Abstract—Heterogeneous graphs generally refers to graphs with different types of nodes and edges. A common approach for extracting useful information from heterogeneous graphs is to use meta-graphs, which can be seen as a special kind of directed acyclic graph (DAG) with same node and edge types as the heterogeneous graph. However, how to design proper meta-graphs is challenging. Recently, there have been many works on learning suitable meta-graphs from a heterogeneous graph. Existing methods generally introduce continuous weights for edges that are independent of each other, which ignores the topological structure of meta-graphs and can be ineffective. To address this issue, we propose a new viewpoint from tensor on learning meta-graphs. Such a viewpoint not only helps interpret the limitation of existing works by CANDECOMP/PARAFAC (CP) decomposition, but also inspires us to propose a topology-aware tensor decomposition, called TENSUS, that reflects the structure of DAGs. The proposed topology-aware tensor decomposition is easy to use and simple to implement, and can be taken as a plug-in part to upgrade many existing works, including node classification and recommendation on heterogeneous graphs. Experimental results on different tasks demonstrate that the proposed method can significantly improve the state-of-the-arts for all these tasks.

Index Terms—Heterogeneous graph, Graph neural network, Tensor decomposition.

I. INTRODUCTION

Heterogeneous graphs [1] refer to graphs where nodes and edges can have multiple types. Since it can model different types of relations, heterogeneous graph naturally appears in many real-world scenarios. An example is the academic network (e.g. the Microsoft Academic Graph [2]). The nodes here can have multiple types, e.g., “paper”, “author” or “institution”, and edges indicate different relations, e.g. an edge between an “author” node and a “paper” node indicates “authorship” relationship, while an edge between an “author” node and an “institution” node indicates “affiliation” relationship. Another example is a social network [3], which is also a heterogeneous graph if we allow two users (nodes) to have different interactions (edges).

Due to the presence of multiple node types and edge types, a heterogeneous graph potentially contains a lot of semantic information [4]–[7]. An early attempt to exploit such information is by using meta-paths [4]. A meta-path is a path with edge types from a heterogeneous graph. It can be seen as a generalization of edge and defines a composite relation between nodes. Thus, different meta-paths will define different composite relations and extract different semantic information from the heterogeneous graph. There are many methods utilizing meta-paths to extract information from heterogeneous graphs. For example, metapath2vec [8] proposes to obtain embeddings for different nodes by performing random walks along meta-paths. HAN [9] and MAGNN [10] improve upon this idea and use a graph neural network (GNN) [11] to obtain node embeddings.

However, the path structure can be too restricted to define complex relations between nodes. To alleviate this problem, meta-graphs [6], [7] generalizes meta-path to more flexible structures other than path. A meta-graph is represented by a directed acyclic graph (DAG), whose nodes and edges have the same types as the heterogeneous graph. Similar to the meta-path, a meta-graph also define a composite relation between nodes in the heterogeneous graph. And since it uses a more flexible DAG structure, it can define more complex relations and help extract semantic information from the heterogeneous graph. Nevertheless, the meta-graphs still need to be predefined, which requires prior knowledge and huge human efforts to design. Besides, the performance of these methods are also sensitive to the choices of meta-graphs [7], [12].

To eliminate human efforts in designing meta-graphs, recent works try to directly learn an informative meta-graph [12]–[14] from a given heterogeneous graph. Observed that meta-graphs are derived from a plain DAG by assigning different types to edges. Given a plain DAG, the meta-graph learning problem can be seen as learning the edge type for each edge in a given plain DAG. By assigning each edge a set of weights for its edge types, we can transform this problem to a continuous optimization problem. This provides us a unified framework for these recent works. For example, GTN [13] considers a plain DAG with a path-like structure, and uses the same transformation introduced before to make it a continuous optimization problem. HGT [15] computes mutual attention scores for different types of edges, which can be seen as a different way to optimize weights on edge types. GEMS [14] considers a general plain DAG than GTN and uses genetic search to find a proper meta-graph. While GEMS can learn meta-graphs instead of only meta-paths like GTN, its computational cost is much higher due to the genetic search algorithm for discrete optimization. In recent years, neural network architecture search (NAS) [16] has demonstrated powerful capabilities in graphs [17], [18]. Some NAS-based methods for heterogeneous graph have been researched and applied to learning tasks of heterogeneous...
graphs [12], [19] DiffMG [12] is current the state-of-the-art on designing meta-graph. By parameterization choices of edge types as a differentiable propagation matrix in GNN, it learns the meta-graph in an end-to-end manner efficiently by stochastic gradient descent.

However, existing methods do not consider the effect of different DAG topological structures. For example, consider the two plain DAGs in Fig. 1 whose edges have no specific edge types. While they both have the same number of edges, the relations between their edges are definitely not the same and worth consideration. While GTN simply cannot learn meta-graphs, the genetic search in GEMS and differentiable parameterization in DiffMG both ignore above topological difference.

Motivated by this limitation, we propose a new meta-graph learning method that is aware of the topological structures of different DAGs. We first view the meta-graph learning as a problem on tensor, and demonstrate that GTN/DiffMG can indeed be seen as using the simple rank-1 CP (CANDDECOMP / PARAFAC) tensor decomposition to express a tensor [20], [21], which only has limited expressive power. From the tensor perspective, we propose to introduce a family of tensor decompositions that can change with the topological structure of different DAGs. While a number of tensor decompositions [22], [23] have been developed to incorporate structure information into tensor decompositions, they are mainly designed for simple structures and not suitable for learning meta-graphs, which can have very different structures. Moreover, existing applications of tensor decompositions mainly focus on the approximation of a given tensor, whereas here the goal is to learn the tensor from data by imposing a tensor structure based on the associated meta-graphs. Extensive empirical results on different downstream tasks of heterogeneous graphs show that it outperforms the state-of-the-arts.

