G5: A Universal GRAPH-BERT for Graph-to-Graph Transfer and Apocalypse Learning

Jiawei Zhang
IFM Lab, Florida State University, Tallahassee, FL, USA
jiawei@ifmlab.org

Abstract—The recent GRAPH-BERT model introduces a new approach to learning graph representations merely based on the attention mechanism. GRAPH-BERT provides an opportunity for transferring pre-trained models and learned graph representations across different tasks within the same graph dataset. In this paper, we will further investigate the graph-to-graph transfer of a universal GRAPH-BERT for graph representation learning across different graph datasets, and our proposed model is also referred to as the "G5" for simplicity. Many challenges exist in learning G5 to adapt the distinct input and output configurations for each graph data source, as well as the information distributions differences. G5 introduces a pluggable model architecture: (a) each data source will be pre-processed with a unique input representation learning component; (b) each output application task will also have a specific functional component; and (c) all such diverse input and output components will all be conjuncted with a universal GRAPH-BERT core component via an input size unification layer and an output representation fusion layer, respectively.

The G5 model removes the last obstacle for cross-graph representation learning and transfer. For the graph sources with very sparse training data, the G5 model pre-trained on other graphs can still be utilized for representation learning with necessary fine-tuning. What’s more, the architecture of G5 also allows us to learn a supervised functional classifier for data sources without any training data at all. Such a problem is also named as the Apocalypse Learning task in this paper. Two different label reasoning strategies, i.e., Cross-Source Classification Consistency Maximization (CCCM) and Cross-Source Dynamic Routing (CDR), are introduced in this paper to address the problem. The preliminary experimental results on several benchmark graph datasets can demonstrate the effectiveness of G5 on graph-to-graph transfer and representation learning.

Index Terms—Graph-Bert; Representation Learning; Apocalypse Learning; Transfer Learning; Graph Mining; Data Mining

I. INTRODUCTION

A brand new graph neural network named GRAPH-BERT (Graph based BERT) is introduced in [35] for graph data representation learning. Different from conventional graph neural networks [11], [29], [13], [26], [14], via linkless subgraph batching, GRAPH-BERT redefines the conventional graph representation learning problem as the target node instance representation learning within individual learning context instead. One of the great advantages of such a new learning setting is that GRAPH-BERT can effectively get rid of many common learning effectiveness and efficiency problems, e.g., suspended animation [24] and hard to parallelize, with the existing graph neural networks. Also it enables the pre-training and fine-tuning of GRAPH-BERT across different learning tasks on the same graph dataset, which has transformative impacts on building functional model pipelines for graph learning.

In this paper, we will further explore the transfer of GRAPH-BERT across different graph datasets, which still remains a great challenge and an open problem by this context so far. To be more precise, we propose to learn GRAPH-BERT with multiple different graph datasets, which have totally different properties, e.g., graph sizes, graph structures, input feature space and output label space. What’s more, the learned GRAPH-BERT on one or several source graph dataset(s) can be further transferred as the pre-trained model for other graph dataset(s) suffering from the lack of training data. For each of these graph data datasets, multiple different application tasks can also be studied concurrently, which may or may not have correlations with each other.

To address such a problem, a novel learning model, i.e., G5, will be introduced in this paper, where the five Gs correspond to the “graph-to-graph transfer of a universal GRAPH-BERT for graph representation learning across different graph datasets”. G5 effectively extends the GRAPH-BERT model for the cross-graph representation learning, which brings about lots of new challenges and new opportunities at the same time.

On the one hand, to learn the G5 model, we may need to explore many great challenges in handling the different graph property differences and the different objectives of diverse learning tasks. To be more specific, G5 introduces a pluggable model architecture: (a) each data source will be pre-learned with a unique input component for data pre-processing; (b) each output application task will also have a specific functional component for computing the output; and (c) all such diverse input and output components will be conjuncted with a universal GRAPH-BERT core component in G5 via an input size unification layer [33] and an output representation fusion layer [35], respectively.

On the other hand, in addition to building the functional model pipelines across graphs for representation learning, a successfully learned G5 will also allow us to explore some new yet challenging problems. Besides the model transfer to graph sources with limited training data, the architecture of G5 also allows us to learn a supervised functional classifier for certain graph sources without any training data at all, which is also named as the Apocalypse Learning (AL) problem formally in this paper. It should be easy to identify that the apocalypse learning task is different from the well-studied zero-shot learning task [25]. Here, we would like to further
clearly illustrate their differences: (1) **apocalypse learning** is for multi-dataset but **zero-shot learning** focuses on one dataset; (2) **apocalypse learning** uses no training data in the target data source but **zero-shot learning** uses training data; and (3) **apocalypse learning** usually needs to know prior class representations or correlations in advance.

We summarize our contributions in this paper as follows:

- **A Universal GNN**: We introduce a new graph neural network model in this paper for multi-graph concurrent representation learning. To adapt the diverse input and output configuration distinctions, G5 introduces a pluggable model architecture which can be tied up with many different input and output components. All such diverse input and output components will be conjuncted with a universal GRAPH-BERT core component in G5 via the input size unification layer and output representation fusion layer, respectively.

- **Pre-Train & Transfer & Fine-Tune**: To learn various application task objectives, G5 will be pre-trained on multiple graphs in a hybrid manner with multiple different learning tasks, which also define the output component pool involving various supervised and unsupervised learning tasks. Meanwhile, a pre-trained G5 can also be transferred and applied to new graph data sources either directly or with necessary fine-tuning in a similarly hybrid manner. There is no specific correlation requirements on these fine-tuning tasks, which can be totally different from those pre-training tasks on the source graph(s) actually.

- **Apocalypse Learning**: Besides investigating the model transfer to graph sources with limited training data, in this paper, we also introduce a new learning problem, i.e., **apocalypse learning**, which aims to build a classifier on certain target graph source without any training data at all. Based on the learning results of the hybrid tasks on other graph datasets, G5 introduces two different strategies, i.e., Cross-Source Classification Consistency Maximization (CCCM) and Cross-Source Dynamic Routing (CDR), to reason for the labels in the target graph source in this paper.

