GraphKAN: Enhancing Feature Extraction with Graph Kolmogorov Arnold Networks

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Abstract

Massive number of applications involve data with underlying relationships embedded in non-Euclidean space. Graph neural networks (GNNs) are utilized to extract features by capturing the dependencies within graphs. Despite groundbreaking performances, we argue that Multi-layer perceptrons (MLPs) and fixed activation functions impede the feature extraction due to information loss. Inspired by Kolmogorov Arnold Networks (KANs), we make the first attempt to GNNs with KANs. We discard MLPs and activation functions, and instead used KANs for feature extraction. Experiments demonstrate the effectiveness of GraphKAN, emphasizing the potential of KANs as a powerful tool. Code is available at `https://github.com/Ryanfzhang/GraphKan`.

1 Introduction

The recent success of neural networks O'shea and Nash [2015], Deng et al. [2009] has greatly stimulated research in the fields of pattern recognition Wang et al. [2017], Stahlberg [2020] and data miningHe et al. [2017]. Especially, in many applications Cui et al. [2019], Fout et al. [2017], data are generated from non-Euclidean domains. Complicated relationships between objects are represented as graphs. For example, in biology, protein can be viewed as graphs Gligorijević et al. [2021], and their structure needs to be identified for protein-protein interaction; in social networks Fan et al. [2019], interactions between peoples indicate similar interests or attributes.

Unfortunately, complexity of graph data has presented significant challenges for traditional deep learning algorithms Zhou et al. [2020]. Nodes in an irregular graph have varying numbers of neighbors. Handing complex patterns of neighbors and extracting feature of each node are troublesome Xu et al. [2018]. Consequently, there has been considerable scholarly interest in harnessing deep learning techniques for the purpose of feature extraction from intricate graph structures.

As an excellent feature extractor for graph, graph neural networks (GNNs) Scarselli et al. [2008] are capable of handing the characteristics of the graph due to the message passing framework Vignac et al. [2020]. Concretely, message passing framework for node representation iteratively (1) **aggregates** information from the neighbors and (2) **extracts** the representations of nodes. Previous studies have made significant efforts in aggregating information, such as GCN Zhang et al. [2019a], GAT Veličković et al. [2017] and so on. Diverse aggregation approaches facilitate the incorporation of

multiple features, including node importance and heterogeneity Zhang et al. [2019b], thereby leading to enhanced efficiency in information passing.

Despite advancements, there are still inherent limitations in the process of extracting representations (Step 2 in message passing framework). In general, the majority of methods utilize Multi-layer Perceptron (MLP) Taud and Mas [2018] for feature extraction. To enhance the nonlinearity capability, an activation function is commonly incorporated between two graph convolutional layer. Regrettably, MLP in the majority of the aforementioned models suffer from poor scaling laws Friedland and Krell [2017]. Specifically, the number of parameters in MLP networks does not scale linearly with the number of layers, leading to a lack of interpretability Barceló et al. [2020]. Moreover, activation function, such as ReLU, limit the representational capacity Yarotsky [2017], potentially preventing it from learning complex features of nodes. To conclude, MLPs+activation function impede the feature extraction in graph-like data.

A recent study introduces Kolmogorov-Arnold Networks (KANs) Liu et al. [2024], a novel neural network architecture designed to potentially replace traditional MLPs. Unlike MLPs, KANs introduce a novel approach by substituting linear weights with spline-based univariate functions along the edges of the network. These functions are specifically structured as learnable activation functions. KANs offer a solution to the limitations of efficiency and interpretability encountered in MLPs in GNNs. Additionally, KANs address the problem of information loss resulting from the use of activation functions.

In this paper, we firstly introduce KANs to feature extraction in graph-like data, dubbed GraphKAN. We replace all MLPs and activation function with KANs in GNNs. Moreover, we add LayerNorm Xu et al. [2019] to stabilize the learning process. To evaluate the practicality of GraphKAN in real- world scenarios, we assess the performance using real-world graph-like temporal signal data for signal classification. Experiments demonstrate the effectiveness of GranKAN in feature extraction.

2 Problem Statement

To evaluate the practicality of GraphKAN in real-world scenarios, we choose a signal classification task.

