Higher-Order Clustering in Heterogeneous Information Networks

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ABSTRACT
As one type of complex networks widely-seen in real-world application, heterogeneous information networks (HINs) often encapsulate higher-order interactions that crucially reflect the complex nature among nodes and edges in real-world data. Modeling higher-order interactions in HIN facilitates the user-guided clustering problem by providing an informative collection of signals. At the same time, network motifs have been used extensively to reveal higher-order interactions and network semantics in homogeneous networks. Thus, it is natural to extend the use of motifs to HIN, and we tackle the problem of user-guided clustering in HIN by using motifs. We highlight the benefits of comprehensively modeling higher-order interactions instead of decomposing the complex relationships to pairwise interaction. We propose the MoCHIN model which is applicable to arbitrary forms of HIN motifs, which is often necessary for the application scenario in HINs due to their rich and diverse semantics encapsulated in the heterogeneity. To overcome the curse of dimensionality since the tensor size grows exponentially as the number of nodes increases in our model, we propose an efficient inference algorithm for MoCHIN. In our experiment, MoCHIN surpasses all baselines in three evaluation tasks under different metrics. The advantage of our model when the supervision is weak is also discussed in additional experiments.

KEYWORDS
Heterogeneous information networks, user-guided clustering, network motifs, meta-graphs, higher-order interaction, non-negative tensor factorization.

1 INTRODUCTION

Heterogeneous information network (HIN) has been shown to be a powerful approach to model linked objects in real-world scenarios with rich and informative type information [44, 52]. Many HIN-based methodologies have been proposed for applications such as classification, clustering, recommendation, and outlier detection [44, 52]. Meanwhile, complex real-world networks often embody mechanism backed by the underlying higher-order interactions [3, 5, 34, 39, 48, 61, 63], where the “players” in the interactions are nodes in the network. Researchers have since been using network motifs to reveal such higher-order interactions. Leveraging motifs is shown to be useful in tasks such as clustering [5, 65], ranking [67] and representation learning [41, 66]. Note that the term higher-order interaction is sometimes used interchangeably with high-order interaction in the literature [69], and the problem of clustering using signals from higher-order interactions is referred to as higher-order clustering [5, 64, 65]. We also remark that motifs in the context of HINs are sometimes referred to as the meta-graphs, and we choose motifs over meta-graphs in this paper primarily because meta-graph has been used under a different definition in the study of clustering [35, 40, 50] as to be discussed in Section 2.

Clustering is a traditional and fundamental task in network mining [17]. In the context of HINs, the problem of user-guided clustering is particularly of interest, because HINs with nodes and edges of different types can have multiple semantic facets and user guidance on the intended semantic facet is often needed to generate more specific and meaningful clustering results [16, 23, 33, 44, 55]. Exploiting higher-order interactions revealed by motifs offers us the opportunity to provide better solutions to this important problem.

Figure 1: Overview of the proposed method MoCHIN that directly models all players in higher-order interactions. Each type of nodes in the HIN corresponds to a color and a shape in the figure. To leverage signals from higher-order interactions without collapsing them into pairwise interactions, MoCHIN transcribes such information into a series of tensors. The order of each tensor is identical to the number of nodes in the corresponding motif. The tensors constructed in this way are sparse. In the task of user-guided clustering in HINs, the tensors constructed as such can provide a rich pool of fine-grained semantics, which can thereby fit a wider spectrum of guidance provided by different users.
work, and this observation is to be corroborated in Section 7.6. We will further discuss this point by real-world example in Section 4 and experiments in Section 7.

Furthermore, while it is easy to come up with semantically meaningful HIN motifs as with meta-paths [14, 20, 55], motifs in HINs can have more complex topology compared to motifs in homogeneous networks do, which are very often restricted to be triadic [5, 38, 65]. In order to fully unleash the power of HIN motifs and leverage the signals extracted by them, we are motivated to propose a method that applies to arbitrary forms of HIN motifs without additional constraints.

To tackle these challenges, we propose to directly model the higher-order interactions by first comprehensively transcribing them via motifs into a series of tensors. In this way, all nodes involved in the higher-order interactions will contribute to the effort in finding clusters. Based on this intuition, we propose the MoCHiN model, short for Motif-based Clustering in HINs, with an overview illustrated in Figure 1. MoCHiN first transcribes information revealed by motifs into a series of tensors and then performs clustering by joint non-negative tensor decomposition with an additional mechanism to reflect user guidance. This approach does not rely on the pairwise clustering methods and can hence better retain the information captured by different motifs to suit the needs of user-guided clustering in the semantic-rich HINs.

In this direction, an additional challenge arises from inducing tensors via corresponding motifs, because the size of the tensor grows exponentially as the number of nodes involved in the motif increases. Fortunately, motif instances are often sparse in real-world networks just as the number of edges is usually significantly smaller than the number of node pairs in a large real-world network, and this observation is to be corroborated in Section 7.6. We hence develop an efficient inference algorithm taking advantage of the sparsity of the derived tensors and the structure of the proposed MoCHiN model. Two real-world datasets and three tasks validate the effectiveness of the proposed model and the inference algorithm. We will release the codes and the processed data used in the experiment once the paper is published. Lastly, we summarize our contributions as follows:

1. We identify the utility of modeling higher-order interaction without collapsing it into pairwise interactions to avoid losing the rich and subtle information captured by motifs.
2. We propose the MoCHiN model that captures higher-order interaction via motif-based comprehensive transcription and applies to arbitrarily many, arbitrary forms of HIN motifs. We also develop an efficient inference algorithm for MoCHiN, leveraging the sparse nature of motif instances in real-world networks.
3. Experiments on two real-world HINs and three tasks demonstrated the effectiveness and efficiency of the proposed method as well as the utility of motifs and the tensor-based modeling approach in the task of HIN clustering.