The remaining parts of this paper are organized as follows. Definitions of several important terminologies and the formulation of the studied problem will be provided in Section II. Detailed information about the G5 model will be introduced in Section III and the two reasoning strategies to address the apocalypse learning problem will be discussed in Section IV. The effectiveness of G5 will be tested in Section V. Finally, we will introduce the related work in Section VI and conclude this paper in Section VII.

II. NOTATIONS, TERMINOLOGY DEFINITION AND PROBLEM FORMULATION

In this section, we will first introduce the notations used in this paper. After that, we will provide the definitions of several important terminologies and the studied problem.

A. Notations

In the sequel of this paper, we will use the lower case letters (e.g., \( x \)) to represent scalars or mappings, lower case bold letters (e.g., \( \mathbf{x} \)) to denote column vectors, bold-face upper case letters (e.g., \( X \)) to denote matrices, and upper case calligraphic letters (e.g., \( \mathcal{X} \)) to denote sets or high-order tensors. Given a matrix \( X \), we denote \( X(i,:) \) and \( X(:,j) \) as its \( i \)th row and \( j \)th column, respectively. The \((i,j)\) entry of matrix \( X \) can be denoted as either \( X(i,j) \). We use \( X^{\top} \) and \( x^{\top} \) to represent the transpose of matrix \( X \) and vector \( x \). For vector \( x \), we represent its \( L_p \)-norm as \( \|x\|_p = (\sum_i |x(i)|^p)^{\frac{1}{p}} \). The Frobenius-norm of matrix \( X \) is represented as \( \|X\|_F = (\sum_{i,j} |X(i,j)|^2)^{\frac{1}{2}} \). The element-wise product of vectors \( x \) and \( y \) of the same dimension is represented as \( x \odot y \), whose concatenation is represented as \( x \uplus y \).

B. Terminology Definitions

Several terminologies will be used in this paper to present the proposed method, which include graph, multi-source graph set and linkless subgraph.

**Definition 1. (Graph)**: Formally, we can represent the studied graph data as \( G = (\mathcal{V}, \mathcal{E}, w, x, y) \), where \( \mathcal{V} \) and \( \mathcal{E} \) denote the sets of nodes and links, respectively. Mapping \( w: \mathcal{E} \rightarrow \mathbb{R} \) projects links to their weights; whereas mappings \( x: \mathcal{V} \rightarrow \mathcal{X} \) and \( y: \mathcal{V} \rightarrow \mathcal{Y} \) can project the nodes to their raw features and labels, respectively.

Given a graph \( G \), its size can be represented by the number of involved nodes, i.e., \( |\mathcal{V}| \). Notations \( \mathcal{X} \) and \( \mathcal{Y} \) used in the above definition denote the feature space and label space, respectively. In this paper, they can also be represented as \( \mathcal{X} = \mathbb{R}^{d_x} \) and \( \mathcal{Y} = \mathbb{R}^{d_y} \) (with dimensions \( d_x \) and \( d_y \)) for simplicity. For node \( v_i \), we can also simplify its raw feature and label vector representations as \( x_i = x(v_i) \in \mathbb{R}^{d_x \times 1} \) and \( y_i = y(v_i) \in \mathbb{R}^{d_y \times 1} \). In this paper, we are studying the transfer of GRAPH-BERT across multiple graphs, and the studied graphs can be denoted as the multi-source graph set as follows.

**Definition 2. (Multi-Source Graph Set)**: Formally, we can represent the set of \( n \) different input graphs that we are studying in this paper as \( \mathcal{G} = \{G^{(1)}, G^{(2)}, \ldots, G^{(n)}\} \), among which some of them may have very limited or even no training data (i.e., labeled nodes). All these \( n \) input graphs can have different properties, e.g., graph sizes, graph structures, node feature space and label space.

Given a node, e.g., \( v_i^{(m)} \in \mathcal{V}^{(m)} \), in graph \( G^{(m)} \in \mathcal{G} \), based on the approach introduced in [35], we will be able to sample a unique linkless sub-graph for it involving node \( v_i \) and its surrounding node context.

**Definition 3. (Linkless Subgraph)**: Given an input graph \( G^{(m)} \), we can denote the sampled linkless subgraph for each node \( v_i^{(m)} \) in the graph as \( g_i^{(m)} = (\mathcal{V}_i^{(m)}, \emptyset) \). Here, the node set
\[ V_i^{(m)} = \{ v_i^{(m)} \} \cup \Gamma( v_i^{(m)}, k^{(m)}) \] covers both \( v_i \) and its top \( k^{(m)} \) intimate nearby nodes, and the link set is empty. Furthermore, the batch of linkless subgraphs sampled for all the nodes in graph \( G^{(m)} \) can be denoted as \( G^{(m)} = \{ g_i^{(m)} \} \), \( v_i^{(m)} \in \mathcal{V}^{(m)}. \)

Therefore, for all the graphs covered in \( \mathcal{G} \), we can represent their sampled subgraph batches as \( \{ G^{(1)}, G^{(2)}, \ldots, G^{(n)} \} \). According to the experimental studies provided in [35], different graphs may have different optimal parameters to control the sampled subgraph size, e.g., \( k^{(m)} \) for graph \( G^{(m)} \). Therefore, the subgraphs sampled in batch \( G^{(l)} \) will usually have different sizes from those in \( G^{(m)}, \forall l, m \in \{ 1, 2, \cdots, n \} \land l \neq m. \)

C. Problem Formulation

Based on the above terminology definitions, we can define the problem studied in this paper as follows:

**Problem Statement:** Formally, given the multi-source graph set \( \mathcal{G} = \{ G^{(1)}, G^{(2)}, \ldots, G^{(n)} \} \) with \( n \) different graphs, we aim to learn a shared representation learning mapping \( f : \bigcup_{m=1}^{n} \mathcal{V}^{(m)} \rightarrow \mathbb{R}^{d_h} \) to learn the representations of nodes in all these \( n \) graphs concurrently. Such learned node representations will be further utilized in various downstream application tasks for either pre-training or fine-tuning the model. Furthermore, depending on the learning settings, the mapping pre-trained based on some graphs can also be further transferred to the other graphs with limited even no supervision information directly or with necessary fine-tuning. In this way, it can hopefully help address the labeled data sparsity problem or even the *apocalypse learning* problem for some input graph datasets.