For a dataset $D = (X_1, Y_1), (X_2, Y_2), \cdots, (X_n, Y_n)$, X and Y represent the raw one-dimension (1-D) sampling signals and fault categories, respectively. We transform 1-D signals into the form of graph. The detailed construction process can refer as . And the constructed graph is named as basic graph (BG), which can be defined as Zhang et al. [2024a,b], where V represents the nodes of G, E is the edge connections between nodes, A indicates the adjacency matrix, and F means the feature matrix of G. As a result, our goal is now focused on recognizing node labels. We can evaluate the model's performance based on diagnosis accuracy. It is important to highlight that the node classification task we have adopted is not tailored to a specific design, and the proposed GraphKAN can enhance feature extraction capabilities as a versatile tool.

3 Methodology

In this section, we detail the overall architecture of our GraphKAN. Kolmogorov-Arnold Network provides a powerful information aggregation in Graph Neural Network. Due to the enhanced representation ability, GraphKAN is more suitable for Graph-like tasks, such as node classification, graph classification and so on.

3.1 Kolmogorov-Arnold Network (KAN)

Contrary to universal approximation theorem, Kolmogorov-Arnold representation theorem demonstrates that any multivariate continuous function f on a bounded domain can be represented as the finite composition of simpler 1-D continuous functions:

$$f(x_1, \cdots, x_n) = \sum_{q=1}^{2n+1} \Phi_q(\sum_{p=1}^{n} \phi_{q,p}(x_p)), \tag{1}$$

where $\phi_{q,p}$ is a mapping $[0,1] \to \mathbb{R}$ and Φ_q is a mapping $\mathbb{R} \to \mathbb{R}$. However, these one-dimensional functions can exhibit non-smoothness and even fractal characteristics, making them impractical to learn in practice.

Liu et al. [2024] devise a neural network that explicitly incorporates this equation. This network is designed in such a way that all learnable functions are univariate and parameterized as B-splines, thereby enhancing the flexibility and learnability of the model.

Specifically, the Kolmogorov-Arnold Network (KAN) can be given by

$$x_{l+1} = \Phi_l x_l, \tag{2}$$

where Φ_l is a matrix

$$\begin{pmatrix} \phi_{1,1} & \phi_{1,2} & \cdots & \phi_{1,n} \\ \phi_{2,1} & \phi_{2,2} & \cdots & \phi_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{m,1} & \phi_{m,2} & \cdots & \phi_{m,n} \end{pmatrix}. \tag{3}$$

3.2 GraphKAN Layer

Graph neural networks (GNNs) are capable of handing the characteristics of the graph due to the message passing framework. GNNs can process the graph-like data which contains of node features x_v and edge features e_{vw}. In general, node features denote the attributes of node and edge features represent the intra-node relations in the form of adjacency matrix.

Message passing framework for node representation can be divided into two steps:

1) **Aggregates** information from the neighbors. The message function is used to aggregate the neighboring features of the target node, including the target node's own features h_v^t, the features of its neighboring nodes h_w^t, and the edge features connecting it to its neighboring nodes e_{vw}^t. This aggregation forms a message vector m_v^t that is then passed to the target node. The formula is as follows:

$$m_v^{t+1} = \sum_{w \in N(v)} M^t(h_v^t, h_w^t, e_{vw}^t) \tag{4}$$

where m_v^{t+1} is the information received by the node in the next layer $t + 1$, M^t is the message function, h_v^t represents the node features in the current layer, $N(v)$ represents the set of neighboring nodes for a node v, h_w^t represents the node features of the neighboring nodes in the current layer, and e_{vw}^t represents the edge features from node to node.

2) **Extracts** the node representation. The node update function is used to update the node features of the next layer, combining the features of the current layer's nodes and the messages obtained from the message function. The formula is as follows:

$$h_v^{t+1} = U^t(h_v^t, m_v^{t+1}) \tag{5}$$

where U^t is the node update function, which takes the original node state and the message as inputs and generates the new node state.

Note that, the majority of methods utilize Multi-layer Perceptron (MLP) for feature extraction. To enhance the nonlinearity capability, an activation function is commonly incorporated in the Phase 2) above. Activation function, such as ReLU, limit the representational capacity, potentially preventing it from learning complex features of nodes. To conclude, MLPs+activation function impede the feature extraction in graph-like data.

Hence, we propose to improve the $Extracts$ the node representation phase by replacing MLP with KAN for U^t. Our new representation extraction can be formalized as:

$$h_v^{t+1} = KAN^t(h_v^t, m_v^{t+1}) = \Phi^t(h_v^t, m_v^{t+1}). \tag{6}$$

Moreover, we utilize the B-spline function as the Φ^t. Despite many variants of KAN, such as FourierKAN and ChebyKAN, are proposed, we found that they are not effective for graph tasks.