2 RELATED WORK

Network motifs. The formation of complex networks is often partially attributed to the higher-order interactions among objects in real-world scenarios [3, 5, 34, 63]. The modeling of such interactions has been shown to be useful in many research areas such as neuroscience [48], biological networks [59], and social networks [61]. Network motifs, or graphlets, are usually used to identify such higher-order interaction [5, 65]. One popular direction of research on network motifs has centered on efficiently counting motif instances such as triangles and more complex motifs [1, 6, 21, 49]. Applications of motifs have also been found in tasks such as network partition and clustering [5, 24, 59, 65] as well as ranking [67]. Researchers have also studied enriching motif with additional attributes, such as temporal information, which has been shown to be instrumental in various network mining tasks [29, 38].

Motifs in heterogeneous information networks. In the context of HINs, network motifs are sometimes referred to as meta-graphs or meta-structures and have been studied recently [14, 15, 20, 23, 31, 32, 41, 66, 68, 70]. A large portion of these works studies pairwise relationship such as relevance or similarity [14, 15, 20, 31, 32, 68, 70], and some other addresses the problem of representation learning [41, 66]. Note that some of these prior works define meta-graphs or meta-structures to be directed acyclic graphs [20, 66, 68, 70], while we do not enforce this restriction on the definition of HIN motifs in general. We also remark that the term “meta-graph” is sometimes defined as a derived graph with indicator vectors being its vertices (nodes) [50], and clustering problem based on this definition of meta-graph has been studied for more than a decade [35, 40, 50]. Therefore, we stick to the term “motif” to refer to the higher-order structural pattern of interest in this paper.

Clustering in heterogeneous information networks. As a fundamental data mining problem, clustering has been studied for HINs [28, 44, 45, 51, 52, 54–56]. One line of HIN clustering study leverages the synergetic effect of simultaneously tackling ranking and clustering [9, 45, 54, 56]. Clustering on specific types of HINs such as those with additional attributes has also been studied [28, 51]. As in our paper, Wu et al. [62] resort to tensors to
represent HINs for clustering. Their solution employs one tensor to describe one HIN as a whole and does not model different semantics implied by different structural patterns.

User guidance, or semi-supervision, brings significantly more potentials to HIN clustering by providing a small portion of seeds. [44, 55]. This is because HINs often carry rich semantics from different facets, and user-guided clustering enables users to inject intention on the semantics of clustering results. To reveal the different semantics in an HIN, pioneering works exploit the meta-path, a special case of the motif, and reflect user-guidance by using the corresponding meta-paths [33, 55].

To the best of our knowledge, there are no existing studies on motif-based HIN clustering applicable to arbitrarily many, arbitrary forms of HIN motifs. A meta-graph–guided random walk algorithm is shown to have superior performance than the performance of only using meta-paths, which requires the used motifs to have undirected edges to ensure symmetry in the transition matrix [23]. Also, this method does not distinguish the semantic of motif AP4TPA from that of APTPA, as to be shown in Section 4, due to the design on how a random walk is sampled under a motif. Sankar et al. [41] propose a convolutional neural network method based on motifs which can potentially be used for user-guided HIN clustering. This approach restricts the motifs of concern to those with a target node, a context node, and auxiliary nodes. Gujral et al. [16] propose a method based on tensor constructed from stacking a set of adjacency matrices, which can successfully reflect user guidance and different semantic aspects. While in practice, one can derive an adjacency matrix by counting instances under one meta-path or higher-order motif, this tensor-based method essentially leverages features derived for node pairs, instead of directly modeling higher-order interactions among multiple nodes.

**Matrix and tensor factorization for clustering.** By factorizing edges that represent pairwise interactions in a network, matrix factorization has been shown to be able to reveal the underlying composition of objects [26]. In this direction, a large body of study has been carried out on clustering networks using non-negative matrix factorization (NMF) [13, 27, 30]. As a natural extension beyond pairwise interaction, tensor has been used to model interaction among multiple objects for decades [18, 60]. A wide range of applications have also been discussed in the field of data mining and machine learning [25, 37].

For the study of clustering and related issues, many algorithms have been developed for homogeneous networks by factorizing a single tensor [4, 7, 8, 42, 43]. A line of work transforms a network to a 3-rd order tensor via triangles, which is essentially one specific type of network motif [4, 43]. Researchers have also explored weak supervision in guiding tensor factorization based analysis [7]. A large number of non-negative tensor factorization methods have been proposed for practical problems in computer vision [42]. Besides, tensor-based approximation algorithms for clustering also exist in the literature [8, 57]. One recent work on local network clustering considering higher-order conductance shares our intuition since it operates on tensor transcribed by a motif without decomposing into pairwise interactions [69]. This method is designed for the scenario where one motif is given. Different from the approach proposed in our paper, all the above methods are not designed for heterogeneous information networks, where the use of multiple motifs is usually necessary to reflect the rich semantics in HINs. Finally, we remark that to the best of our knowledge existing tensor-based clustering methods for HINs [16, 62] either do not jointly model multiple motifs or would essentially decompose the higher-order interactions into pairwise interactions.

### 3 PRELIMINARIES

In this section, we define related concepts and notations.

**Definition 3.1 (Heterogeneous information network and schema [52]).** An information network is a directed graph $G = (V, E)$ with a node type mapping $\phi : V \rightarrow T$ and an edge type mapping $\psi : E \rightarrow R$. When the number of node types $|T| > 1$ or the number of edge types $|R| > 1$, the network is referred to as a heterogeneous information network (HIN). The schema of an HIN is an abstraction of the meta-information of the node types and edge types of the given HIN.

As an example, Figure 2a illustrates the schema of the DBLP network we are to use in Section 7. Additionally, we denote the set of all nodes with the same type $t \in T$ by $V_t$.

**Definition 3.2 (HIN motif and HIN motif instance).** In an HIN $G = (V, E)$, an HIN motif is a structural pattern defined by a graph on the type level with its node being a node type of the original HIN and an edge being an edge type of the given HIN. Additional constraints can be optionally added such as two nodes in the motif cannot be simultaneously matched to the same node instance in the given HIN. Further given an HIN motif, an HIN motif instance under this motif is a subnetwork of the HIN that matches this pattern.