Our contributions are summarized as:

- We give a tensor view on meta-graph learning, and highlight the drawbacks of existing methods from the perspective of tensor decomposition;
- Based on tensor decomposition, we propose a novel parameterization that is aware of the topological structures of different DAGs;
- We conduct experiments on various downstream applications of heterogeneous graph as well as the logic rule learning problem on knowledge graph. Results demonstrate the performance gain of our topology-aware parameterization.

Notations. We use boldface lowercase letters (e.g., \( \mathbf{u} \)) to denote vectors, boldface uppercase letters (e.g., \( \mathbf{T} \)) to denote matrices, and calledigraph uppercase letter (e.g., \( T \)) to denote tensors. The \( i \)-th element of a vector \( \mathbf{u} \) is denoted \( u(i) \). element \((i, j)\) of a matrix \( \mathbf{A} \) is denoted \( A(i, j) \), and element \((i_1, \ldots, i_k)\) of a tensor \( T \) is denoted \( T(i_1, \ldots, i_k) \). We also use : (e.g., \( \mathbf{A}(i,:) \) or \( T(i_1, \ldots, i_k) \)) to denote all elements in a matrix or tensor along a specific axis.

II. BACKGROUND: HETEROGENEOUS GRAPHS

Definition 1 (Heterogeneous Graph [1]). A heterogeneous graph is a graph \( G = \{V, E, N, R, f_N, f_R\} \), where \( V \) is the set of nodes, \( E \) is the set of edges, \( N \) is the set of node types, \( R \) is the set of edge types, \( f_N : V \rightarrow N \) is a mapping from nodes to node types, and \( f_R \) is a mapping from edges to edge types.

When \(|N| = |R| = 1\), a heterogeneous graph reduces to a homogeneous graph. In this paper, we focus on the case where both \(|N|\) and \(|R|\) are larger than 1. An example is shown in Fig. 1(a) which has 4 types of nodes (author (A), paper (P), institution (I), venue (V)), and 6 types of edges specifying the types of nodes connected (A-I/I-A, A-P/P-A, P-V/V-P).

Given a heterogeneous graph with \( C \) edge types, we have a set of \( C \) adjacency matrices \( \mathbf{A} = \{\mathbf{A}^1, \ldots, \mathbf{A}^C\} \), one for each edge type. A naive approach is to ignore the edge types, which reduces the heterogeneous graph to a homogeneous graph. Standard graph data mining algorithms (such as DeepWalk [24]) or graph neural networks (GNN) (such as GCN [11] or GAT [25]) can then be used. However, edge types are often critical, and ignoring them can lead to poor performance.

To utilize edge type information, a common approach is to use meta-paths:

Definition 2 (Meta-path [4]). A meta-path \( \mathcal{P} \) is a sequence of node and edge types: \( \mathcal{P} = t_0 \xrightarrow{e_1} t_1 \xrightarrow{e_2} \cdots \xrightarrow{e_{M-1}} t_M \), where \( t_0, \ldots, t_M \in N \) and \( e_1, \ldots, e_{M-1} \in R \).

Fig. 1(b) shows an example meta-path “A-P-V-P-A”. Specifically, it expresses the relationship that two authors publish papers in the same venue. A natural and more powerful extension of the meta-path is the meta-graph, which uses a more flexible DAG structure.

Definition 3 (Meta-graph [5], [6]). A meta-graph \( \mathcal{M} \) is a directed acyclic graph (DAG), where its node types and edge types are subsets of \( N \) and \( R \), respectively.

To be consistent with the meta-path, we also restrict the meta-graph to have only a single source node and a single target node. Fig. 1(c) shows an example meta-graph, which describes a complex relation in which two authors publish papers in the same venue. A natural and more powerful extension of the meta-path is the meta-graph, which uses a more flexible DAG structure.

A. Tensor Decomposition

A tensor is a high-dimensional array describing multilinear relations among objects. Consider an \( M \)-order tensor \( \mathbf{T} \) of size \( C_1 \times \cdots \times C_M \). As \( M \) increases, obviously it becomes more expensive to store all its entries. In recent decades, a number of tensor decompositions with more efficient storage have been developed [21], [22], [23], [24]. A classic example is the CP (CANDDECOMP/PARAFAC) decomposition [20], [21].

The \( (i_1, i_2, \ldots, i_M)-\)th entry of \( \mathbf{T} \) is given as:

\[
T(i_1, \ldots, i_M) = \sum_{r=1}^{d} \prod_{m=1}^{M} G_m(i_m, r),
\] (1)
where each \( G_m \in \mathbb{R}^{C_m \times d} \), and \( d \) is the rank. Another well-known example is the Tucker decomposition \([21],[28]\). However, its number of parameters still scales exponentially with the tensor order, and can be problematic even for a moderate \( M \).