Table 1: Settings of four input graphs.

| Graph | Labeled node amount | | Unlabeled Amount |
	Label 0	Label 1-5	
BG_1	200	100	700
BG_2	200	80	700
BG_3	200	60	700
BG_4	200	40	700

Table 2: Model structural settings.

Name	Model structural settings	Kernel size
GCN GraphKAN	GCN structure: 512-256-128, layer normalization	$k_1 = 3, k_1 = 3, k_1 = 3$

3.3 A Simple GraphKAN for Node Classification

To evaluate the ability of representation extraction of GraphKAN, we contrive a simple GraphKAN based on Graph Convolutional Neural Network (GCN).

Concretely, the formula of GraphKAN layer based on GCN is as follows:

1) message function M^t is

$$(deg(v)deg(w))^{-1/2}A_{uw}h_w^t, \tag{7}$$

where deg computes the degree of node.

2) node representation extraction function U^t is

$$U^t(h_v^t, m_v^{t+1}) = \Phi^t m_v^{t+1} \tag{8}$$

.

To stabilize the training, we leverage the LayerNorm between GraphKAN layers.

4 Experimental Verification

A node classification task is constructed to validate the superiority of GraphKAN. It derives from a pattern recognition task for one-dimensional signals that collected from one axial-flow pump [3]. A specific graph construction method is designed in [1], demonstrating the relationship between samples. In this part, the constructed graphs named basic graphs (BGs) are used for node classification to validate the improvement effect of GraphKAN. According to the difference of the number of labeled samples, we constructed four graphs, as shown in Table. 1. The labeled nodes can be used for model training and model validation, and the testing nodes within these four graphs are the same. Two models, i.e., GraphKAN and GCN are separately conducted for processing the BGs. Their hyper-parameters are all set to the same value, as shown in Table 2. In this study, we adopted the CosineAnnealingLR learning rate scheduler in PyTorch to dynamically adjust the learning rate. We set the maximum number of epochs to 200 and constrained the minimum learning rate to 1e-4. This configuration aims to adjust the learning rate through cosine annealing to balance the model's convergence speed and performance during training. The above settings are valid for both models.**?**

