just treated as a complex, unknown and nonlinear function parameterized by weights and biases.

In this study, we investigate some of the desired characteristics a neural network architecture should have for solving a classification task. We derive our results based on the topology of the space of training data and how this topology changes as data is transformed by each layer.

Topology is a field of mathematics that studies the shape of objects and associated invariances like connectedness, number of holes of different dimensions etc. Weibel (1999). It is observed that many real datasets when viewed as point cloud dataset in a high dimensional space follow certain topology. For example the study in Carlsson (2009) shows that the image patches obtained from natural images follow the topology of a Klein bottle Stillwell (1993).

Topological data analysisCarlsson (2009); Chazal and Michel (2021) uses topological tools, like persistent homology Edelsbrunner et al. (2008), for analyzing point cloud dataset in order to identify and characterize underlying structures in a dataset.

In their recent study, Naitzat et al. (2020) uses Betti numbers Weibel (1999) to quantify topological complexity. In their study, they make the following important observations:

1. Topological changes to data across layers of a network remain robust under different instances of training.

2. Compared to smooth activation functions like sigmoid and tanh, non-homeomorphic activation functions like ReLU helps in changing the topology of data faster.

Our work is motivated by Naitzat et al. (2020) where the transfer function of each layer is looked at, based on how the layer changes the topology of the data. Most real world datasets have non-trivial complex topology, and in order to perform classification each layer of the neural network transforms the entire space of data to a simpler topology. This leads us to the conclusion that in order to achieve classification, each layer of the neural networks should be able to change the topology of data and hence a non-homeomorphic transformation is needed at each layer. This is achieved by activation functions with discontinuity like ReLU. However, ReLU has only a single point of discontinuity. We hypothesize that an activation function with multiple discontinuities can result in faster training (less number of epochs).

We followed the approach in Naitzat et al. (2020) and used Betti numbers to quantify topological complexity of the point cloud dataset.

In addition to the above insight, that the activation function should be non-homeomorphic, we also hypothesize that a non-bijective (many-to-one) transfer function can help to bring samples from the same class closer in the transformed space.

Based on the above two hypotheses, we introduce a new parameterized family of activation functions with multiple **many-to-one** regions and **multiple** discontinuities.

Results of our experiments show that, with the proposed activation function, the network converges faster as compared to commonly used activation functions like ReLU. It is also observed that the Betti numbers, computed using persistent homology Naitzat et al. (2020), reduce faster with the proposed activation function.

The main contribution of this paper is to provide new guidelines for designing activation functions for supervised classification tasks. We illustrate the guideline by proposing a new family of activation functions.

2. Related Work

2.1. Topological Data Analysis

Topological Data Analysis, Chazal and Michel (2021); Smith et al. (2021), is an approach for characterizing a dataset topologically using persistent homology Edelsbrunner et al. (2008). In 2008, Carlsson et al. (2008) conducted a qualitative study on 3 × 3 image patches taken from natural images and results of their study showed that the manifold of high contrast natural image patches is homeomorphic to that of Klein bottle.

With the use of deep neural networks for implementing machine learning tasks, like image classification, object detection and segmentation, when the data dimensionality and sample size is huge the challenge of determining the right architecture for a given dataset became a hot area of research interest. Geometric deep learning, refers to the application of deep neural networks for huge datasets with complex manifold space, not necessarily Euclidean. The Study in Bronstein et al. (2017) provides a survey of geometric deep learning. Saucan et al. (2007) introduces a new sampling technique for sampling manifolds in high dimensional spaces.

2.2. Activation function and Training convergence

Since the introduction of ReLU activation function in Krizhevsky et al. (2012) as an alternative for sigmoid and tanh functions, many different variations of it like Leaky ReLU, PReLU, ELU, Threshold ReLU etc. has been tried out for faster training convergence and better classification accuracy. Bounded ReLU activation function was suggested by Liew et al. (2016) for better generalizability and training convergence. In 2017, Ramachandran et al. (2017) used automatic search techniques to look for new activation functions. They evaluated their best reported activation function $f(x) = x.sigmoid(\beta x)$ on Imagenet using existing best performing architecture and reported 0.9% improvement on classification accuracy.