To avoid the curse of dimensionality in high-order tensors, a class of more complex tensor decompositions called tensor networks have been proposed \([22],[23]\). A popular example is the tensor train (TT) \([27]\), which decomposes \( T \) as:

\[
T(i_1, \ldots, i_M) = \sum_{r_1=1}^{d_1} \cdots \sum_{r_M=1}^{d_{M-1}} W_1(i_1, r_1) W_2(i_2, r_1, r_2) \cdots W_{M-1}(i_{M-1}, r_{M-2}, r_{M-1}) W_M(i_M, r_{M-1}),
\]

where \( W_i \in \mathbb{R}^{C_i \times d_i}, W_M \in \mathbb{R}^{C_M \times d_{M-1} \times d_M} \), and \( W_i \)'s are 3-order tensors with size \( C_m \times d_{m-1} \times d_m \). These matrices and tensors are called core tensors, and \( d_m \)'s are the ranks. As the name implies, the TT has a train-like (sequential) computation process.

The TT decomposition has been successfully used in many applications \([27],[29],[30]\). However, it assumes a simple line structure in the tensor, and is not suitable for more complicated tensor structures. Recently, Li and Sun \([31]\) attempt to directly search for an appropriate tensor decomposition by genetic search. Nevertheless, this is very expensive.

### III. RELATED WORKS

#### A. Learning with given meta-path / meta-graph

The edge types in the meta-path can help guide the GNN graph convolutions and thus produce more informative node embeddings. For example, MAGNN \([10]\) updates the node embedding \( H^{(k)} \) at the \( k \)th iteration as:

\[
H^{(k)} = f(H^{(k-1)}; A^{i_k}), \quad k = 1, 2, \ldots, K,
\]

where \( K \) is the number of edges in a given meta-path, \( H^{(0)} \) is the initial node embedding (usually set to the node feature matrix \( X \)), \( f(H; A) = \sigma(AH\Theta) \) is the standard graph convolution \([11]\) with parameter \( \Theta \), and \( A^k \) (with \( i_k \in \{1, \ldots, C\} \)) is the adjacency matrix of the \( k \)th edge in the meta-path. Fig. 2 shows an example with \( K = 4 \). Similarly, meta-graphs can also be used to help the GNN to learn node embeddings.

#### B. Meta-path / meta-graph learning

Section III-A rely on predefined meta-paths or meta-graphs. However, designing meta-paths and/or meta-graphs require domain knowledge, and can be expensive or even infeasible. A natural extension is to directly learn the meta-path or meta-graph from the heterogeneous graph. Earlier works such as GTN \([13]\) and HGT \([15]\) focus on the learning of meta-paths. Since the edge type to be used in each segment of the meta-path is not known (Fig. 3(a)), the update in (3) is extended and the node embedding is obtained as a weighted combination of the convolution outputs from all \( C \) candidate edge types:

\[
H^{(k)} = \sum_{i=1}^{C} \alpha^{(k-1,k)}_i f(H^{(k-1)}; A^i), \quad k = 1, \ldots, K,
\]

where \( \{\alpha^{(k-1,k)}_i\}_{i=1}^{C} \) are the weights (which sum to 1) that are learned together with the graph convolution parameter \( \Theta \). After convergence, for each edge \( H^{(k-1)} \rightarrow H^{(k)} \), the edge type \( i \) with the largest weight \( \alpha^{(k-1,k)}_i \) is chosen to form the meta-path.

**Fig. 1:** An example heterogeneous graph, and an associated meta-path and meta-graph. In this example, the edge type is implicitly specified by the two node types that the edge connects.

**Fig. 2:** Computation of node embeddings (top) using a given meta-path (bottom).
More recently, meta-graph learning methods (such as GEMS \cite{13} and DiffMG \cite{12}) learn meta-graphs with general structures (Fig. 3(b)). Here, we focus on the state-of-the-art DiffMG. At the \(k\)th iteration, DiffMG updates the node embedding by using node embeddings \(\{H^{(b)},\ldots,H^{(k-1)}\}\) at all previous iterations:

\[
H^{(k)} = \sum_{i=1}^{C} \sum_{j=0}^{k-1} \alpha_i^{(j,k)} f(H^{(j)}, A^{(k)}), \quad k = 1, \ldots, K,
\]

where the learnable weights \(\alpha_i^{(j,k)}\) satisfy \(\sum_{i=1}^{C} \alpha_i^{(j,k)} = 1\) for each \((j, k)\) pair. After convergence, DiffMG also obtains a meta-graph by choosing the edge type \(i\rightarrow j,k\) with the largest \(\alpha_i^{(j,k)}\) in each \(H^{(j)} \rightarrow H^{(k)}\) edge.

IV. Tensor Formulation for Meta-Graph Learning

In this section, we formulate meta-graph learning in terms of tensors. Section IV-A first shows the connection between some existing works on meta-path/meta-graph learning with rank-1 CP decomposition. Section IV-B then proposes a novel tensor decomposition for meta-path/meta-graph learning. Section IV-C introduces how the proposed decomposition is used for meta-graph learning.

