HyperFM: Fact-Centric Multimodal Fusion for Link Prediction over Hyper-Relational Knowledge Graphs

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Abstract

With the ubiquity of hyper-relational facts in modern Knowledge Graphs (KGs), existing link prediction techniques mostly focus on learning the sophisticated relationships among multiple entities and relations contained in a fact, while ignoring the multimodal information, which often provides additional clues to boost link prediction performance. Nevertheless, traditional multimodal fusion approaches, which are mainly designed for triple facts under either entity-centric or relation-guided fusion schemes, fail to integrate the multimodal information with the rich context of the hyper-relational fact consisting of multiple entities and relations. Against this background, we propose **HyperFM**, a **Hyper**-relational **F**act-centric **M**ultimodal Fusion technique. It effectively captures the intricate interactions between different data modalities while accommodating the hyper-relational structure of the KG in a fact-centric manner via a customized Hypergraph Transformer. We evaluate HyperFM against a sizeable collection of baselines in link prediction tasks on two real-world KG datasets. The results show that HyperFM consistently achieves the best performance, yielding an average improvement of 6.0-6.8% over the best-performing baselines on the two datasets. Moreover, a series of ablation studies systematically validate our fact-centric fusion scheme.

1 Introduction

Knowledge Graphs (KGs) are semantic networks that represent relationships between entities. They have underpinned a wide range of real-world applications, including commonsense reasoning (Lin et al., 2019), recommender systems (Wang et al., 2019), and urban computing (Zhao et al., 2022a). While early KGs are usually limited to binary relationships and represent facts as triplets, modern KGs such as Freebase (Bollacker et al., 2008) and Wikidata (Wikidata, 2022) often consist of hyper-relational facts, which comprises a base triplet (h, r, t) along with additional key-value pairs (k, v) further enriching the information about the base triplet, expressed as $(h, r, t,\ k_1,\ v_1,\ ...)$. For instance, one hyper-relational fact in Figure 1 can be presented as *(Microsoft, industry, software industry, in the scope of, operating system)*. To effectively make use of such KGs, link prediction is widely adopted as a promising solution for KG completion and reasoning, aiming to predict missing entities or relations in a fact (Bordes et al., 2013).

Recent studies have substantiated the efficacy of hyper-relational KG embeddings in link prediction. They strive to capture the structural information of the KG by learning the correlation between entities and relations in each fact with Convolutional Neural Networks (CNNs) (Rosso et al., 2020), Graph Neural Networks (GNNs) (Galkin et al., 2020), or Transformers (Wang et al., 2021). However, existing approaches often overlook the significance of multimodal data in the KG, which can provide crucial information to distinguish the subtle differences between entities beyond the KG structure, thus leading to more accurate link prediction. For instance, suppose that the task is to predict the missing triplet *(Apple, headquarters location, ?)* as shown in Figure 1. It is easy to make the wrong prediction *Redmond* based on the structural information only, since the entity *Apple* presents a similar structural role to the entity *Microsoft* with the common relation *industry*, tail *software industry*, and key-value pair *(in the scope of, operating system)*. Nevertheless, by incorporating the visual and textual modalities, the image and textual description of *Apple* both prompt the answer *Cupertino*. The visual modality includes the image of *Apple*'s headquarters, while the textual description highlights specific information about its location. Therefore, multimodal information can be used to distinguish

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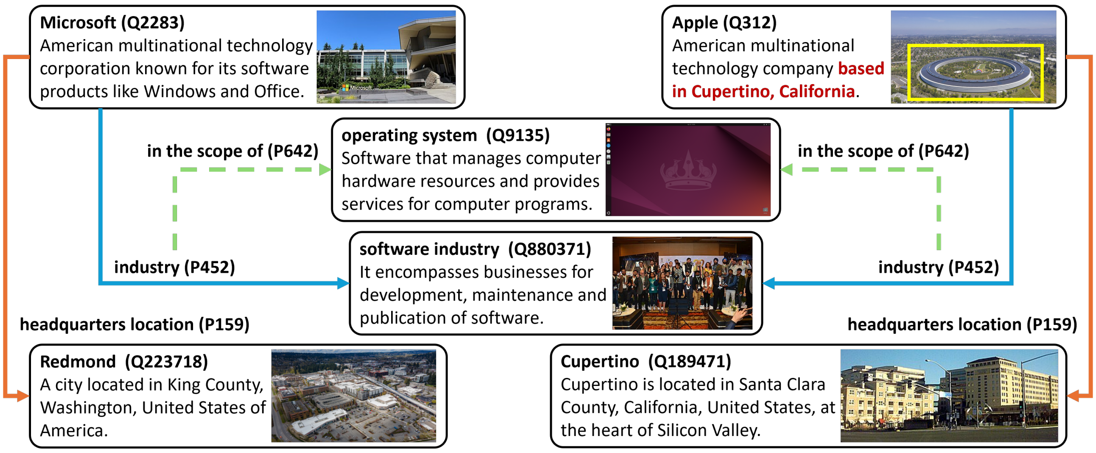

Microsoft (Q2283)
American multinational technology corporation known for its software products like Windows and Office.
Apple (Q312)
American multinational technology company based in Cupertino, California.
operating system (Q9135)
Software that manages computer hardware resources and provides services for computer programs.
in the scope of (P642)
in the scope of (P642)
software industry (Q880371)
It encompasses businesses for development, maintenance and publication of software.
industry (P452)
industry (P452)
headquarters location (P159)
headquarters location (P159)
Redmond (Q223718)
A city located in King County, Washington, United States of America.
Cupertino (Q189471)
Cupertino is located in Santa Clara County, California, United States, at the heart of Silicon Valley.