We randomly select 20% of labeled nodes for model validation, and the validation accuracy serves as a criterion to determine the model's convergence. 700 unlabeled nodes are utilized for model testing. Ten trials involving model training, validation, and testing were carried out, and the average test accuracy and time duration using various input graphs are illustrated in Fig. 1. Clearly, the time consumption of GraphKAN is notably higher than that of the original GCN, attributed to the more time-consuming computation of KAN. However, it can be observed that the test accuracy of GraphKAN is superior to that of GCN, particularly in BG_3 and BG_4. Although the time consumption has increased significantly, the improvement in accuracy is even more valuable. Moreover, the time
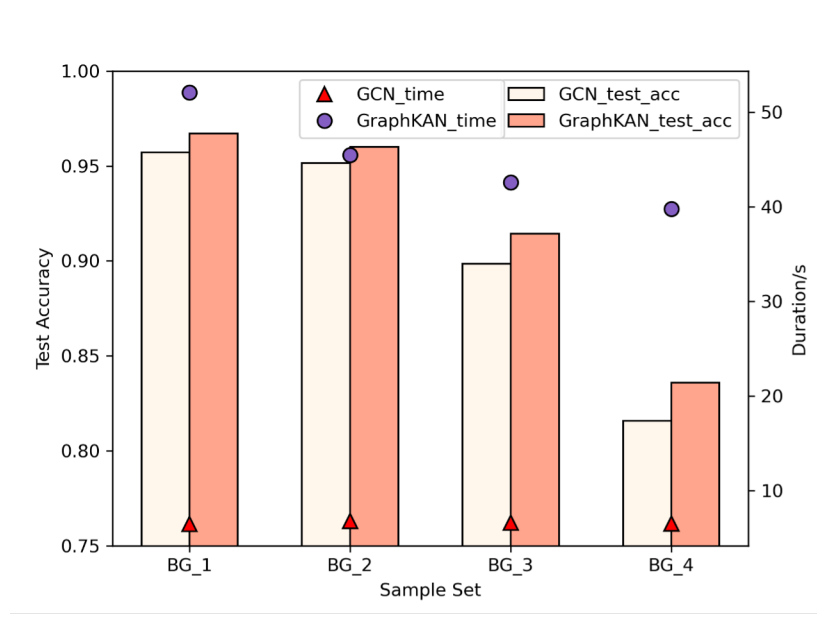
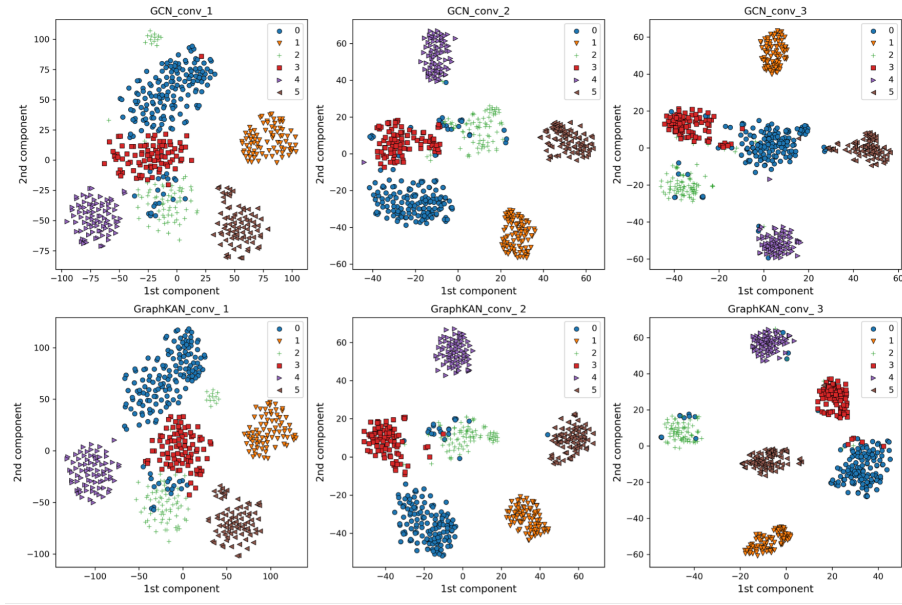Figure 1: Comparison on testing accuracy and time consumption

Figure 2: Clustering comparison of intermediate features for testing nodes within BG_1

consumption remains within a manageable range, less than one minute. At the same time, we also noticed that the improvement effect of GraphKAN is more significant when the input graph has less labeled nodes, such as BG_3 and BG_4. It probably indicates that GraphKAN holds potential significance for few-shot classification tasks.

We also used t-SNE algorithm to cluster the intermediate features of GNN models. Specifically, the output features of three graph convolutional layers for testing nodes are extracted and clustered in Fig. 2-5 , with different input graphs. It can be seen that in the clustering of outputs at the corresponding layers of these two models, GraphKAN always manages to cluster features of the same type more closely, while clusters of different types are farther apart. This indicates that GraphKAN's feature extraction capability surpasses that of GCN, thereby enhancing the classification accuracy.
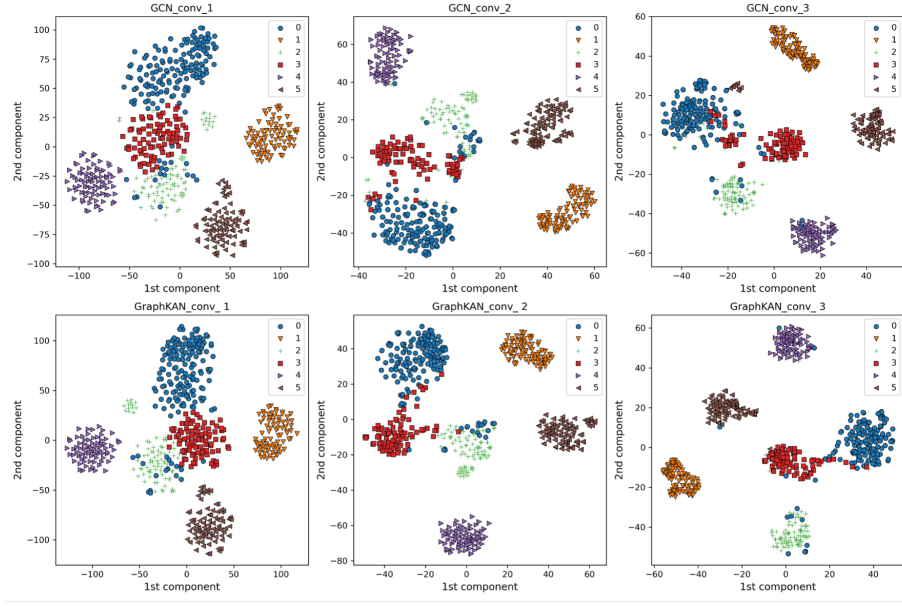
5