A. Existing Meta-Graph Learning as Rank-1 CP Decomposition

Since each \(H^{(k)}\) in (5) is computed from \(\{H^{(0)},\ldots,H^{(k-1)}\}\), the computation graph for \(\{H^{(0)},\ldots,H^{(K)}\}\) has \(M = K(K+1)/2\) edges. We index these \(M\) edges as \(\{(g_1,\ldots,g_M)\}\), in which each \(g_m = (j,k)\) corresponds to the edge \(H^{(j)} \rightarrow H^{(k)}\). There are thus a total of \(C^M\) candidate meta-graphs. Each such candidate can be specified by the \(M\)-tuple \((i_{g_1},i_{g_2},\ldots,i_{g_M})\), where \(i_{g_m} \equiv i_{j,k} \in \{1,\ldots,C\}\) represents the edge type used for edge \(g_m\) connecting \(H^{(j)}\) to \(H^{(k)}\). As noted above, existing methods (such as GTN, HGT and DiffMG) form the meta-path/graph by selecting the edge type \(i\rightarrow j,k\) with the largest weight for each \((j, k)\) pair in (5). This is equivalent to finding the meta-graph \(M\) which maximizes the score 

\[
w_{M} = \prod_{k=1}^{K} \prod_{j=0}^{k-1} \alpha_{i,j,k}^{(j,k)}
\]

(for GTN \cite{13}, this reduces to the form

\[
w_{M} = \prod_{k=1}^{K} \alpha_{i}^{(k-1,k)}.
\]

A compact way to store the scores of all candidate meta-graphs is to use a \(M\)-order tensor \(T\), with:

\[
T(i_{g_1},\ldots,i_{g_M}) = \prod_{k=1}^{K} \prod_{j=0}^{k-1} \alpha_{i,j,k}^{(j,k)}.
\]

Note that this is a rank-1 CP decomposition in \(\mathcal{R}\), with \(d = 1\) and \(G_m(i_{j,k},1) = \alpha_{i,j,k}^{(j,k)}\). In other words, DiffMG is implicitly using a rank-1 CP decomposition. However, it is known that rank-1 CP decomposition only has limited expressive power \cite{21}.

B. Encoding Meta-Path/Meta-Graph Structure by Tensor Decomposition

In this section, we propose a novel tensor decomposition, called TENSUS (Tensor Meta-graph Learning). It is more powerful than the rank-1 CP decomposition, and performs meta-path/meta-graph learning by taking the local graph structures into consideration.

1) Encoding Meta-Paths: We first consider the special case of meta-path learning. The simplest meta-path involves only two node embeddings: \(H^{(0)}\) and \(H^{(1)}\) (Fig. 4(a)). As there is only one edge \((H^{(0)} \rightarrow H^{(1)})\), the weights for all \(C\) candidate edge types can be stored in a vector \(W_{0,1} \in \mathcal{R}^C\), where the subscripts correspond to the node embedding indices.

Next, consider the case with 3 node embeddings \(H^{(0)}, H^{(1)}\) and \(H^{(2)}\), in which \(H^{(1)}\) is computed from \(H^{(0)}\) and then \(H^{(2)}\) computed from \(H^{(1)}\). Recall from (6) that \(T(i_{0,1},i_{1,2}) = \alpha_{i_{0,1}}^{(0,1)} \alpha_{i_{1,2}}^{(1,2)}\). The tensor \(T\) (which reduces to a \(C \times C\) matrix here) thus equals \(\alpha_{i}^{(0,1)}(\alpha_{i}^{(1,2)})^T\) (where \(\alpha_{i}^{(0,1)} = [\alpha_{i}^{(0,1)}]\)  and \(\alpha_{i}^{(1,2)} = [\alpha_{i}^{(1,2)}]\) and is rank-1. In the following, we propose to replace this by a rank-\(d\) matrix, which is more expressive than a rank-1 matrix but less expensive than a full matrix:

\[
T(i_{0,1},i_{1,2}) = \sum_{r_1=1}^{d} W_{0,1}(i_{0,1},r_1)W_{1,2}(i_{1,2},r_1),
\]

where \(W_{0,1},W_{1,2} \in \mathcal{R}^{C \times d}\) are learnable matrices corresponding to the edges \(H^{(0)} \rightarrow H^{(1)}\) and \(H^{(1)} \rightarrow H^{(2)}\), respectively.

When there are 4 node embeddings, \(T\) becomes a 3-order tensor. We propose to use the tensor train (TT) decomposition
(Section [II-A]) which follows a path-like computation similar to meta-path. Using (2), the tensor $T$ is (Fig. 4(b)):

$$
T(i_{0,1}, i_{1,2}, i_{2,3}) = \sum_{r_1=1}^{d} \sum_{r_2=1}^{d} W_{0,1}(i_{0,1}, r_1) W_{1,2}(i_{1,2}, r_1, r_2) W_{2,3}(i_{2,3}, r_2).
$$

(8)

Similar to (7), each $W_{i,j,k}$ in (8) corresponds to the edge $H^{(j)} \rightarrow H^{(k)}$, and each index $r_k$ corresponds to an intermediate $H^{(k)}$. When $d = 1$, (8) reduces to $T(i_{0,1}, i_{1,2}, i_{2,3}) = W_{0,1}(i_{0,1}, 1) W_{1,2}(i_{1,2}, 1, 1) W_{2,3}(i_{2,3}, 1)$, which is equivalent to $\alpha_{i_{0,1}} \alpha_{i_{1,2}} \alpha_{i_{2,3}}$ in (6), with only a difference in notations.

For the general case with node embeddings $H^{(0)}, \ldots, H^{(K)}$, we again use the TT decomposition on higher-order tensors. Similar to (8), we have:

$$
T(i_{0,1}, \ldots, i_{K-1}, K) = \sum_{r_1=1}^{d} \cdots \sum_{r_{K-1}=1}^{d} W_{0,1}(i_{0,1}, r_1) W_{1,2}(i_{1,2}, r_1, r_2) \cdots W_{K-1,K}(i_{K-1,K}, r_{K-1}).
$$

(9)

When $d = 1$, this also becomes equivalent to (6).