III. THE PROPOSED METHOD

In this section, we will introduce the G5 model architecture in detail.

A. The Key Challenges

As introduced in Section [II-B] for the multi-source input graphs \( \mathcal{G} \), a batch of linkless subgraphs can be sampled from them for target node representation learning. To enable the concurrent learning of the G5 model with all these \( n \) graphs in \( \mathcal{G} \), several important differences among these graph datasets cannot be ignored:

- **Input Space Difference:** For any two nodes from two different graphs, their raw features can be very different in (1) data types: their feature vectors can be in totally different data types, e.g., image, text, or tags; (2) feature length: the vectors can also have different length; (3) feature domain: for the features of the same type and have the same dimensions, they may also from totally different domains and carry different information, e.g., medical images vs traffic images; and (4) feature distribution: for the identical features in different graph sources, they may follow distinct distributions.

- **Model Configuration Difference:** In addition to the input feature space differences aforementioned, there may also exist a lot of model configuration differences in the favored Graph-BERT component in G5 by different graph datasets. For instance, according to [35], the sampled subgraph size parameter \( k \) may affect the learning performance of Graph-BERT a lot; whereas different graph datasets may also prefer different parameter \( k_s \), which may lead to different model configurations.

- **Output Space Difference:** Meanwhile, for the downstream application tasks to be studied in G5 on the same/different graph datasets, they tend to have different output space actually, which may cast certain task-oriented requirements on the representation learning process. For instance, the node raw feature reconstruction and graph structure recovery tasks actually focus more on embedding node attributes and graph structures into the learned representations, respectively; whereas the node classification aims at learning a classifier to project nodes to the label space instead.

To handle these above differences properly, as illustrated in Figure [1] we design the G5 model with a pluggable architecture containing several key parts: (1) pluggable input dataset-wise processing components, (2) input size unification interlayer, (3) the universal Graph-BERT model shared across graphs, (4) representation fusion interlayer, (5) pluggable task-wise output components for each dataset, and (6) reasoning component for *apocalypse learning*. For each input graph data, it will have a unique input component to handle its initial embeddings based on their unique subgraph batches, which will accommodate the input feature space differences and information distribution differences for G5. Meanwhile, each graph dataset will have several output components as multiple pre-train/fine-tune tasks will be studied concurrently, which can handle the output space difference problem. The input size unification interlayer introduced in this paper can effectively accommodate the configurations of diverse inputs from different datasets prior to feeding them into the universal Graph-BERT model; whereas the representation fusion interlayer will aggregate the learned representations to generate the fused representations for the output components.

The G5 model will be effectively pre-trained based on the graph datasets with sufficient supervision information, which can be further transferred to the graph datasets lacking enough labeled data with fine-tuning. Furthermore, if certain fine-tuning task on the target graph dataset doesn’t contain any supervision information, the *apocalypse learning* based component will be used for label reasoning. In this section, we will introduce the first five components in G5, except the reasoning component for *apocalypse learning*, which will be introduced in the next Section [V] in detail.

B. Input Accommodation Component

For presentation simplicity, in this part, we will first ignore the script index for the graphs in the notations. Formally, given the sampled subgraph batch from an input graph \( G \), for the target nodes \( v_i \) together with their learning context
(with \( k \) nodes), according to [35], we can represent its initial embedding vector as

\[
\mathbf{h}_i^{(0)} = \text{Aggregate}\left(\mathbf{e}_i^r, \mathbf{e}_i^l, \mathbf{e}_i^d, \mathbf{e}_i^f\right),
\]

where \( \mathbf{e}_i^r, \mathbf{e}_i^l, \mathbf{e}_i^d \) and \( \mathbf{e}_i^f \) are embeddings based on the raw features, WL based roles, relative positions and the hop based distance as introduced in [35], respectively. In the notation, \( k \) denotes the subgraph sampling parameter, and \( d_e \) is the raw embedding feature dimension in the graph. The Aggregate\((·)\) function will effectively aggregate the input vectors together, which can be defined in different ways. In this paper, we will follow the previous work, and just define it as the vector summation.

It is easy to know that the raw embedding feature dimension, i.e., \( d_e \), in the graph datasets can be different form each other. Also the initial embedding features can lie in different feature spaces for different graph datasets. Therefore, instead of directly feeding vector \( \mathbf{h}_i^{(0)} \) to the universal Graph-BERT model, to accommodate the input feature space, G5 introduces an input component for each graph dataset based on the graph-transformer to project the inputs to a shared feature space of dimension \( d_h \), as follows:

\[
\begin{align*}
\mathbf{H}_i^{(0)} &= \left[\mathbf{h}_i^{(0)}, \mathbf{h}_i^{(0)}, \cdots, \mathbf{h}_i^{(0)}\right]^T, \\
\mathbf{H}_i^{(l)} &= \text{G-Transformer}\left(\mathbf{H}_i^{(l-1)}\right), \forall l \in \{1, 2, \cdots, D\},
\end{align*}
\]

where \( D \) denotes the input component depth and the nodes in set \( \{v_{i,1}, v_{i,2}, \cdots, v_{i,k}\} = \Gamma(v_i, k) \) denotes the learning context of \( v_i \) in its sampled subgraph. Notation G-Transformer\((·)\) denotes the graph-transformer layers consisting of both the transformer and graph residual terms as introduced in [35], which will also be defined in the following Equation (4) in detail. Formally, the finally learned representation matrix \( \mathbf{H}_i^{(D)} \in \mathbb{R}^{(k+1) \times d_h} \) for the subgraph \( g_i \) will be the representation input of the subgraph to the follow-up universal Graph-Bert model.