Figure 2b gives an example of a motif in the DBLP network with four distinct terms, which we refer to as AP4TPA. If a motif is a path graph, it could also be considered as a meta-path [53, 55]. The motif, AP4TPA, in Figure 2c is one such example.

**Definition 3.3 (Tensor, k-mode product, mode-k matricization [37].** A tensor is a multidimensional array. For an $N$-th-order tensor $X \in \mathbb{R}^{d_1 \times \ldots \times d_N}$, we denote its $(j_1, \ldots, j_N)$ entry by $X_{j_1, \ldots, j_N}$. The $k$-mode product of $X$ and a matrix $A \in \mathbb{R}^{d_k \times d}$ is denoted by $Y = X \times_k A$, where $Y \in \mathbb{R}^{d_1 \times \ldots \times d_{k-1} \times d_{k+1} \times \ldots \times d_N}$, and
Additionally, we define authors graduated from other groups. Under meta-path APTPA, motif instances can only be found between Eric Xing and authors from multiple groups. However, if we use motif AP4TPA, motif instances can provide more subtle information than meta-paths do, and if a user wishes to cluster authors by research groups, motif AP4TPA can be very informative.

Furthermore, if we look into the AP4TPA motif instances that are matched to Xing and Blei, the involved terms such as dirichlet are very specific to their group’s research interest. Modeling the interaction among dirichlet and other nodes can kick in more information even if users ultimately only wish to obtain clustering results on authors. If one only used motifs to generate features for node pairs without more comprehensive modeling of the higher-order interaction revealed by motifs, such information would be lost. In Section 7, we will further quantitatively validate the utility of comprehensive modeling of the higher-order interaction.

5 THE MOCHIN MODEL

In this section, we describe the proposed MoCHIN model step by step with an emphasis on its intention to more comprehensively model higher-order interaction while availng user guidance.

5.1 Revisit on Clustering by Non-Negative Matrix Factorization

Non-negative matrix factorization (NMF) has been a popular method for the problem of network clustering [13, 27, 30]. While additional constraints or regularization terms are usually enforced to ensure unique solution or certain other properties, the basic NMF-based clustering algorithm solves the following optimization problem for given adjacency matrix $M$

$$
\min_{V_1, V_2 \geq 0} \| M - V_1^T V_2 \|_F^2,
$$

where $\| \cdot \|_F$ is the Frobenius norm, $A \geq 0$ denotes matrix $A$ is non-negative, and $V_1, V_2$ are two $|V| \times C$ matrices with $C$ being the number of clusters. In this model, the $j$-th column of $V_1$ or that of $V_2$ gives the inferred cluster membership of the $j$-th node in the network. The intuition of the model stems from using the inner product of the cluster membership of the $j_1$-th node and that of the $j_2$-th node to reconstruct the existence of the edge represented by non-zero entry $(j_1, j_2)$ in the adjacent matrix.

5.2 Single-Motif–Based Clustering in HINs

Recall that an edge essentially characterizes the pairwise interaction between two nodes. To model higher-order interaction revealed by motifs without first collapsing it into pairwise interactions in the problem of clustering, a natural solution is to use the inferred cluster membership of all nodes involved in a motif instance to reconstruct the existence of this motif instance. This solution can be formulated by non-negative tensor factorization (NTF), and a line of research on NTF itself [37, 42] and clustering algorithm by factorizing a single tensor [4, 8, 43] can be found in the literature.

Specifically, given a single motif $m$ with $N$ nodes having node type $t_1, t_2, \ldots, t_N$ of the HIN, we transcribe the higher-order interaction revealed by this motif to a $N$-th–order tensor $X$ with dimension $|V_{t_1}| \times |V_{t_2}| \times \ldots \times |V_{t_N}|$. We set the $(j_1, j_2, \ldots, j_N)$...
entry of $X$ to 1 if a motif instance is found to be matched to the following $n$ nodes: $j_1$-th of $V_{t_1}$, $j_2$-th of $V_{t_2}$, ..., $J_N$-th of $V_{t_N}$; and set it to 0 otherwise. By extending Eq. (1), whose objective can be equivalently written as $\|M - V_1^m V_2^m\|_F^2$ with $m$ being the identity matrix, we can approach the clustering problem by solving

$$\begin{align*}
\min_{V_1, V_2 \geq 0} \|X - I \times_{j=1}^N V_j\|_F^2 + \lambda \sum_{i=1}^N \|V_i\|_1,
\end{align*}$$

(2)

where $I$ is the $N$-th order identity tensor with dimension $C \times C \times \ldots \times C$, $\|\cdot\|_1$ is the entry-wise l-1 norm introduced as regularization to avoid trivial solution, and $\lambda$ is the regularization coefficient. We also note that this formulation is essentially CP decomposition [19, 37] together with additional l-1 regularization and non-negative constraints. In this paper, we write the CP decomposition part of the formulation in a way different from its most common form for notation convenience in the inference section (Section 6) considering the presence of regularization and constraints.

### 5.3 Proposed Model for Motif-Based Clustering in HINs

Real-world HINs often contain rich and diverse semantic facets due to its heterogeneity [46, 52, 55]. To reflect the different semantic facets of an HIN, a set $\mathcal{M}$ of more than one candidate motifs are usually necessary for the task of user-guided clustering. With additional clustering seeds provided by users, the MoCHIN model selects the motifs that are both meaningful and pertinent to the seeds.