2) Encoding Meta-Graphs: In this section, we consider the encoding of meta-graphs. When there are only 2 nodes, the meta-graph is the same as a meta-path as we only have one edge. When there are 3 nodes, recall from (5) that $H^{(2)}$ is computed by summing the graph convolutions due to $H^{(0)}$ and $H^{(1)}$ (Fig. 4(c)). Let $T_1(i_{0,1}, i_{1,2})$ and $T_2(i_{0,2})$ be the matrix and vector containing the scores for $H^{(0)} \rightarrow H^{(1)} \rightarrow H^{(2)}$ and $H^{(0)} \rightarrow H^{(2)}$ and $H^{(0)} \rightarrow H^{(2)}$ are independent, their scores can be simply multiplied together to obtain the score of the whole graph as:

$$
T(i_{0,1}, i_{0,2}, i_{1,2}) = T_1(i_{0,1}, i_{1,2}) T_2(i_{0,2}).
$$

(10)

To represent all possible $(i_{0,1}, i_{0,2}, i_{1,2})$ combinations, $T_1$ can be stored as a $C \times C$ matrix, and $T_2$ as a $C$-dimensional vector. Similar to (7), we propose to express $T_1$ by rank-$d$ decomposition, i.e.,

$$
T_1(i_{0,1}, i_{1,2}) = \sum_{r_1=1}^{d} W_{0,1}(i_{0,1}, r_1) W_{1,2}(i_{1,2}, r_1),
$$

with $W_{0,1}, W_{1,2} \in \mathbb{R}^{C \times d}$. Thus, (10) becomes:

$$
T(i_{0,1}, i_{0,2}, i_{1,2}) = \sum_{r_1=1}^{d} W_{0,1}(i_{0,1}, r_1) W_{1,2}(i_{1,2}, r_1) w_{0,2}(i_{0,2}).
$$

(11)

As in section [IV-B1] when $d = 1$, (10) reduces to $T(i_{0,1}, i_{1,2}, i_{2,3}) = W_{0,1}(i_{0,1}, 1) W_{1,2}(i_{1,2}, 1, 1) w_{0,2}(i_{0,2})$, which is equivalent to $\alpha_{i_{0,1}} \alpha_{i_{1,2}} \alpha_{i_{0,2}}$ in (6), with only a difference in notations.

Fig. 4(c) shows the computation in (11) graphically. $W_{0,1}$ and $W_{1,2}$ in (11) share an index $r_1$ as the edges correspond to $H^{(0)} \rightarrow H^{(1)}$ and $H^{(1)} \rightarrow H^{(2)}$ share an internal node. Thus, index $r_1$ can be viewed as corresponding to the intermediate $H^{(1)}$, as in (9).

For the general case with node embeddings $H^{(0)}, \ldots, H^{(K)}$, we can similarly extend the correspondence in (9) and (11) by introducing indices $r_k$ for node embedding $H^{(k)}$, and core tensor $W_{i,j,k}$ for the edge $H^{(j)} \rightarrow H^{(k)}$. Since the computation for $H^{(K)}$ is also different now, $T$ also takes a different form and becomes:

$$
T(i_{0,1}, \ldots, i_{K-1}, K) = \sum_{r_1=1}^{d} \cdots \sum_{r_{K-1}=1}^{d} W_{0,1}(i_{0,1}, r_1) \cdots W_{0,K-1}(i_{0,K-1}, r_{K-1}) W_{1,2}(i_{1,2}, r_1, r_2) \cdots W_{K-2,K-1}(i_{K-2,K-1}, r_{K-2}, r_{K-1}) w_{0,K}(i_{0,K}) W_{1,K}(i_{1,K}, r_1) \cdots W_{K-1,K}(i_{K-1,K}, r_{K-1}).
$$

(12)

By keeping only the edges $H^{(0)} \rightarrow H^{(1)}, H^{(1)} \rightarrow H^{(2)}, \ldots, H^{(K-1)} \rightarrow H^{(K)}$, the above is reduced to:

$$
T(i_{0,1}, \ldots, i_{K-1}, K) = \sum_{r_1=1}^{d} \cdots \sum_{r_{K-1}=1}^{d} W_{0,1}(i_{0,1}, r_1) W_{1,2}(i_{1,2}, r_1, r_2) \cdots W_{K-1,K}(i_{K-1,K}, r_{K-1}),
$$

which is of the same form in (9).
C. Optimization Algorithm

To obtain the final node embedding \( H^{(K)} \), we solve the following optimization problem:

\[
\min_{\Theta, \{W_{j,k}\}} \mathcal{L}(H^{(K)})
\]

\[
\text{s.t. } \sum_{i_1=1}^{C} \cdots \sum_{i_m=1}^{C} T(i_{g_1}, \ldots, i_{g_m}) = 1, \quad (14)
\]

\[
T(i_{g_1}, \ldots, i_{g_m}) \geq 0, \quad (15)
\]

where \( \Theta \) is the GNN model parameter, and \( \mathcal{L} \) is an appropriate loss function. The constraints ensure that the scores in \( \mathcal{T} \) are non-negative and sum to a constant.