According to the above descriptions, we can accommodate the input representations for all the sampled subgraphs from all the input graphs, i.e., \( \mathcal{G} = \{G^{(1)}, G^{(2)}, \cdots, G^{(n)}\} \). For instance, by adding the graph index superscript into the notations, we can represent such learned nodes’ representations from graph \( G^{(m)} \) as \( \left\{\mathbf{H}_i^{(m)}\right\}_{v_i^{(m)} \in \mathcal{V}(m)} \), where \( \mathbf{H}_i^{(m)} \in \mathbb{R}^{(k^{(m)}+1) \times d_h} \). Here, we may need to add a remark: the input components for the different graphs in \( \mathcal{G} \) will not share the weight parameters, and they can also be in different depths (i.e., \( D^{(m)} \)) depending on their unique requirements.

### C. Input Size Unification Interlayer

According to the previous subsection, for the input feature dimension, feature domain and distribution differences, they can be effectively handled with the input components consisting of several graph-transformer layers. Meanwhile, it is easy to observe that the accommodated input representations for subgraphs from different graph source still have different configurations, since the subgraph size parameter used in them are usually different, i.e., \( k^{(l)} \neq k^{(m)} \) for \( G^{(l)}, G^{(m)} \in \mathcal{G} \). Therefore, prior to feeding them to the universal Graph-BERT model, we introduce one more layer to accommodate the input subgraph representation sizes from different graph datasets, which is called the input size unification interlayer. There exist different input size unification approaches that can be used, e.g., full-input strategy, padding/pruning strategy and segment shifting strategy as introduced in [33]. We can take the padding/pruning strategy as an example to introduce here, but the other two strategies can be used as well depending on the specific learning settings.

Formally, we can denote the dimension of the inputs for the universal Graph-BERT model (to be introduced in...
the next subsection) as $\mathbb{R}^{(k+1) \times d_h}$, where the parameter $k$ without superscript denotes the objective subgraph node context size desired by the universal Graph-BERT model. Meanwhile, depending on the input subgraph representations and their subgraph size parameters $k^{(m)}$ for graph $G^{(m)}$, the padding/pruning strategy based size unification layer will handle them as follows:

- **Pruning**: If $k^{(m)} > k$, the input has more feature entries than that the universal Graph-BERT model can handle. Therefore, the size unification layer will prune the last $k^{(m)} - k$ vector entries from the input, which correspond to the context nodes less relevant to the target node.

- **No Action**: If $k^{(m)} = k$, the inputs can be handled by the universal Graph-BERT directly and no action is necessary to be performed at the size unification layer.

- **Padding**: If $k^{(m)} < k$, necessary dummy vectors will be needed to be padded to the inputs to increase the involved subgraph node number from $k^{(m)}$ to $k$. We will use the zero padding for simplicity in this paper, which will not dramatically affect the learning results according to [33] but can introduce more learning time costs.

Formally, given the input representation matrix $H^{(m,D^{(m)})}$ learned for subgraph $g^{(m)}$ from graph $G^{(m)}$, we can denote its size-unified output representations as

$$Z^{(m,0)}_i = \text{Unify} \left( H^{(m,D^{(m)})}_i \right) \in \mathbb{R}^{(k+1) \times d_h}, \quad (3)$$

Similar operators can be applied to all the remaining subgraphs sampled from all these $n$ input graph datasets.

### D. Universal Graph-BERT

The universal Graph-BERT model is shared for all the input graph datasets, which can learn the representations based on the inputs iteratively with several layers. Here, we can denote the inputs to Graph-BERT from the input size unification layer as $Z^{(0)} \in \mathbb{R}^{(k+1) \times d_h}$ without indicating its node index or the graph index in the subscript/superscript. The representation learning component in Graph-BERT also contains several layers of the graph-transformers. Formally, at the $l_{th}$ layer, we can represent the learned representation as follows:

$$Z^{(l)} = \text{G-Transformer} \left( Z^{(l-1)} \right)$$

$$= \text{softmax} \left( \frac{Q^{(l)} (K^{(l)})^T}{\sqrt{d_h}} \right) V^{(l)} + \text{G-Res} \left( Z^{(l-1)}, X \right), \quad (4)$$

where

$$\begin{align*}
Q^{(l)} &= Z^{(l-1)} W^{(l)}_Q, \\
K^{(l)} &= Z^{(l-1)} W^{(l)}_K, \\
V^{(l)} &= Z^{(l-1)} W^{(l)}_V.
\end{align*} \quad (5)$$

In the above equation, $W^{(l)}_Q, W^{(l)}_K, W^{(l)}_V \in \mathbb{R}^{d_h \times d_h}$ denote the involved variables in the $l_{th}$ layer. In this paper, to simplify the presentation and notations, the hidden representations at different layers in the universal Graph-BERT are assumed to have the identical dimension $d_h$ by default. Notation G-Res $\left( Z^{(l-1)}, X \right)$ defines the graph residual term introduced in [34], and $X$ is the raw features of all nodes in the subgraph.

For both the shared universal Graph-BERT component and the individual graph input components introduced in Section III-B, we will use the “graph-raw” residual term in this paper by default. The universal Graph-BERT component involved in G5 will contain $D$ layers, and we can denote the output by the $D_{th}$ layer as $Z^{(D)} \in \mathbb{R}^{(k+1) \times d_h}$.

### E. Output Representation Fusion Interlayer

As illustrated in Figure 1, one more fusion layer is stacked on the universal Graph-BERT model to fuse such learned representations to define the ultimate representation vector of the target node, which can be denoted as:

$$z = \text{Fusion} \left( Z^{(D)} \right) = \frac{1}{k+1} \sum_{i=1}^{k+1} Z^{(D)}(i, :). \quad (6)$$

Many advanced fusion strategies can also be used here, e.g., fusion with further node selections or weighted fusion based on certain attention scores. However, in this paper, we will not explore them and a simple averaging function can be used here to define the above fusion component across all the nodes in the sampled subgraphs. Based on the above descriptions, by bringing the node and graph index subscript/superscript back, we can represent the outputted representations of all the nodes in graph $G^{(m)}$ by the universal Graph-BERT component as $\{z_i^{(m)} \}_{i \in \mathcal{V}^{(m)}}$, which will be fed to the following functional components to study various downstream application tasks.