Our work differs from all of these as we are using topological simplification as a basis for deriving new activation. We propose that an activation function with many-to-one regions can reduce topological complexity of data and hence can result in faster training convergence.

3. Proposed Method

3.1. Problem Formulation

We restrict our analysis to the task of supervised classification of 1) 3-dimensional synthetic datasets using Multi Layer Perceptron(MLP) and 2) images using Convolutional Neural Network. The classification task can be viewed as a many-to-one mapping, $f : R^d \mapsto$

$\{c_1, c_2, \ldots c_k\}$. The set of all samples forms a point cloud dataset on d-dimensional space ($d = H \times W$ in the case of an image of height H and width W). As identified in Naitzat et al. (2020), for classification task a non-homeomorphic transfer function is required for each layer as it can change the topology of the point cloud dataset. In order to achieve classification, it is necessary to change the topology from an initial complex topology to a simpler and contractible topology for each class. Another important characteristic of layer transfer function, in a classification network, is that each layer reduces the dimensionality of the input data. This helps the networks to carry forward only the information relevant for classification while discarding all other information.

This study focuses on an important aspect of neural network design – design of an optimum non-linear activation function for supervised classification tasks. See subsection 3.5 for details.

3.2. Dataset

We use two 3-dimensional simulated datasets, nine ring dataset and nine sphere dataset used in Naitzat et al. (2020). The nine ring dataset, as shown in Figure 1a, consists of two classes of data, colored Green and Red, interlocked together. The nine sphere dataset consists of nine Green spheres and 18 Red Spheres enclosing each other as shown in Figure 1b. Both the datasets contain 16000 samples for training and 2000 samples for testing.

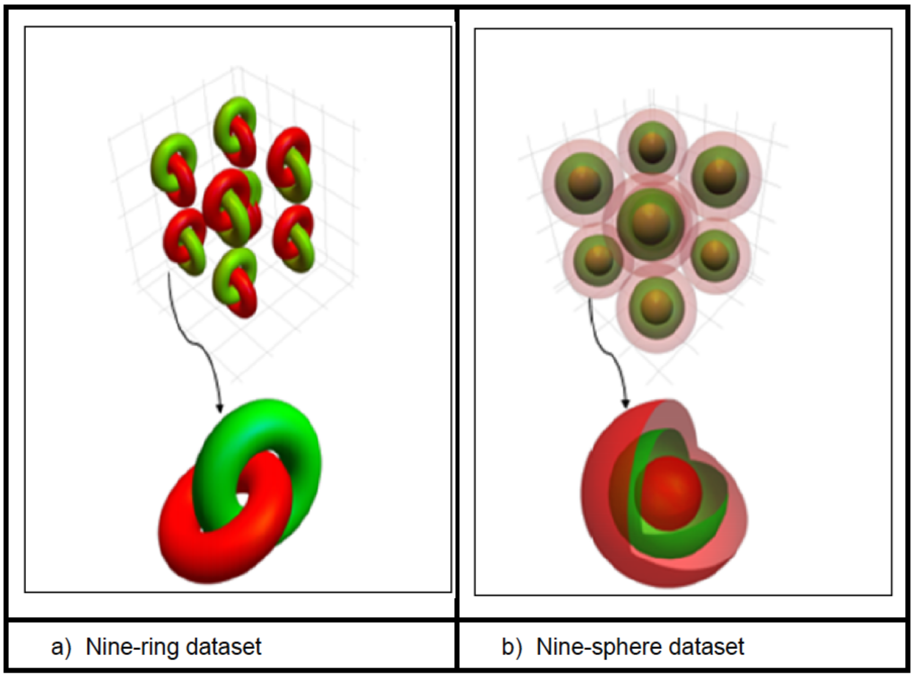


Figure 1: 3-dimensional synthetic datasets with two different classes(Red and Green) used for training MLP.
Source: https://arxiv.org/abs/2004.06093

In addition, we also perform experiments and provide results on the following real datasets:

1. Cat-Dog dataset in Kaggle – The dataset consists of images of size 32 × 32. The dataset is divided into training and testing sets, with 8000 training images and 2000 testing images, each set with an equal number of images of cats and dogs.
2. Fashion MNIST – The dataset consists of 70,000 grayscale images of size 28 × 28 with 10 different categories. The dataset is divided into training and testing sets, with 60,000 training images and 10,000 test images.
3. CIFAR-10 – The dataset consists of 60,000 colour images of size 32 × 32 with 10 different categories. Each category consists of 6000 images. The dataset is divided into training and testing sets, with 50,000 training images and 10,000 test images.

Sample images from each of the above datasets are shown in Figures 2, 3 and 4. The datasets were converted to gray scale and normalized. No other preprocessing was performed.

source:https://www.kaggle.com/c/dogs-vs-cats/

Figure 2: Sample images from Cat-Dog dataset

3.3. Layer Transfer Function

The layer transfer function is composed of an affine transformation and a non-linear activation function. The generic form of the layer transfer function in MLP and CNN is given in Equations 1 and 2 below.

$$X^{l+1} = f(W^T X^l + b) \tag{1}$$

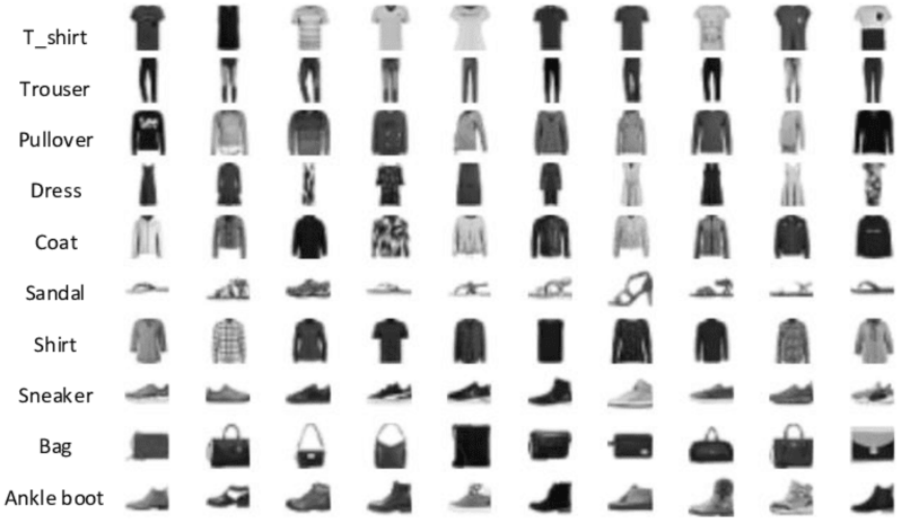


Figure 3: Sample images from each of the 10 categories in Fashion MNIST dataset.