1) Differentiable transformation: To enforce the constraints \( (14) \) and \( (15) \), DiffMG uses the softmax trick. However, this cannot be directly used here, as there are additional indices \( r_j \)'s in \( (12) \). We re-formulate the constraints by re-parametrizing \( W_{j,k} \)'s as:

\[
\begin{align*}
W_{j,k}(r_j, r_k) &= \text{softmax}(B_{j,k}(r_j, r_k)), \\
W_{0,0}(r_k) &= \text{softmax}(B_{0,0}(r_k)),
\end{align*}
\]

\[
\begin{align*}
W_{j,k}(r_j) &= \text{softmax}(B_{j,k}(r_j)), \\
W_{0,k}(r_j) &= \text{softmax}(B_{0,k}(r_j)),
\end{align*}
\]

\[
W_{j,k}(r_j) = \frac{\exp(B_{j,k}(r_j, r_k))}{\sum_{r'_j} \exp(B_{j,k}(r'_j, r_k))}.
\]

The following proposition shows that all the tensor elements are non-negative and sum to a constant.

**Proposition 1.** For \( \mathcal{T} \) in \( (12) \) with \( W_{j,k} \)'s in \( (16)-(18) \), we have \( T(i_{g_1}, \ldots, i_{g_m}) \geq 0 \), and \( \sum_{i_1=1}^{C} \cdots \sum_{i_m=1}^{C} T(i_{g_1}, \ldots, i_{g_m}) = d^{K-1} \).

Thus, to satisfy the constraints in \( (14) \) and \( (15) \), we only need to divide \( (12) \) by the constant \( d^{K-1} \), as follows:

\[
\begin{align*}
\mathcal{T}(i_{0,1}, \ldots, i_{K-1}) &= \frac{1}{d^{K-1}} \sum_{r_1=1}^{d} \cdots \sum_{r_{K-1}=1}^{d} W_{0,1}(i_{0,1}, r_1) \cdots W_{0,K-1}(i_{0,K-1}, r_{K-1}) \\
W_{1,2}(i_{1,2}, r_1, r_2) \cdots W_{K-2,K-1}(i_{K-2,K-1}, r_{K-2}, r_{K-1}) \\
W_{0,K}(i_{0,K}) W_{1,K}(i_{1,K}, r_1) \cdots W_{K-1,K}(i_{K-1,K}, r_{K-1}, r_{K-1})
\end{align*}
\]

\[
(20)
\]

2) Gradient-based Algorithm: For DiffMG, similar to \( \mathcal{T} \), the node embeddings \( H^{(K)} \) are iteratively computed as:

\[
H^{(K)} = \sum_{i=1}^{C} W_{0,k}(i, r_k) f(H^{(0)}, A^i)
\]

\[
+ \sum_{0<j<k} \frac{1}{d} \sum_{r_j=1}^{d} \sum_{r_k=1}^{d} W_{j,k}(i, r_j, r_k) f(H^{(j)}, A^i)
\]

\[
H^{(K)} = \sum_{i=1}^{C} W_{0,k}(i) f(H^{(0)}, A^i)
\]

\[
+ \sum_{0<j<K} \frac{1}{d} \sum_{r_j=1}^{d} \sum_{r_k=1}^{d} W_{j,k}(i, r_j, r_k) f(H^{(j)}, A^i),
\]

where the subscript \( r_k \) in \( H^{(K)} \) is the same as the index \( r_k \) in the decomposition \( (12) \). We can see that this reduces to DiffMG \( (12) \) if we have \( d = 1 \), and the decomposition in \( (12) \) can also reduce to the rank-1 CP decomposition. A higher-rank CP decomposition can also have more expressive power, because tensors networks having higher ranks can restore higher-order tensors more precisely. However, this generalization overlooks how we compute the node embedding \( H^{(K)} \)'s, and leads to worse results that will be demonstrated in experiments V-C3. These weights \( W \)'s, which are given by learnable parameters \( B \)'s, are simultaneously optimized with the convolutional parameters \( \Theta \).

3) Space and Time Complexities: The decomposition in \( (20) \) contains at most \( C M d^2 \) parameters. If we do not set \( d \) too large, this will be negligible compared with the number of parameters in other parts of the model (e.g., \( \Theta \) in the graph convolution part), which can easily have thousands of parameters.

For the time complexity, if we assume computing \( f_{j,k} \) (resp. \( f_{j,k}^{(j)} \)) takes unit time, then the time complexity should be \( O(N^2 d^2) \) for TENSUS and \( O(N^2) \) for DiffMG where \( f \) is message passing functions like GCN \( (11) \). We will also compare the impact of different \( d \)'s on the performance and computational cost in Section V-C3.

V. Experiments

In this section, we empirically verify the improvement of our proposed topology-aware parameterization. We integrate our parameterization with existing methods, as is introduced in Section IV-C. For the proposed method, we set \( d = 2 \) unless otherwise specified. Experiments are implemented by PyTorch and run on a machine with a single NVIDIA RTX 2080 Ti GPU.

A. Node Classification

Experiments are performed on three standard benchmark data sets \( \{9, 13\} \): DBLP, ACM and IMDB (Table III). The DBLP dataset has three types of nodes: paper (P), author (A), and conference (C) where authors are labeled by their research areas; the ACM dataset has nodes: paper (P), author (A), and subject (S) where papers are labeled by research areas; and the IMDB dataset has nodes: movies (M), actors (A), and directors (D) where movies are labeled by genres. The nodes use the bag-of-words representation as input features.