### F. Output Application Components

To learn such representations together with the model variables, necessary optimization objective function will be needed. In this paper, we introduce a hybrid learning task combo by following [35], which covers unsupervised node attribute reconstruction, unsupervised graph structure recovery and supervised node classification.

- **Node Attribute Reconstruction**: Based on the learned node representations, via several fully connected layers (with necessary activation functions), we will be able to project the learned representation vectors to their raw features, i.e., the node raw attribute reconstruction. By minimizing the difference between nodes’ original raw attributes versus the reconstructed ones, we will be able to learn the G5 model.

- **Graph Structure Recovery**: Given any two nodes from the same graph, based on their learned representations, via either fully connected layers or simple similarity metrics, we will be able to project the node pair representation vectors to their corresponding link labels or similarity scores. Also by minimizing the differences between such learned link scores versus the graph link ground truth, G5 can also be effectively learned.
A. Reasoning Strategy #1: CCCM

One approach proposed in this paper for the potential label reasoning for nodes in graph without supervision information is called the cross-source classification consistency maximization (CCCM). Formally, as illustrated in Figure 2, let’s take one of the target graph $G^{(m)}$ as an example, which contains no node labels, and we are studying the node classification task based on it. Given the pre-trained G5 model with several other graph datasets (containing supervised application functional components), via necessary fine-tuning with the other unsupervised learning tasks on $G^{(m)}$, e.g., node attribute reconstruction and graph structure recovery, we can still learn the representations of the nodes in the graph with G5, which can be representations as $\{z_{i}^{(m)}\}_{v_{i}^{(m)} \in V^{(m)}}$. Furthermore, for node $v_{i}^{(m)}$ with representation $z_{i}^{(m)}$, via several fully connected layers, we can represent the node’s label to be

$$\hat{y}_{i}^{(m)} = \text{softmax} \left( \text{FC}^{(m)} \left( z_{i}^{(m)} \right) \right).$$ \hspace{1cm} (7)

According to the previous descriptions, with the input processing components for each dataset, the learned node representations from different graphs will lie in identical feature spaces actually. Based on such an intuition, via the learned G5 models on the other graph datasets like $G^{(l)}$, given the node representation $z_{i}^{(m)}$, we can also define their inferred labels by G5 directly as $\{\hat{y}_{i}^{(l)}\}_{l \neq m}$, where

$$\hat{y}_{i}^{(l)} = \text{softmax} \left( \text{FC}^{(l)} \left( z_{i}^{(m)} \right) \right).$$ \hspace{1cm} (8)

Meanwhile, based on the inferred label vector $\hat{y}_{i}^{(m)}$, we propose to project it to the other graph datasets via several FC layers, and the projected label vectors in the other datasets can be denoted as $\{\hat{y}_{i}^{(l)}\}_{l \neq m}$, where

$$\hat{y}_{i}^{(l)} = \text{softmax} \left( \text{FC}^{(m \rightarrow l)} \left( \hat{y}_{i}^{(m)} \right) \right).$$ \hspace{1cm} (9)

In this paper, we assume that its learned class labels should carry consistent information across all these different graphs, since they are learned within the identical framework. Therefore, to learn the nodes label vectors in graph $G^{(m)}$ as well as the involved fully connected layers, we propose to minimize the below classification consistency loss term:

$$\min_{v_{i}^{(m)} \in V^{(m)}} \sum_{l \neq m} \sum_{i=1}^{n} \left\| \hat{y}_{i}^{(l)} - \hat{y}_{i}^{(l)} \right\|_{2}.$$ \hspace{1cm} (10)

B. Reasoning Strategy #2: CDR

The CCCM approach may need to learn several fully connected layers for the node label reasoning based on the classification result consistency assumption across graphs for common representation inputs. Here, in this part, we will introduce another reasoning approach based on the dynamic routing algorithm instead, which works very differently. Formally, for any node $v_{i}^{(m)}$ in graph $G^{(m)}$, we can denote its representation in $G^{(m)}$ as vectors $z_{i}^{(m)}$. Furthermore, by feeding $z_{i}^{(m)}$ as the...
input for classifiers in other graph sources, we can represent their learned label vectors as \( \{ y_{i}^{(l)} \}_{i=1}^{n} \), respectively. The cross-source dynamic routing (CDR) approach reasons nodes’ labels in \( G^{(m)} \) iteratively as follows:

\[
\begin{align*}
    c_{i}^{(l \rightarrow m)} &= \text{softmax} \left( b_{i} \right), \\
    u_{i}^{(l \rightarrow m)} &= W^{(l \rightarrow m)} y_{i}^{(l)}, \\
    s_{i}^{(l \rightarrow m)} &= \sum_{j=1}^{k} c_{i}^{(l)} u_{j}^{(l \rightarrow m)}, \\
    v_{i}^{(l \rightarrow m)} &= \| s_{i}^{(l \rightarrow m)} \|_{2}, \\
    b_{i}^{(l \rightarrow m)} &= b_{i}^{(l)} + v_{i}^{(l \rightarrow m)}.
\end{align*}
\]

(11)

where \( W^{(l \rightarrow m)} \in \mathbb{R}^{d_{y}^{(m)} \times d_{y}^{(l)}} \) denotes the label vector dimension adjustment variable between graphs \( G^{(l)} \) and \( G^{(m)} \). Formally, the vector \( v_{i} \), outputted by such a process will represent the reasoned label vector of node \( v_{i}^{(m)} \). By minimizing its difference with the inferred label by \( G_{5} \), i.e., as defined in Equation (7), we will be able to represent the introduced reasoning loss function as follows:

\[
\min \sum_{v_{i}^{(m)} \in \mathcal{V}^{(m)}} \left\| \hat{y}_{i}^{(m)} - y_{i} \right\|_{2}^2.
\]

(12)

More information about the experimental studies of these two apocalypse learning oriented reasoning strategies will be provided in the following section in detail.