To this end, we assign motif-specific weights $\mu = (\mu_1, \ldots, \mu_{|\mathcal{M}|})$, such that $\sum_{m \in \mathcal{M}} \mu_m = 1$ and $\mu_m \geq 0$ for all $m \in \mathcal{M}$. Denote $X^{(m)}$ the tensor constructed by motif $m$, $V^{(m)}$ the cluster membership matrix for the i-th node in motif $m$, $o(m)$ the number of nodes in motif $m$, and $\phi(m, i)$ the node type of the i-th node in motif $m$. For each node type $t \in \mathcal{T}$ of the HIN, we put together cluster membership matrices concerning this type with motif weights considered to construct the consensus matrix

$$V^*_t := \sum_{\phi(m, i)=t} \frac{\mu_m V^{(m)}_i}{\sum_{i=1}^|M| \phi(m, i)=\phi(m, i)},$$

where $\mathbb{1}[P]$ equals to 1 if $P$ is true and 0 otherwise. With this notation, $\sum_{i=1}^|M| \mathbb{1}[\phi(m, i)=\phi(m, i)]$ is simply the number of nodes in motif $m$ that are of type $t$.

Furthermore, we intend to let (i) each cluster membership $V_t^{(m)}$ be close to its corresponding node-type-specific consensus matrix $V^*_t$ and (ii) the consensus matrices not assign seed nodes to the wrong cluster. We hence propose the following overall objective for the MoCHIN model with the third and the fourth term modeling the aforementioned two intentions

$$O = \sum_{m \in \mathcal{M}} \left\|X^{(m)} - I \times_{i=1}^N V_i^{(m)}\right\|_F^2 + \lambda \sum_{m \in \mathcal{M}} \sum_{i=1}^o(m) \left\|V_i^{(m)}\right\|_1 + \theta \sum_{m \in \mathcal{M}} \sum_{i=1}^o(m) \left\|V_i^{(m)} - V^*_t\right\|_F^2 + \rho \sum_{t \in \mathcal{T}} \left\|M^{(t)} \odot V^*_t\right\|_F^2,$$

(3)

where $\odot$ is the Hadamard product and $M^{(t)}$ is the seed mask matrix for node type $t$. Its $(i, c)$ entry $M^{(t)}_{i,c} = 1$ if the i-th node of type $t$ is a seed node and it should not be assigned to cluster $c$ according to user guidance, and $M^{(t)}_{i,c} = 0$ otherwise.

Finally, solving the problem of HIN clustering by modeling higher-order interaction and automatically selecting motifs can be converted to solving the following problem

$$\begin{align*}
\min_{\{V_t^{(m)} \geq 0, \mu \in \Delta\}} O,
\end{align*}$$

(4)

where $\Delta$ is the standard simplex. To the best of our knowledge, there is no method similar to ours that simultaneously model multiple motifs in an HIN without decomposing higher-order interactions into pairwise interactions.

### 6 THE INFERENCE ALGORITHM

In this section, we first describe the algorithm for solving the optimization problem as in Eq. (4). Then, a series of speed-up tricks are introduced to circumvent the curse of dimensionality, where direct computation on the tensors would be problematic since a motif involving many nodes would induce a tensor with a formidable large number of entries.

#### 6.1 Update $V^{(l)}_k$ and $\mu$

Each clustering membership matrix $V^{(l)}_k$ with non-negative constraints is involved in all terms of the objective function (Eq. (3)), where $l \in \mathcal{M}$ and $k \in \{1, \ldots, o(l)\}$. We hence develop multiplicative update rules for $V^{(l)}_k$ that guarantees monotonic decrease at each step, accompanied by projected gradient descent (PGD) [36] to find global optimal of $\mu = (\mu_1, \ldots, \mu_{|\mathcal{M}|})^\top$ by exploiting its convexity. Overall, we solve the optimization problem by alternating between $\{V^{(l)}_k\}$ and $\mu$.

To update $V^{(l)}_k$ when $\{V^{(m)}_i\}_{i, \phi(m, i)=\phi(l,k)}$ and $\mu$ are fixed under non-negative constraints, we derive the following theorem. For
notation convenience, we further denote \( V^*_m = \sum_{q(i,m) = t} \eta^*_q V^{(m)}_i \), where \( \eta^*_q = \frac{\mu_m}{\sum_{r \neq q} \mu_r} \).

**Theorem 6.1.** The following update rule for \( V^{(l)}_k \) monotonically decreases the objective function.

\[
V^{(l)}_k \leftarrow V^{(l)}_k 
\begin{align*}
&- \frac{\chi^{(l)}(k) \otimes \phi^{(l)}(k) V^{(l)}_k \top}{\sum_{i=1}^{2} \eta_q (V^{(m)}_i \top + V^{(m)}_i) \top} + \eta^*_q V^{(m)}_i + \eta^*_q V^{(m)}_i + \\
&\times \left( 1 - \frac{1}{\eta^*_q (V^{(m)}_i \top + V^{(m)}_i)} + \eta^*_q V^{(m)}_i + \lambda \
&\times \left( 1 - \eta^*_q (V^{(m)}_i \top + V^{(m)}_i) + \frac{1}{\eta^*_q V^{(m)}_i \top + V^{(m)}_i} + \lambda \
&\right), \right)
\end{align*}
\]

where for any matrix \( A, [A]^+ := \frac{|A + A|}{2}, [A]^- := \frac{|A - A|}{2} \).

Inspired by prior art on non-negative matrix factorization [27], we provide the proof for this theorem on non-negative tensor factorization as follows.

**Proof.** With the equivalency given by Lemma 3.4

\[
\|X^{(m)} - \hat{X}^{(m)} \|_F \leq \|X^{(m)} - V^{(m)} I^{(m)} \|_F
\]

we construct the following auxiliary function

\[
\begin{align*}
Z(V^{(l)}_k, \hat{V}) &:= \sum_{s,t} \left( \{X^{(l)}(k) \otimes \phi^{(l)}(k) V^{(l)}_k \top \} \otimes \phi^{(l)}(k) V^{(l)}_k \top \} \right) \times (V^{(m)}_i \top + V^{(m)}_i) \top \\
&- 2(X^{(l)}(k) \otimes \phi^{(l)}(k) V^{(l)}_k \top) \times (V^{(m)}_i \top + V^{(m)}_i) \top \\
&+ \theta \left( \frac{1}{\eta^*_q (V^{(m)}_i \top + V^{(m)}_i)} + \frac{1}{\eta^*_q V^{(m)}_i \top + V^{(m)}_i} + \lambda \
&\times \left( 1 - \eta^*_q (V^{(m)}_i \top + V^{(m)}_i) + \frac{1}{\eta^*_q V^{(m)}_i \top + V^{(m)}_i} + \lambda \
&\right), \right)
\end{align*}
\]