We compare our proposed method TENSUS with DiffMG \( (12) \) as well as the following baselines in \( (12) \): meta-path2vec \( (8) \), GCN \( (11) \), GAT \( (25) \), HAN \( (9) \), MAGNN \( (10) \), GTN \( (13) \) and HGT \( (15) \). The experimental setting follows GTN \( (13) \) and DiffMG \( (12) \). These baselines are selected by DiffMG \( (12) \), and we follow the setup of this paper. The embedding dimension is 64. We use the Adam optimizer \( (32) \) with its hyper-parameters (learning rate, weight decay and input dropout) tuned according to the validation set. For performance evaluation, we use the average macro-F1 score over 5 runs with different random seeds.

Table [I] shows the macro-F1 scores. Note that HAN and MAGNN, which rely on manually-designed meta-paths, do
TABLE I: Macro F1 scores on node classification for different heterogeneous graphs. (results of baseline were copied from DiffMG [12])

|       | metapath2vec* | GCN* | GAT* | HAN* | MAGNN* | GTN | HGT* | DiffMG* | TENSUS |
|-------|---------------|------|------|------|--------|-----|------|---------|--------|
| DBLP  | 85.53         | 87.30| 93.71| 92.83| 92.81  | 93.98| 93.67| 94.45   | 95.92  |
| ACM   | 87.61         | 91.60| 92.33| 90.96| 91.15  | 91.89| 91.83| 92.65   | 94.02  |
| IMDB  | 35.21         | 56.89| 58.14| 56.77| 57.13  | 59.68| 59.35| 61.04   | 64.16  |

![Learning curves of different methods](image)

Fig. 5: Learning curves of different methods.

TABLE II: AUC (%) on the recommendation task on different heterogeneous graphs. (results of baseline were copied from DiffMG [12])

|       | metapath2vec* | GCN* | GAT* | HAN* | MAGNN* | GEMS* | GTN | HGT* | DiffMG* | TENSUS |
|-------|---------------|------|------|------|--------|-------|-----|------|---------|--------|
| Amazon| 58.17         | 66.64| 55.70| 67.35| 68.26  | 70.66 | 71.82| 74.75| 75.28   | 77.72  |
| Yelp  | 51.98         | 58.98| 56.55| 64.28| 64.73  | 65.12 | 66.27| 68.07| 68.77   | 70.38  |
| Douban| 51.60         | 77.95| 77.58| 82.65| 82.44  | 83.00 | 83.26| 83.38| 83.78   | 84.44  |

TABLE III: Statistics of the graph datasets for node classification.

|       | DBLP | ACM  | IMDB |
|-------|------|------|------|
| # nodes | 18405| 8994 | 12772|
| # edges | 67946| 25922| 37288|
| # edge types | 4    | 4    | 4    |
| # features | 334  | 1902 | 1256 |
| # training | 800  | 600  | 300  |
| # test    | 2857 | 2125 | 2339 |

not have good performance as compared to GTN, HGT, and DiffMG. This indicates that manually designed meta-graphs can be limited in mining task-dependent semantic information. DiffMG consistently achieves better performance than GTN and HGT due to the use of meta-graphs with flexible topologies, and TENSUS achieves the best performance among all these methods by encoding the topological structure of meta-graphs into parametrization.

Fig. 5(a) shows the learning curves on the IMDB dataset. As can be seen, meta-graphs learned by TENSUS lead to better performance than the baseline method.

B. Link Prediction

In this experiment, we consider three commonly used recommendation datasets: Yelp, Douban movie, and Amazon (Table IV). The Yelp dataset is a platform where users review businesses, Douban is a social media community where users share reviews about movies, Amazon is a large e-commerce platform which contains users’ ratings for items.

TABLE IV: Statistics of the graph datasets for recommendation task. Boldface indicates the target edge type we want to predict.

| dataset | relation (A-B) | # A | # B | # A-B |
|---------|---------------|-----|-----|-------|
| User-Business (U-B) | 16239 | 14284 | 198397 |
| User-User (U-U) | 16239 | 16239 | 158590 |
| Yelp User-Compliment (U-Co) | 16239 | 11 | 76875 |
| Business-City (B-C) | 14284 | 47 | 14267 |
| Business-Category (B-Ca) | 14284 | 511 | 40009 |
| Douban User-Movie (U-M) | 13367 | 12677 | 1068278 |
| User-Group (U-G) | 13367 | 2449 | 11276 |
| User-Actor (U-A) | 13367 | 2449 | 11276 |
| Movie-Director (M-D) | 12677 | 2449 | 11276 |
| Movie-Type (M-T) | 12677 | 38 | 27668 |
| Amazon User-Item (U-I) | 6170 | 2753 | 195791 |
| Item-View (I-V) | 2753 | 3857 | 5694 |
| Item-Category (I-C) | 2753 | 22 | 5508 |
| Item-Brand (I-B) | 2753 | 334 | 2753 |

We compare TENSUS with the same baselines in Section V-A and GEMS [14], which adopts a parallel genetic algorithm to search meta-structures for recommendation task and propose an attention based method to fuse information from
meta-structures. We follow the data preprocessing and experimental settings in DiffMG [12]. The embedding dimension is 64. We use the Adam optimizer [32] with its hyper-parameters (learning rate, weight decay and input dropout) tuned according to the validation set. For performance evaluation, we use the average AUCs over 10 runs with different random seeds.