V. EXPERIMENTS

To test the effectiveness of \( G_{5} \) on graph representation learning, in this section, we will report some preliminary experimental results of \( G_{5} \) that we obtain on three real-world benchmark graph datasets. More experimental results will be provided in the followup updated version of this paper as well.

A. Dataset and Learning Settings

The graph benchmark datasets used in the experiments include Cora, Citeseer and Pubmed [31], which are used in most of the recent state-of-the-art graph neural network research works [11], [29], [13], [26], [14], [34]. For fair comparison, the experimental settings, e.g., train/validation/test set partition, will be identical as these existing research papers as well. Based on the input graph data, we will first pre-compute the node intimacy scores, based on which subgraph batches will be sampled subject to the subgraph size \( k \) for each dataset. In addition, we will also pre-compute the node pairwise hop distance and WL node codes. In this paper, we aim to examine the transfer of the universal Graph-BERT across different graph datasets based on the \( G_{5} \) framework. Considering that different datasets will have different learning settings, instead of summing the loss functions of all the datasets, we propose to train \( G_{5} \) with multiple graph datasets iteratively. To be more specific, the pre-training of \( G_{5} \) will last for several iterations. In each iteration, we will train the corresponding components in \( G_{5} \) with Cora, Citeseer and Pubmed sequentially subject to their unique parameter settings shown as follows. The default evaluation metric used in the experiments is Accuracy.

TABLE I

| Methods       | Datasets (Accuracy) |
|---------------|---------------------|
|               | Cora    | Citeseer | Pubmed |
| LP ([31])     | 0.680   | 0.453    | 0.630  |
| ICA ([16])    | 0.751   | 0.691    | 0.739  |
| ManiReg ([14])| 0.595   | 0.601    | 0.707  |
| SemiEmb ([30])| 0.590   | 0.596    | 0.711  |
| DeepWalk ([22])| 0.672  | 0.432    | 0.653  |
| Planetoid ([31])| 0.757  | 0.647    | 0.772  |
| MoNet ([20])  | 0.817   | -        | 0.788  |
| GCN ([11])    | 0.815   | 0.703    | 0.790  |
| GAT ([29])    | 0.830   | 0.725    | 0.790  |
| LoopyNet ([22])| 0.826  | 0.716    | 0.792  |
| GRAPH-BERT ([35])| 0.843 | 0.712    | 0.793  |
| G5 (isolated) | 0.841   | 0.715    | 0.789  |

(k = 7) (k = 5) (k = 30)

Default Parameter Settings: If not clearly specified, the results reported in this paper are based on the following parameter settings of \( G_{5} \): subgraph size: \( k = 7 \) (Cora), \( k = 5 \) (Citeseer), \( k = 30 \) (Pubmed); hidden size: \( D = 32 \); attention head number: \( 2 \); hidden layer number: \( D = 2 \); learning rate: 0.01 (Cora) and 0.001 (Citeseer) and 0.001 (Pubmed); weight decay: \( 5e^{-4} \); intermediate size: \( 32 \); hidden dropout rate: 0.5; attention dropout rate: 0.3; graph residual term: graph-raw; optimizer: Adam; training epoch: 150 (Cora), 500 (Pubmed), 2000 (Citeseer). For the universal Graph-BERT, we evaluate the learning performance by changing its parameter \( k \) with different values from \( \{5, 7, 15, 30\} \) in the experiments, where \( 5, 7, 30 \) are the optimal parameters for these three datasets, respectively, and value 15 can balance among all the datasets.

Experiment Organization: We intend to use the experiments to answer several questions that readers may have in mind:

- \textbf{Q1}: Can \( G_{5} \) still work well for isolated graph input?
- \textbf{Q2}: Can \( G_{5} \) be applicable to multiple graph inputs, which all have abundant training data actually?
- \textbf{Q3}: How will the pre-trained \( G_{5} \) perform when being transferred to target graphs lacking enough training data?
- \textbf{Q4}: How is the learning performance of two reasoning strategies in \( G_{5} \) on addressing the apocalypse learning task?

The following experiments will be designed to address these above above questions specifically.

B. Isolated \( G_{5} \) on Node Classification

Prior to showing the learning performance of \( G_{5} \) across multiple graph datasets, we will first provide the learning results of \( G_{5} \) on node classification based on each graph dataset in an isolated learning mode in Table I. The isolated version of \( G_{5} \) is very similar to Graph-BERT studied in [35] actually, except that \( G_{5} \) will have two more graph-transformer layers (i.e., the input processing component for each dataset) besides the shared universal Graph-BERT component. To
| Input Graphs & $k$ | Graphs | datasets (Accuracy) |
|-------------------|--------|---------------------|
|                   |        | Cora | Citeseer | Pubmed |
|                   | $k$    | 5    | 0.834 | 0.707 | — |
|                   |        | 7    | 0.835 | 0.717 | — |
|                   |        | 15   | 0.828 | 0.702 | — |
|                   |        | 30   | 0.822 | 0.698 | — |
|                   | $k$    | 5    | 0.832 | —     | 0.772 |
|                   |        | 7    | —     | 0.728 | 0.666 |
|                   |        | 15   | 0.829 | —     | 0.782 |
|                   |        | 30   | 0.816 | —     | 0.791 |

To make the comparison more complete, in addition to GRAPH-BERT [35], we also provide the learning results of several classic graph classification methods, e.g., LP [38], ICA [16], ManiReg [2], SemiEmb [30], recent graph embedding methods, DeepWalk [22], Planetoid [31], MoNet [20], and the latest graph representation learning approaches, e.g., GCN [11], GAT [29], LoopyNet [32]. According to the results, the scores achieved by G5 are very close to those of GRAPH-BERT, which are much higher than the scores obtained by the other baseline methods.