Straightforward derivation can show the following three relations hold: (i) \( Z(V^{(l)}_k, \hat{V}) = O(V^{(l)}_k) \), (ii) \( Z(V^{(l)}_k, \hat{V}) \geq O(\hat{V}) \), and (iii) \( Z(V^{(l)}_k, \hat{V}) \) is convex with respect to \( \hat{V} \). Therefore, by setting \( \frac{\partial}{\partial \hat{V}} Z(V^{(l)}_k, \hat{V}) = 0 \), one can find \( Z(V^{(l)}_k, \hat{V}) \) is minimized at \( \hat{V} = \hat{V}_{\text{opt}} \), where \( \hat{V}_{\text{opt}} \) is the righthand side of Eq. (5), and \( O(V^{(l)}_k) \geq Z(V^{(l)}_k, \hat{V}_{\text{opt}}) \geq O(\hat{V}_{\text{opt}}) \). It follows that setting \( V^{(l)}_k \) to \( \hat{V}_{\text{opt}} \) monotonically decreases the objective function \( O \) which is exactly the update rule in Theorem 6.1.

For fixed \( V^{(m)}_i \), the objective function Eq. (3) is convex with respect to \( \mu \). We therefore use PGD to update \( \mu \) by performing projection onto the standard simplex after each step of gradient descent, where the gradient can be derived with straightforward calculation, which we omit due to space limitations.

### 6.2 Computational Speed-Up

In this section, we describe a series of speed-up tricks, with which the complexity would be governed no longer by the dimension of the tensors but by the number of motif instances in the network. Unlike the scenario where researchers solve the NTF problem with tensors of fixed order regardless of the applied dataset, our problem is specifically challenging because a motif can involve multiple nodes. For instance, the APATPA motif discussed in Section 4 is one real-world example involving 8 nodes. Using this motif in the model would induce an 8-th order tensor. Consequently, the fact that the tensor size grows exponentially with the order of the tensor poses a special challenge to conducting motif-based clustering via tensor factorization.

In the proposed inference algorithm, the direct computation of these terms involve complexity subject to the size of the tensor: the first term in the numerator of Eq. (5), \( X^{(l)}(k) \otimes \phi^{(l)}(k) V^{(l)}_k \top \), the first term in the denominator of Eq. (5), \( V^{(l)}_k \top \otimes \phi^{(l)}(k) V^{(l)}_k \top \), and the first term of the objective function Eq. (3),

\[
\|X^{(m)} - \hat{X}^{(m)} \|_F \leq \|X^{(m)} - V^{(m)} I^{(m)} \|_F
\]

Fortunately, the computation of all these terms can be significantly simplified by exploiting the sparsity of tensor \( X^{(l)}(X^{(m)}) \) and the composition of dense matrix \( \phi^{(l)}(k) V^{(l)}_k \top \).

Consider the example that motif \( l \in M \) involves 5 nodes, each node type has 10,000 node instances, and the nodes are to be clustered into 10 clusters. Then the induced dense matrix \( \phi^{(l)}(k) V^{(l)}_k \top \) would have \( \Pi_{i=1}^{10} |V_{\phi(m,i)}| \cdot |\phi(i)| - 1 = 10^{4} \cdot 10^{4} = 10^{8} \) entries, and tensor \( X^{(l)} \) would have \( \Pi_{i=1}^{10} |V_{\phi(m,i)}| = 10^{5} \) entries. As a result, directly computing the first term in the numerator of Eq. (5), \( X^{(l)}(k) \otimes \phi^{(l)}(k) V^{(l)}_k \top \), would involve matrix multiplication of a dense \( 10^{2} \) entry matrix. However, given the sparsity of \( X^{(l)} \), one may denote \( n_{x}(X) := \{j \in \{1, \ldots, 10\} \mid X_{j_{1}, \ldots, j_{5}} \neq 0 \} \) the set of indices of the non-zero entries in tensor \( X \) and derive the

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**Algorithm 1:** The MoCHIN inference algorithm

**Input:** \( X^{(m)} \), supervision \( M^{(l)} \), the number of clusters \( C \), hyperparameters \( \theta, \rho, \lambda \)

**Output:** the cluster membership matrices \( \{V^{*}_{m}\} \)

1. Begin
2. While not converged do
3. For \( m \in M \) do
4. Find local optimum of \( V^{(m)} \) by Eq. (5).
5. Find global optimum of \( \mu \) by PGD.
6. End
7. End
following equivalency

\[
X^{(l)}_{(k)} \circ_k V^{(l)}_{i k} = \sum_{j \in \text{nz}(X^{(l)})} X^{(l)}_{j i} \cdot h(j) \prod_{i \in k} (V^{(l)}_{i k})_{j i},
\]

where \( \prod \) is Hadamard product of a sequence and \( h(j) \) is one-hot column vector of size \( |V_{i k}| \) that has entry 1 at index \( j \).

Computing the right-hand side of this equivalency involves the summation over Hadamard product of a small sequence of small vectors, which has a complexity of \( O(\text{nnz}(X^{(l)})) \cdot (o(l) - 1) \cdot C \) with \( \text{nnz}(\cdot) := |\text{nz}(\cdot)| \) being the number of non-zero entries of a tensor. In other words, if the previous example comes with 1,000,000 matched motif instances, the complexity would decrease from manipulating a 10\( \cdot \)entry dense matrix to a magnitude of \( 4 \times 10^7 \).