Figure 3: Clustering comparison of intermediate features for testing nodes within BG_2
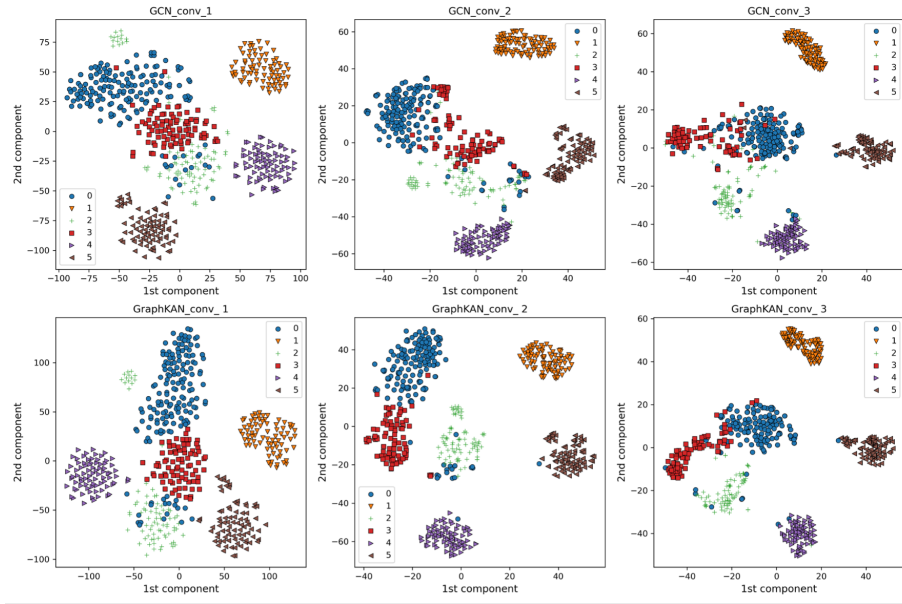

Figure 4: Clustering comparison of intermediate features for testing nodes within BG_3

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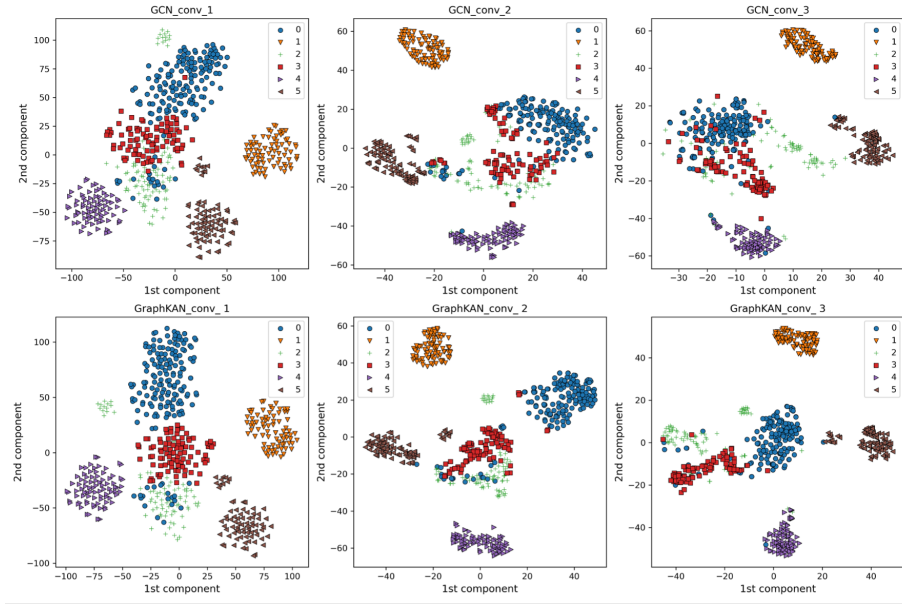
Figure 5: Clustering comparison of intermediate features for testing nodes within BG_3

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