### C. Results of G5 on Mixed Graph Input

In Table II, we provide the learning results of G5 learned with multiple graph inputs. To be more specific, given the input graphs, we will pre-train G5 with the hybrid application tasks on these graph datasets. Such pre-trained G5 model will be further fine-tuned on each graph for the node classification task. For each graph, the parameter $k$ of its input pre-processing component is assigned with the default parameter as introduced before. Meanwhile, for the universal GRAPH-BERT involved in G5, we change its input size parameter $k$ with values in $\{5, 7, 15, 30\}$, where 5, 7 and 30 are the optimal parameter $k$ for Citeseer, Cora and Pubmed, respectively, and value 15 balances among these optimal parameters.

According to the results, we observe that training G5 concurrently with multiple input graphs and hybrid application tasks will have some minor impacts on its performance on the node classification task. In some cases, compared with Table I there are some drops of the scores, e.g., G5 on Cora. Meanwhile, in some other cases, the learning performance of G5 can also be very good, which are highlighted in the table. What’s more, parameter $k$ of the universal GRAPH-BERT model does have an impact on the performance of G5, where Cora and Citeseer favor small $k$, whereas Pubmed prefers larger $k$ instead. To achieve the balanced performance, we will set $k = 15$ for the following studies on G5 transfer across different graph datasets.

### D. Transfer of G5 to Sparsely Labeled Graph

In Table III we provide the learning results of G5 on graphs with sparse labels. To be more specific, we will pre-train G5 on the source graphs with the hybrid application tasks and transfer the pre-trained model to the target graph(s) for evaluation. Since we focus on the graphs with sparse labels, a small portion of the labeled data are sampled from the target graph for model fine-tuning, where the sampling ratio changes with value in $\{5\% , 10\%, \ldots, 50\% \}$. Meanwhile, for comparison completeness, we also provide the results of G5 without pre-training in the table, where the parameter $k$ of the universal component is assigned with the optimal values favored by the graph datasets. According to the results, in most of the cases, G5 with pre-training can out-perform that without pre-training consistently.

### E. Reasoning of G5 for Apocalypse Learning

In Table IV we provide the learning results of G5 based on the apocalypse learning settings, where the target graph has no labeled data at all. All the existing graph neural networks will fail to work in such a learning setting. To enable G5 can work to address the node classification problem on the target graph, we pre-train G5 on the source graphs to learn the universal GRAPH-BERT component shared across graphs. Furthermore, such pre-trained G5 will be further fine-tuned on the target graph with the unsupervised learning tasks, i.e., node attribute reconstruction and graph recovery, so as to learn the input component for the target graph in G5. Based on the CCCM and CDR reasoning strategies, G5 will still be able to reason for the potential labels for the nodes in the target graph. For comparison, we also provide the results of random guess in the table, and the scores achieved by G5 with these two reasoning strategies are both much higher than random guess.

### VI. Related Work

Several interesting research topics are related to this paper, which include graph neural network and BERT.

**Graph Neural Network:** In addition to the graph convolutional neural network [11] and its derived variants [29], [26], [14], many great research works on graph neural networks have been witnessed in recent years for graph representation learning [11], [36], [8], [37]. Many existing graph neural network models will suffer from performance problems with deep architectures. In [34], [13], [26], [7], the authors explore to build deep graph neural networks with residual learning, dilated convolutions, and recurrent network, respectively. In [35], the authors introduce a new type of graph neural network based on graph transformer and BERT, i.e., the GRAPH-BERT model. Different from the node representation learning [11], [29], GNNs proposed for the graph representation learning aim at learning the representation for the entire graph instead [21]. To handle the graph node permutation invariant challenge, solutions based various techniques, e.g., attention [3], [18], pooling [18], [24], [9], capsule net [17], Weisfeiler-Lehman kernel [12] and sub-graph pattern learning and matching.
TABLE III

| Source Graph(s) & Target Graph & k | Training Data Sampling Ratio (Accuracy) |
|-----------------------------------|----------------------------------------|
|                                   | 5%  | 10%  | 15%  | 20%  | 25%  | 30%  | 35%  | 40%  | 45%  | 50%  |
| Cora                              |     |      |      |      |      |      |      |      |      |      |
| Citeseer                          | 0.418 | 0.569 | 0.541 | 0.546 | 0.557 | 0.600 | 0.593 | 0.607 | 0.623 | 0.661 |
| Pubmed                            | 0.530 | 0.649 | 0.669 | 0.692 | 0.692 | 0.687 | 0.692 | 0.697 | 0.710 | 0.743 |
| Citeseer                          | 0.262 | 0.420 | 0.546 | 0.619 | 0.684 | 0.662 | 0.706 | 0.727 | 0.729 | 0.748 |
| Pubmed                            | 0.524 | 0.692 | 0.697 | 0.682 | 0.725 | 0.717 | 0.756 | 0.749 | 0.749 | 0.741 |

TABLE IV

| Source & Target Graph(s) | Reasoning Strategies |
|--------------------------|----------------------|
| Source(s)                | CCCM | CDR | Random |
| Cora                     | 0.280 | 0.312 | 0.167 |
| Citeseer                 | 0.531 | 0.544 | 0.333 |
| Pubmed                   | 0.505 | 0.515 | 0.333 |
| Citeseer                 | 0.332 | 0.358 | 0.143 |
| Pubmed                   | 0.323 | 0.358 | 0.143 |
| Citeseer & Pubmed        | 0.342 | 0.304 | 0.143 |
| Cora & Citeseer          | 0.323 | 0.331 | 0.167 |
| Cora & Pubmed            | 0.342 | 0.304 | 0.143 |
| Citeseer & Pubmed        | 0.327 | 0.319 | 0.143 |

VII. Conclusion

In this paper, we have studied the graph-to-graph transfer of a universal GRAPH-BERT for graph representation learning across different graph datasets. To address the problem, we introduce a new learning model named G5, whose pluggable architecture containing several key parts, i.e., (1) pluggable input dataset-wise components, (2) input size unification interlayer, (3) the universal Graph-Bert model shared across graphs, (4) representation fusion interlayer; (5) pluggable task-wise output components for each dataset, and (6) reasoning component for apocalypse learning. Furthermore, based on the G5 model, we also investigate a special and novel learning task, i.e., the apocalypse learning problem, which aims at learning a classifier without using any labeled data. Two different reasoning strategies, i.e., CCCM and CDR, are proposed to reason for the potential labels for the nodes. To test the effectiveness of G5, some preliminary experiments have been done on real-world graph datasets and the results also demonstrate the effectiveness of both G5 and these two proposed reasoning strategies.