The first term in the denominator of Eq. (5) again involves matrix multiplication of the huge dense matrix \([\otimes_{i=1}^{o(l)} V^{(l)}_{i}]^T H^{(l)}_{(k)}\). Leveraging the composition of \([\otimes_{i=1}^{o(l)} V^{(l)}_{i}]^T H^{(l)}_{(k)}\), one can show that

\[
V^{(l)}_{k i} \cdot h(j) \prod_{i \in k} (V^{(l)}_{i k})_{j i} = \sum_{i \in k} a(l) \begin{pmatrix} |V^{(l)}_{i i} V^{(l)}_{i i}| \end{pmatrix}.
\]

As such, instead of multiplying a huge dense matrix, one may only compute Hadamard product and matrix multiplication over a few relatively small matrices. Note that in the previous example, \([\otimes_{i=1}^{o(l)} V^{(l)}_{i}]^T H^{(l)}_{(k)}\) has 10\( \cdot \) entries, while \( |V^{(l)}_{i i}| = 10^5\) entries and \( o(l) = 5 \).

Thirdly, evaluating the loss function Eq. (3) for determining convergence involves the computation of the Frobenius norm of its first term, i.e., \( \|X^{(m)} - I^{(m)} \otimes C \|_F \), which is a huge, dense tensor. Again by exploiting the desirable sparsity property of \( X^{(m)} \), we can calculate the Frobenius norm of \( \|X^{(m)} - I^{(m)} \otimes C \|_F \) as follows

\[
\|X^{(m)} - I^{(m)} \otimes C \|_F = \left\| X^{(m)} \right\|_F^2 - 2 \left\| X^{(m)} \otimes C \|_F \right\|_F + \left\| I^{(m)} \otimes C \|_F \right\|_F^2.
\]

\[
\|X^{(m)} \|_F^2 - 2 \sum_{j i} (X^{(m)}_{j i} I^{(m)}_{i}) + C \sum_{i \in k} |V^{(m)}_{i i}| + \sum_{c i} \sum_{c j} \sum_{c k} |V^{(m)}_{i i}| \cdot (V^{(m)}_{i i})_{c i} \cdot (V^{(m)}_{i i})_{c j} \cdot (V^{(m)}_{i i})_{c k}.
\]

This equivalency transform the computation of a dense and potentially high-order tensor to that of a sparse tensor accompanied by a couple of matrix manipulation. The complexity of the first and the second term in the above formula are \( O(\text{nnz}(X^{(m)})) \) and \( O(C \cdot \text{nnz}(X^{(m)})) \), respectively, thanks to the sparsity of \( X^{(m)} \).

With the complexity of the third term being \( O(C^2 \cdot \sum_{i \in k} |V^{(m)}_{i i}|) \), the overall complexity is reduced from \( O(\prod_{i = 1}^{o(l)} |V^{(m)}_{i i}|) \) to \( O(C \cdot \text{nnz}(X^{(m)}) + C^2 \cdot \sum_{i \in k} |V^{(m)}_{i i}|) \). That is, considering the previous example, the complexity of evaluating this Frobenius norm would decrease from a magnitude of \( 10^{20} \) to a magnitude of \( 10^8 \).

It is worth noting that the trick introduced in the last equivalency, Eq. (6), has already been proposed in the study of Matrixized Tensor Times Khatri-Rao Product (MTTKRP) [2, 11, 47]. MTTKRP and our model share a similarity in this trick because, unlike update rule Eq. (5), evaluating the loss function Eq. (3) does not involve the non-negative constraints.

Finally, we remark that the above computation can be highly parallelized, which has further promoted the efficiency of the proposed algorithm in our implementation. An empirical efficiency study on two datasets is to be presented in Section 7.6. We summarize the algorithm in Algorithm 1.

7 EXPERIMENTS

In this section, we present the quantitative evaluation results on two real-world datasets through multiple tasks and carry out case studies to analyze the performance of the proposed MoCHIN model under various circumstances.

7.1 Datasets and Evaluation Tasks

Datasets. We use two real-world HINs for experiments.

- **DBLP** is a heterogeneous information network that serves as a bibliography of researchers in computer science area [58]. The network consists of 5 types of nodes: author (A), paper (P), key term (T), venue (V) and year (Y). The key terms are extracted and released by Chen et al. [10]. The edge types include authorship, term usage, venue published, year published, and the reference relationship. The first four edge types are undirected, and the last one is directed. The schema of the DBLP network is shown in Figure 2a. In DBLP, we select two candidate motifs for all applicable methods, including AP4TPA and APPA, where APPA is also a meta-path representing author writes a paper that refers another paper written by another author and AP4TPA was introduced in Section 4.

- **YAGO** is a knowledge graph constructed by merging Wikipedia, GeoNames and WordNet. YAGO dataset consists of 7 types of nodes: person (P), organization (O), location (L), prize (P), work (W), position (S) and event (E). There are 24 types of edges in the network, with 19 undirected edge types and 5 directed edge types as shown by the schema of the YAGO network in Figure 4. In YAGO, the candidate motifs used by all compared methods include \( p^6 O^{23} L, p^7 O^{23} L, p^8 O^{23} L, 2P2W, 3P2W, \) where the first three are also meta-paths with the number in superscript being type of edge given in Figure 4. \( 2P2W \) is the motif that 2 people simultaneously co-created (edge type 14) two pieces of work, and \( 3P2W \) is the motif that 3 people who created (edge type 14), directed (edge type 15) and acted (edge type 16) in a piece of work, respectively.

Evaluation tasks. In order to validate the proposed model’s capability in reflecting different guidance given by different users, we use two sets of labels on authors to conduct two tasks in DBLP similar to previous study [55]. Additionally, we design another task on YAGO with labels on persons. We will release datasets and labels used in the experiment once the paper is published. **DBLP-group** – Clustering authors to 5 research groups where they graduated, which is an expanded label set from the “four-group dataset” [55].
Figure 4: The schema of YAGO [46].