Table II shows the AUCs. Similar to the node classification task, HAN and MAGNN perform worse than those methods that can learn meta-paths or meta-graphs, i.e. GEMS, GTN, HGT, and DiffMG, which demonstrates the necessity of learning meta-graphs. The proposed parameterization TENSUS can improve upon DiffMG by the topology-aware tensor decomposition.

We also plot the learning curves of different methods in Fig. 5(b) for the Douban dataset, which demonstrates that our parameterization TENSUS can help find meta-paths or meta-graphs that have a more stable performance.

C. Ablation Study

1) Visualization of learned meta-graphs: We first visualize the learned meta-graphs from DiffMG and TENSUS in Figures 6(a) and 6(b), respectively. The “I” operation in these figures indicate identity operation, i.e. the node embeddings are directly added to later results. From these two figures, we can see that TENSUS identifies meta-graphs that are less complex and achieve a better performance, as is demonstrated in Table II.

2) Impact of topology information: In this section, we compare the performance of our topology-aware decomposition with the CP decomposition under similar number of parameters by controlling the rank of these two decompositions. Results are shown in Fig. 8. From the figure, we can see that our proposed method achieves a better result than CP with similar number of parameters. This demonstrates that the performance gain of our proposed method comes from modeling topological structures rather than more parameters.

3) Effect of Hyper-Parameter \(d\): Finally, we study the effect of the rank \(d\), which controls the expressive power of the proposed parameterization. Figures 7(a) and 7(b) show the validation and test AUC of TENSUS with different \(d\) on the Douban dataset. For easy reference, we also show the performance of DiffMG [12]. As can be seen, TENSUS outperforms DiffMG over a range of \(d\)’s. As expected, a \(d\) too small limits the expressive power, while a \(d\) too large can make optimization difficult. A large \(d\) also increases the training time as well as the number of parameters, as is shown in Figures 7(c) and 7(d), respectively. However, the total number of parameters here is only about 1000 even when \(d\) is set to 5, which is very small if compared with the parameters in a GNN model.
VI. CONCLUSION

In this paper, we study the problem of learning suitable metagraphs on a given heterogeneous graph. Instead of modeling the edges in a meta-graph independently, which corresponds to CP decomposition, we propose to impose how node embeddings are computed onto the tensor of weights for meta-graphs. The decomposition is inspired by the parsimonious tensor train decomposition, and can be trained efficiently together with another graph data mining model. Empirical results on three diverse tasks demonstrate that the proposed method can find better meta-graphs and outperforms the state-of-the-arts.

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APPENDIX A

PROOF FOR PROPOSITION \[1\]

**Proof.** By the definition of softmax operation, we should have

$$W_{0,k}(i_{0,k}, r_k) > 0, \quad \sum_{i_{0,k} = 1}^C W_{0,k}(i_{0,k}, r_k) = 1,$$

$$W_{j,k}(i_{j,k}, r_j, r_k) > 0, \quad \sum_{i_{j,k} = 1}^C W_{j,k}(i_{j,k}, r_j, r_k) = 1,$$

$$W_{0,N+1}(i_{0,N+1}) > 0, \quad \sum_{i_{0,N+1} = 1}^C W_{0,N+1}(i_{0,N+1}) = 1,$$

$$W_{j,N+1}(i_{j,N+1}, r_j) > 0, \quad \sum_{i_{j,N+1} = 1}^C W_{j,N+1}(i_{j,N+1}, r_j) = 1,$$

hold for all \( r_j, r_k = 1, \ldots, d \). Then obviously we have \( T(i_{0,1}, \ldots, i_{N,N+1}) > 0 \). And to prove \( \sum_{i_{0,1} = 1}^C \cdots \sum_{i_{N,N+1} = 1}^C T(i_{0,1}, \ldots, i_{N,N+1}) = 1 \), we first re-write the summation to follows:

$$\sum_{i_{0,1} = 1}^C \cdots \sum_{i_{N,N+1} = 1}^C T(i_{0,1}, \ldots, i_{N,N+1})
= \sum_{i_{0,1} = 1}^C \cdots \sum_{i_{N,N+1} = 1}^C \frac{1}{d^N} \sum_{r_1 = 1}^d \cdots \sum_{r_N = 1}^d \ W_{0,1}(i_{0,1}, r_1) \cdots W_{0,N}(i_{0,N}, r_N)
\quad \cdots \quad W_{1,2}(i_{1,2}, r_1, r_2) \cdots W_{N-1,N}(i_{N-1,N}, r_{N-1}, r_N)
\quad \cdots \quad W_{0,N+1}(i_{0,N+1}) \cdots W_{1,N+1}(i_{1,N+1}, r_1)
\quad \cdots \quad W_{N,N+1}(i_{N,N+1}, r_N)
$$

Then from the properties of softmax operation, we have:

$$\sum_{i_{0,1} = 1}^C \cdots \sum_{i_{N,N+1} = 1}^C T(i_{0,1}, \ldots, i_{N,N+1})
= \frac{1}{d^N} \sum_{r_1 = 1}^d \cdots \sum_{r_N = 1}^d 1 \cdots 1
= \frac{1}{d^N} d^N = 1$$

where the \( d^N \) comes from the \( N \) summations of \( r_1, \ldots, r_N \) from 1 to \( d \). And this concludes our proof. \( \square \)