[19], have been proposed. To apply GRAPH-BERT on graph instance modeling and handle diverse graph instance sizes, [53] proposes several different graph instance size unification approaches.

BERT: Transformer [28] and Bert [5] based models have almost dominated NLP and related research areas in recent years due to their great representation learning power. Prior to that, the main-stream sequence transduction models in NLP are mostly based on complex recurrent [6], [4] or convolutional neural networks [10]. However, as introduced in [28], the inherently sequential nature precludes parallelization within training examples. To address such a problem, a brand new representation learning model solely based on attention mechanisms, i.e., the transformer, is introduced in [28], which dispense with recurrence and convolutions entirely. Based on Transformer, [5] further introduces BERT for deep language understanding, which obtains new state-of-the-art results on eleven natural language processing tasks. By extending Transformer and Bert, many new BERT based models, e.g., T5 [23], ERNIE [27] and RoBERTa [15], can even out-perform the human beings on almost all NLP benchmark datasets.
REFERENCES

[1] A. Atamma, N. Sokolovska, and J.-C. CRIVELLO. SPI-GCN: A Simple Permutation-Invariant Graph Convolutional Network. working paper or preprint, Apr. 2019.

[2] M. Belkin, P. Niyogi, and V. Sindhwani. Manifold regularization: A geometric framework for learning from labeled and unlabeled examples. J. Mach. Learn. Res., 7:2399–2434, Dec. 2006.

[3] F. Chen, S. Pan, J. Jiang, H. Huo, and G. Long. DAGCN: dual attention graph convolutional networks. CoRR, abs/1904.02278, 2019.

[4] J. Chung, Ç. Gülçehre, K. Cho, and Y. Bengio. Empirical evaluation of gated recurrent neural networks on sequence modeling. CoRR, abs/1412.3555, 2014.

[5] J. Devlin, M. Chang, K. Lee, and K. Toutanova. BERT: pre-training of deep bidirectional transformers for language understanding. CoRR, abs/1810.04805, 2018.

[6] S. Hochreiter and J. Schmidhuber. Long short-term memory. Neural Comput., 9(8), Nov. 1997.

[7] B. Huang and K. M. Carley. Inductive graph representation learning with recurrent graph neural networks. CoRR, abs/1904.08035, 2019.

[8] S. Ivanov and E. Burnaev. Anonymous walk embeddings. CoRR, abs/1805.11921, 2018.

[9] J. Jiang, Z. Cui, C. Xu, and J. Yang. Gaussian-induced convolution for graphs. CoRR, abs/1811.04393, 2018.

[10] Y. Kim. Convolutional neural networks for sentence classification. In Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing (EMNLP), pages 1746–1751, Doha, Qatar, Oct. 2014. Association for Computational Linguistics.

[11] T. N. Kipf and M. Welling. Semi-supervised classification with graph convolutional networks. CoRR, abs/1609.02907, 2016.

[12] N. M. Kriege, P.-L. Giscard, and R. Wilson. On valid optimal assignment kernels and applications to graph classification. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, Advances in Neural Information Processing Systems 29, pages 1623–1631. Curran Associates, Inc., 2016.

[13] Q. Li, Z. Han, and X. Wu. Deeper insights into graph convolutional networks for semi-supervised learning. CoRR, abs/1801.07606, 2018.

[14] G. Lin, J. Wang, K. Liao, F. Zhao, and W. Chen. Structure fusion based on graph convolutional networks for semi-supervised classification. CoRR, abs/1907.02586, 2019.

[15] Y. Liu, M. Ott, N. Goyal, J. Du, M. Joshi, D. Chen, O. Levy, M. Lewis, L. Zettlemoyer, and V. Stoyanov. Roberta: A robustly optimized BERT pretraining approach. CoRR, abs/1907.11692, 2019.

[16] Q. Lu and L. Getoor. Link-based classification. In Proceedings of the Twentieth International Conference on International Conference on Machine Learning, ICML’03, pages 496–503. AAAI Press, 2003.

[17] M. D. G. Mallea, P. Melzner, and P. J. Bentley. Capsule neural networks for graph classification using explicit tensorial graph representations. CoRR, abs/1902.08399, 2019.

[18] P. Melzner, M. D. G. Mallea, and P. J. Bentley. Pinet: A permutation invariant graph neural network for graph classification. CoRR, abs/1905.03046, 2019.

[19] L. Meng and J. Zhang. Isomn: Isomorphic neural network for graph representation learning and classification. CoRR, abs/1907.00495, 2019.

[20] F. Monti, D. Boscaini, J. Masci, E. Rodolà, J. Svoboda, and M. M. Bronstein. Geometric deep learning on graphs and manifolds using mixture model cnns. CoRR, abs/1611.08402, 2016.

[21] A. Narayanan, M. Chandramohan, R. Venkatesan, L. Chen, Y. Liu, and S. Jaiswal. graph2vec: Learning distributed representations of graphs. CoRR, abs/1707.05005, 2017.

[22] B. Perozzi, R. Al-Rfou, and S. Skiena. Deepwalk: Online learning of social representations. CoRR, abs/1403.6652, 2014.

[23] C. Raffel, N. Shazeer, A. Roberts, K. Lee, S. Narang, M. Matena, Y. Zhou, W. Li, and P. J. Liu. Exploring the limits of transfer learning with a unified text-to-text transformer. arXiv preprint arXiv:1910.10683, 2019.

[24] E. Ranjan, S. Sanyal, and P. P. Talukdar. Asap: Adaptive structure aware pooling for learning hierarchical graph representations. arXiv preprint arXiv:1911.07979, 2019.

[25] R. Socher, M. Ganjoo, C. D. Manning, and A. Ng. Zero-shot learning through cross-modal transfer. In C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 26, pages 935–943. Curran Associates, Inc., 2013.