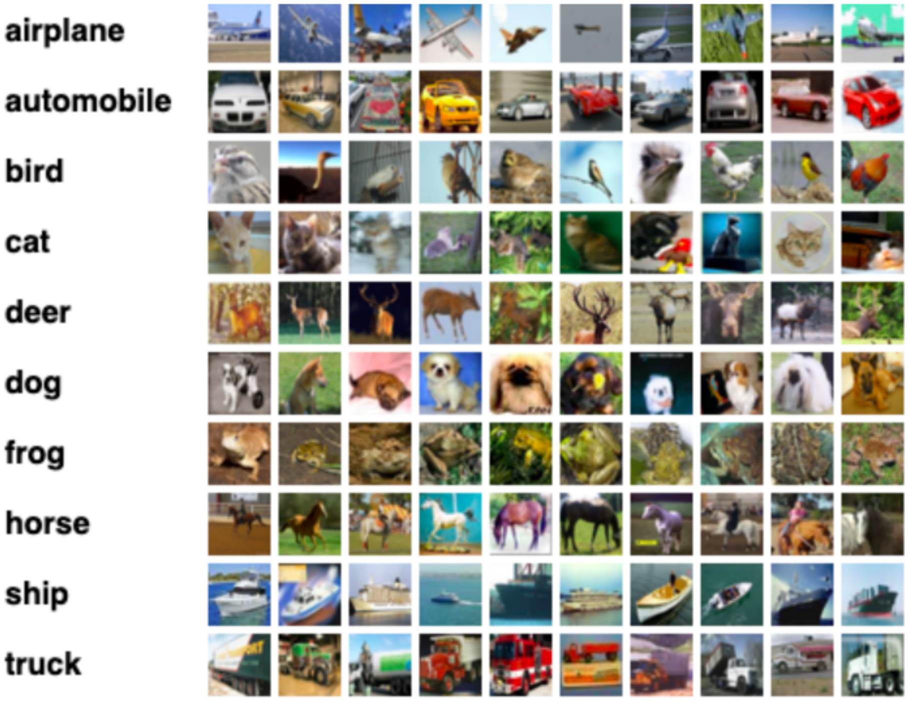


Figure 4: Sample images from CIFAR-10 dataset

where:

$$\begin{aligned} X^{l+1} &= \text{Output of layer } l+1 \\ X^{l} &= \text{Output of layer } l \\ W &= \text{Weight matrix} \\ b &= \text{Bias vector and} \\ f(.) &: \text{Non-linear activation function} \end{aligned}$$

$$x_{ij}^{l+1} = f\Big(\sum_{m,n \in N(i,j)} w_{mn} x_{mn}^{l} + b\Big) \tag{2}$$

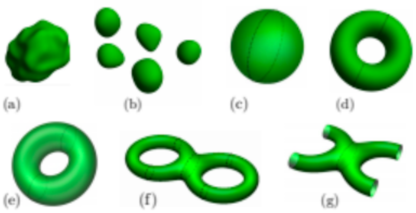
where:

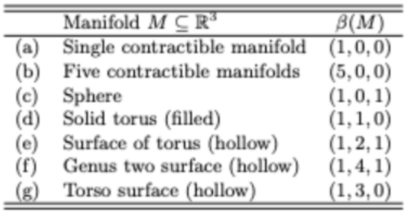
$$\begin{aligned} x_{ij}^{l+1} &= \text{Output value of layer } l+1 \text{ at pixel location } (i,j) \\ N(i,j) &= \text{Set of pixels in a square nieghbourhood centered at pixel } (i,j). \\ w_{mn} &= \text{Convolutional filter weights} \\ b &= \text{Bias} \end{aligned}$$

In the subsections below, we provide the details of desired characteristics for activation function from a topological point of view.

3.4. Significance of Betti numbers on classification

Betti numbers, denoted as $\beta_k(X)$, are used to quantify the topological complexity of a d-dimensional topological space X, where $0 \leq k \leq d-1$. The 0^{th} Betty number, $\beta_0(X)$, is the number of connected components, the first Betti number, $\beta_1(X)$, is the number of one dimensional holes, the second Betti number, $\beta_2(X)$, is the number of two dimensional holes and so on. Figure 5 shows some topological spaces and their corresponding Betti numbers.

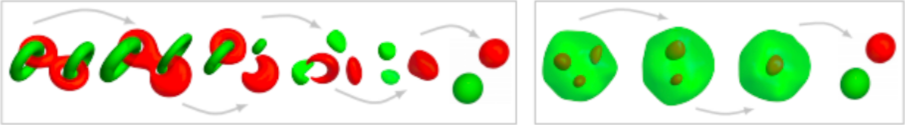




	Manifold $M \subseteq \mathbb{R}^3$	$\beta(M)$
(a)	Single contractible manifold	$(1,0,0)$
(b)	Five contractible manifolds	$(5,0,0)$
(c)	Sphere	$(1,0,1)$
(d)	Solid torus (filled)	$(1,1,0)$
(e)	Surface of torus (hollow)	$(1,2,1)$
(f)	Genus two surface (hollow)	$(1,4,1)$
(g)	Torso surface (hollow)	$(1,3,0)$

Figure 5: Examples of some complex topological spaces and corresponding Betti numbers. Source: https://arxiv.org/abs/2004.06093

For efficient classification, one needs to transform the original point data cloud, X, from a high dimensional space with large Betti numbers to a low dimensional latent representation with $\beta_0(X)$ (number of connected components) equal to the number of classes K and all other Betti numbers to zero. As evident from Figure 6 , this ensures that each connected component corresponds to a single class (either Red or Green) and there are no holes within the connected components. Hence each connected component is contractible to a single point. It is easy to find a decision boundary if there are no holes on the manifold formed by samples from a single class.