The "four-group dataset" includes researchers from four renowned research groups led by Christos Faloutsos, Michael I. Jordan, Jiawei Han, and Dan Roth. Additionally, we add another group of researchers, who have collaborated with at least one of the researchers in the "four-group dataset" and label them as the fifth group with the intention to involve more subtle semantics in the original HIN. 5% of the 250 authors with labels are randomly selected as seeds from user-guidance. We did not use 1% for seed ratio as in the following two tasks because the number of authors to be clustered in this task is small. The resulted HIN processed as such consists of 19,500 nodes and 108,500 edges. **DBLP-area** – Clustering authors to 14 research areas, which is expanded from the "four-area dataset" [55], where the definition of the 14 areas is derived from the Wikipedia page: List of computer science conferences. 1% of the 7,165 authors with labels are randomly selected as seeds from user-guidance. The HIN processed in this way has 16,100 nodes and 30,239 edges. **YAGO** – Clustering people to 10 popular countries in the YAGO dataset. We knock out all edges with edge type wasBornIn, and if a person had an edge with one of the 10 countries, we assign this country to be the label of this person. Additionally, to avoid making our task trivial, we remove all other types of edges between person and location. 1% of the 11,368 people are randomly selected as seeds from user-guidance. There are 17,109 nodes and 70,251 edges in the processed HIN.

**Evaluation metrics.** We use three metrics to evaluate the quality of the clustering results generated by each model: Accuracy (Micro-F1), Macro-F1, and NMI. **Accuracy** refers to a measure of statistical bias. More precisely it is defined by the division of the number of correctly labeled data by the total size of the dataset. Note that in multi-class classification tasks, accuracy is always identical to Micro-F1. **Macro-F1** refers to the arithmetic mean of the F1 score across all different labels in the dataset, where the F1 score is the harmonic mean of precision and recall for a specific label. **NMI** is the abbreviation for normalized mutual information. Numerically, it is defined as the division of mutual information by the arithmetic mean of the entropy of each label in the data. For all these metrics, higher values indicate better performance.

### 7.2 Baselines and Experiment setups

**Baselines.** We use four different baselines to obtain insight on different aspects of the performance of MoCHIN.

- **KNN** is a classification algorithm where the label of each object in the test set is assigned to the most common one among the labels of its nearest neighbors. This is a homogeneous method that does not distinguish different node types. In our scenario, the distance between two nodes is defined as the length of the shortest path between them.
- **KNN+Motifs** serves as a direct comparison to the proposed MoCHIN model, since KNN+Motifs can also use signals generated by arbitrary forms of motifs, but does not directly model all players in higher-order interactions. To extract information from motifs, we construct a motif-based network for each candidate motif, where an edge is constructed if two nodes are matched to a motif instance in the original HIN. The KNN algorithm is then applied again on each motif-based network. Finally, a linear combination is applied to the outcome probability matrices generated by KNN from the motif-based networks and the original HIN. Weights used in the linear combination are tuned to the best. When using this baseline method, we additionally add APVPA into the set of candidate motifs for both DBLP tasks and add $p^{14}O^{14}P, p^{15}O^{15}P,$ and $p^{16}O^{16}P$ for the YAGO task.

- **GNetMine** is a graph-based regularization framework to address the transductive classification problem in heterogeneous information networks [22]. This method only leverages edge-level information without considering structural patterns such as meta-paths or motifs.
- **PathSelClus** is a probabilistic graphical model that performs clustering tasks on heterogeneous networks by integrating meta-path selection with user-guided object clustering [55]. When using this baseline method, we additionally add APVPA, APTPA, APT, AP, and, APAPA into the set of candidate meta-paths for both DBLP tasks as suggested by the original paper [55] and add $p^{14}O^{14}P, p^{15}O^{15}P,$ and $p^{16}O^{16}P$ for YAGO task.

**Experiment setups.** For MoCHIN, we set hyperparameters $\theta = 1, \rho = 100$ and $\lambda = 0.0001$ across all tasks in our experiments. We also add each edge type as an edge-level motif into the set of candidate motifs for MoCHIN. For each baseline, we always tune its hyperparameters to achieve the best performance in each task.

### 7.3 Quantitative Evaluation Result

We quantitatively evaluate the effectiveness of the proposed MoCHIN model against the baselines and report the main results in Table 2.
Table 2: Quantitative evaluation on clustering results under multiple metrics in three tasks.

| Metric    | DBLP-group | DBLP-area | YAGO  |
|-----------|------------|-----------|-------|
| Acc./Micro-F1 | Macro-F1 | NMI | Acc./Micro-F1 | Macro-F1 | NMI | Acc./Micro-F1 | Macro-F1 | NMI |
| KNN       | 0.4249     | 0.2566    | 0.1254 | 0.4107     | 0.4167    | 0.2537 | 0.3268     | 0.0921    | 0.0810 |
| KNN+Motifs| 0.4549     | 0.2769    | 0.1527 | 0.4811     | 0.4905    | 0.3296 | 0.3951     | 0.1885    | 0.1660 |
| GNetMine [22] | 0.5880 | 0.6122    | 0.3325 | 0.4847     | 0.4881    | 0.3469 | 0.3832     | 0.2879    | 0.1772 |
| PathSelClus [55] | 0.5622 | 0.3535    | 0.3246 | 0.4361     | 0.4520    | 0.3967 | 0.3856     | 0.3405    | 0.2864 |
| MoCHIN    | 0.6910     | 0.6753    | 0.5486 | 0.5318     | 0.5464    | 0.4396 | 0.6134     | 0.5563    | 0.4607 |

Overall, MoCHIN uniformly outperformed all baselines in all three tasks under all metrics. We remark that these three metrics measure different aspects of the model performance. One example is that, in the DBLP-area task, PathSelClus outperforms GNetMine under Macro-F1 and NMI, while GNetMine outperforms PathSelClus under Acc./Micro-F1. As a result, achieving superior performance uniformly under all metrics is strong evidence that MoCHIN with higher-order interaction directly modeled is armed with greater modeling capability in the task of user-guided HIN clustering.