Source:https://arxiv.org/pdf/2004.06093.pdf

Figure 6: Simplification of topological space as the data is transformed by successive layers of neural network. The input data (leftmost) has a complex topology with samples from Red and Green classes interlocked together and contains holes. As the data is transformed by successive layers of the classification network, samples from the two classes get disconnected to form multiple connected components. Each connected component has samples from the same class. Transformation by further layers joins different connected components of samples from the same class into one single connected component and removes the holes from each connected component. The final transformed space has two connected components one for each class (right most).

3.5. Design of activation function

It is observed that non-homeomorphic activation functions like ReLU reduce the Betti numbers faster as opposed to traditional activation functions like sigmoid and tanh which are homeomorphic Naitzat et al. (2020). Further, the more the number of discontinuities, the more powerful the activation function will be in terms of reducing the topological complexity. In addition to these findings, we also hypothesize that multiple many-to-one regions in the layer transfer function can reduce the topological complexity of samples within a single class, as it tries to bring more samples together. As shown in Figure 7, we start with a portion of a single half cycle of a sine function, and select a cut-off point $x = \frac{3\pi}{4}$. The selected portion of the sine function is repeated to get the final activation function as shown in the last figure in Figure 7.

The final analytical form of activation function is

$$y = ksin(\frac{3\pi}{4}) + sin(x - \frac{3\pi}{4}) \tag{3}$$

where $k = \left\lfloor \frac{x}{\frac{3\pi}{4}} \right\rfloor$

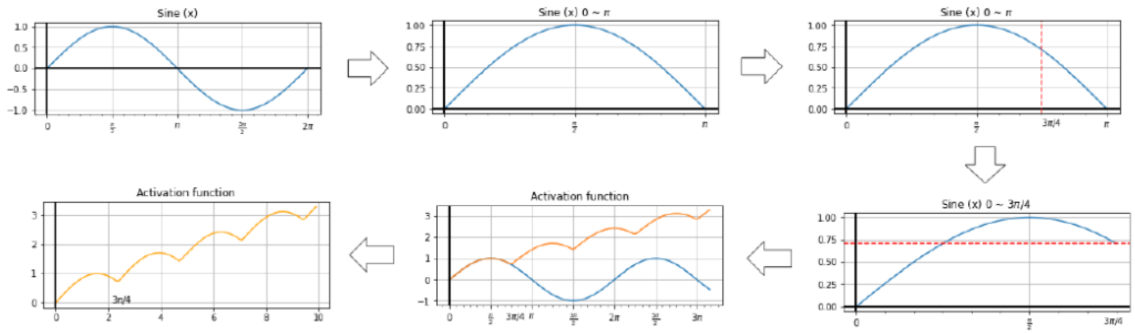


Figure 7: Steps in design of many-to-one activation functions. We start with a single half cycle of a sinusoidal function an decide a cutoff-point $\frac{3\pi}{4}$ and repeat the function in the interval $[0, \frac{3\pi}{4}]$ to get the final activation function.

3.6. Neural Network Architecture

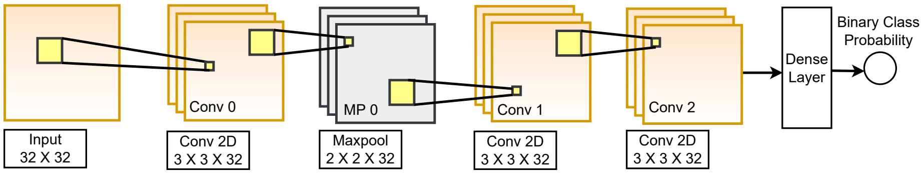
We performed experiments using MLP on nine-sphere and nine-rings datasets. For image datasets, we used Convolutional Neural Networks for running the experiments. The MLP for simulated dataset consists of 9 layers with 25 neurons in each layer. We performed experiments with Leaky ReLU and the proposed activation function. Our empirical results show that the proposed activation function results in faster training convergence compared to Leaky ReLU.

4. Results and Discussion

Figure 8 shows comparison of progression of first Betti numbers (number of connected components) as the data is transformed across layers when Leaky ReLU is is used in all the layers Vs the proposed activation function is used is the final convolutional layer. It is observed, from Figures 8, that with the proposed activation function Betti numbers decrease by a significantly larger amount than Leaky ReLU activation function. Figure 9 shows the comparison of convergence of multi layer perceptron with Leaky ReLU and proposed activation function using nine-sphere and nine-ring datasets. As evident from this figure, the reduction in Betti numbers directly translates to faster training convergence. The new activation functions with multiple many-to-one regions seem to work well on various datasets and help in achieving at-par or better trainability.

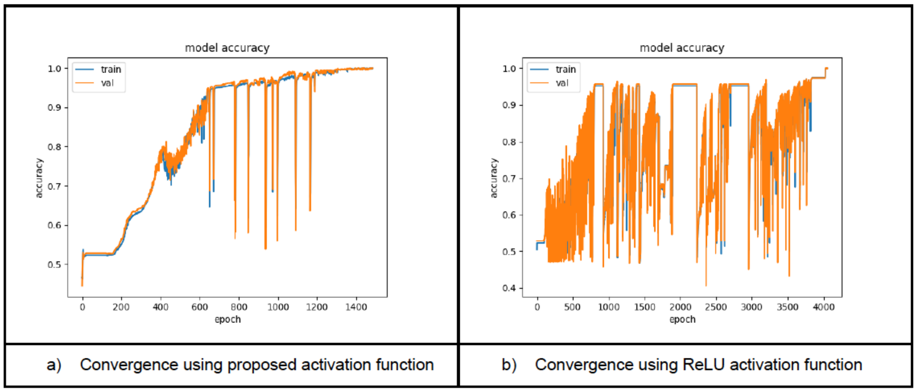
Also, The performance impact becomes more pronounced at larger batch-sizes i.e. with larger batch-sizes the gain tends to reach a factor of 2. On increasing the batch size the training for even simpler datasets takes longer (more epochs) for legacy activation functions. Even though the increase in training epochs is seen for the proposed activation function also, the increase is less pronounced.

We further observed that, in contrast to legacy activation functions like Leaky ReLU, the need to adjust learning rate seems to be little.



Layer	Input	Conv 0	MP 0	Conv 1	Conv 2
Betti Numbers LeakyRelu	68	66	88	56	610
Betti Numbers Proposed Activation	68	65	88	58	**53**

Figure 8: Architecture of CNN for classifying images in CIFAR-10 dataset along with the comparison of progression of first Betti number (Number of connected components) of samples from a single class across the layers using Leaky ReLU and proposed activation function. First row of the table shows Betti numbers using Leaky ReLU. Second row shows the Betti numbers with the proposed activation function added in layer Conv 2. It is observed that Betti number reduce significantly in layer Conv 2.



a) Convergence using proposed activation function

b) Convergence using ReLU activation function

Figure 9: Comparison of training convergence using proposed activation function and Leaky ReLU activation function. It is observed that convergence is faster with the proposed activation function.

5. Conclusion

In this work, we look at topological complexity of data at the output of each layer of deep neural network for binary classification tasks. We propose a new activation function that simplifies the topological complexity of point cloud data (measured using Betti numbers) at each hidden layer which translates to faster training convergence. We evaluate the proposed methods on popular image classification datasets and our results show 1) the proposed activation function results in faster training convergence and 2) removing hidden channels with large Betti numbers does not reduce the test accuracy which indicates that these feature maps are insignificant and can be removed.

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