MoCHIN exploits signals from motifs more comprehensively and achieves superior performance even with fewer motifs. Recall that both MoCHIN and the baseline KNN+Motifs exploit signals from motifs, while KNN+Motifs uses motifs to transform higher-order interactions into signals over node pairs. In our experiments, KNN+Motifs cannot get evaluation results as good as our method, which implies merely using motifs to generate pairwise features cannot fully exploit signals from motifs. In fact, the set of non–edge-level motifs used in the baseline is always a superset of that used in MoCHIN. We interpret this result as follows: although MoCHIN uses fewer motifs, by modeling all players in the higher order interaction, it implicitly captures information carried by other motifs, which justifies the use of a more complex model.

KNN is disadvantaged on imbalanced data when the supervision is weak. Across all the three tasks conducted in the experiments, the ground truth labels in the YAGO dataset are the most imbalanced. As presented in Table 2, KNN performs notably worse on YAGO with 1% seed ratio under Macro-F1 and NMI, which are more sensitive to model performance on rare classes compared to Accuracy (Micro-F1). In other words, KNN tends to achieve inferior results on rare classes when supervision is weak, and data is imbalanced. We recommend using other heterogeneous methods that consider the type information in this scenario. The results in Section 7.5 can further validate this point, where experiments with varied seed ratio are presented.

### 7.4 Impact of Candidate Motif Choice

In this section, we conduct a case study on how the choice of candidate motifs impacts the performance of the proposed MoCHIN model and additionally use the concrete example in Figure 3 of Section 4 to understand the model outputs.

As introduced in Section 7.1, the candidate motifs MoCHIN used in the DBLP tasks are all edge types with two non–edge-level motifs: APPA and AP4TPA. We conducted an ablation study by taking out either or both of the two non–edge-level motifs and compared with the original full model in the DBLP-group task, and the results are reported in Table 3. It can be seen that the full MoCHIN model outperformed all baselines. This result shows that using motifs does make a difference in clustering.

Moreover, we also looked into the concrete example in Figure 3 of Section 4 and check how each model outputted cluster assignment for Eric Xing. The result is also included in Table 3, which shows only model versions equipped with AP4TPA made the correct assignment for Eric Xing. This observation echoes the intuition discussed in Section 4.

### 7.5 Varied Seed Ratio

In addition to using 1% people as seeds for the YAGO task reported in Table 2, we additionally experimented under varied seed ratio 2%, 5%, and 10% for YAGO. The results under Accuracy and Macro-F1 are reported in Figure 5. We omit NMI due to space limitations.

For all methods under all metrics, the performance increased as the seed ratio increased, which was a natural outcome of progressively stronger supervision. Additionally, MoCHIN still outperformed all baselines under all circumstances. Notably, the difference in performance between MoCHIN and the baselines shrunk as seed ratio increased. This suggests when supervision is strong enough, the pairwise edge level signal can provide progressively sufficient information to obtain reasonable results. On the other hand, MoCHIN is particularly attractive when supervision is weak for being able to extract more subtle information from limited data.
7.6 Efficiency Study

In this section, we empirically evaluate the efficiency of the proposed algorithm with a focus on the speed-up tricks described in Section 6.2. Specifically, we estimate the runtime for inferring all parameters involved in one motif while all other parameters are fixed, or equivalently, reaching convergence of the while-loop from line 4 to line 6 in Algorithm 1.

This study was conducted on both the DBLP dataset and the YAGO dataset for each of their respective non-edge-level motifs: APPA and AP4TPA in DBLP; 2P2W and 3PW in YAGO. The non-edge-level motifs are studied because (i) they are more complex in nature and (ii) the tensors induced by edge-level motifs are essentially matrices, the study of which degenerates to the well-studied case of non-negative matrix factorization. To downsample the HINs, we randomly knock out a portion of papers in DBLP or persons in YAGO. The involved edges and the nodes that become dangling after the knock-out are also removed from the network. The reason node type paper and person are used is that they are associated with the most diverse edge types in DBLP and YAGO, respectively. In the end, we obtain a series of HINs with 10%, 25%, 50%, 75%, 100% of papers or persons left.

To more accurately evaluate the efficiency of the proposed algorithm in this study, we turn off the parallelization in our implementation and use only one thread. We record the wall-clock runtime for inferring all parameters of each concerned motif, \( \{v_k^{(l)} \}_{k=1}^a(l) \), while fixing the motif weights \( \mu \) and parameters of other motifs, \( \{v_k^{(m)} \}_{k=1}^m \). The experiment is executed on a machine with Intel(R) Xeon(R) CPU E5-2680 v2 @ 2.80GHz. The result is reported in Figure 6.

The proposed algorithm empirically achieves near-linear efficiency in inferring parameters of each given motif. As presented in Figure 6, the runtime for all motifs on both datasets are approximately linear to the number of involved motif instances. This result is in line with the analysis provided in Section 6.2 and justifies the effectiveness of the speed-up tricks.

Moreover, we also reported the number of motif instances against the number of nodes regardless of type in each downsampled network. For all four studied motifs, we do observe motif instances are sparse and do not explode quickly as the size of the network increases.

8 Conclusion and Future Works

We studied the problem of user-guided clustering in heterogeneous information networks with the intention to model higher-order interactions. To solve this problem, we identified that it is crucial to model higher-order interactions without collapsing them into pairwise interactions in order to avoid losing the rich and subtle information. Based on this intuition, we proposed the MoCHIN model, which models higher-order interaction more comprehensively and applies to arbitrary forms of motifs. An inference algorithm with computational speed-up techniques was also developed. Experiments validated the effectiveness of the proposed model and the utility of comprehensively modeling higher-order interactions without collapsing them into pairwise relation.

Future works include exploring further methodologies to join signals from multiple motifs, which is currently realized by a simple linear combination in the MoCHIN model. Furthermore, as the current model takes user guidance by injecting labels of the seeds, it is also of interest to extend MoCHIN to the scenario where guidance is made available by providing must-link and cannot-link constraints on node pairs.
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