Figure 1: Real-world facts with multimodal information on Wikidata.

the subtle differences between entities based on their unique attributes, thereby boosting the link prediction performance.

In the current literature, existing works targeting multimodal KGs mainly focus on the representation of triplets and are incapable of learning hyper-relational facts (Chen et al., 2024). Moreover, in their multimodal fusion process, most methods adopt an *entity-centric* scheme, neglecting the informative fact context (Li et al., 2023; Lee et al., 2023). For example, the missing tail in the triplet *(Apple, headquarters location, ?)* is inferred to be a location based on the relation *headquarters location*, suggesting that attention should be put on location-specific information within the visual and textual modalities. Although some further methods (Zhang et al., 2024a) incorporate relational context to adaptively adjust the weights of different modalities, such a *relation-guided* scheme oversimplifies the rich context of a hyper-relational fact containing multiple entities and relations, where the interactions among modalities should be assumed on the basis of the hyper-relationality of the fact.

Against this background, we propose a novel **Hyper**-relational **F**act-centric **M**ultimodal Fusion (HyperFM) technique. HyperFM follows a fact-centric design, where multiple entities of a fact and their multi-modality features are integrated under a hypergraph, capturing the intricate interactions between different modalities while accommodating the hyper-relational structure of the KG. To achieve effective multimodal fusion, we design a customized Hypergraph Transformer to comprehensively learn the interaction across multimodal features under the hypergraph setting. For resolving link prediction tasks, an edge-biased self-attention layer is used to further capture the correlation between elements in a fact while accommodating the heterogeneous connections between them. We summarize our contributions as follows:

- We study the problem of link prediction over multimodal hyper-relational KGs by addressing two key drawbacks of existing approaches: 1) hyper-relational KG models often ignore the multimodal information, and 2) multimodal KG models fail to incorporate the hyper-relationality into the multimodal fusion process.
- We propose HyperFM, a **Hyper**-relational **F**act-centric **M**ultimodal Fusion technique for link prediction tasks over multimodal hyper-relational KGs; it can capture the intricate interactions between different data modalities while accommodating the hyper-relational structure of the KG via a customized Hypergraph Transformer.
- We thoroughly evaluate the performance of HyperFM against a wide range of state-of-the-art baselines on two multimodal hyper-relational KG datasets. Results show that HyperFM consistently outperforms all baselines, with an average improvement of 6.0-6.8% over the best-performing baselines on the two datasets. Furthermore, a series of ablation studies systematically validate our fact-centric fusion scheme.

2 Related Work

Hyper-relational KG modeling. Traditional KGs are usually represented by a set of triplets, which fail to capture the ubiquitous hyper-relational facts where multiple entities are connected via multiple relations (Rosso et al., 2020). To address this issue, the n-ary representation has been used to model a hyper-relational fact by transforming it into a set of relation-entity pairs (Wen et al., 2016; Zhang et al., 2018; Guan et al., 2019; Fatemi et al., 2021; Liu et al., 2021). However, the n-ary representation loses essential information encoded by the base triplet, thus showing suboptimal performance in link prediction. In this context, models such as HINGE (Rosso et al., 2020), NeuInfer (Guan et al., 2020), and ShrinkE (Xiong et al., 2023) keep the base triplet of a hyper-relational fact by learning from the base triplet and its associated key-value pairs via different channels. Following this representation, models like GRAN (Wang et al., 2021), HyNT (Chung et al., 2023), and HyperFormer (Hu et al., 2023) employ Transformer to capture the sophisticated correlation between elements in a fact. Recently, the (graph)encoder-(Transformer)decoder architecture has shown promising results in resolving link prediction tasks. In line with this paradigm, models like MSeaHKG (Di and Chen, 2021), StarE (Galkin et al., 2020), Hy-Transformer (Yu and Yang, 2021), QUAD (Shomer et al., 2022), and HAHE (Luo et al., 2023) focus on designing various graph encoders to capture the rich semantics of entities and relations. Different from these existing works that often ignore the multimodal information in hyper-relational KGs, we propose in this paper HyperFM to subtly integrate multimodal information to further boost link prediction performance.

Multimodal KG modeling. Some recent studies have enriched the original KG dataset and attempted to capture multimodal information for link prediction, especially through the incorporation of images and textual descriptions of entities (Xie et al., 2017; Pezeshkpour et al., 2018; Liu et al., 2019). A few early works represent different modalities in a unified space to extract common features; however, they failed to maintain the distinctive characteristics of each modality (Chen et al., 2022; Xu et al., 2022; Wang et al., 2023b). Therefore, models like IMF (Li et al., 2023), VISTA (Lee et al., 2023), NativE (Zhang et al., 2024a), MoSE (Zhao et al., 2022b), and AdaMF (Zhang et al., 2024b) capture complex interactions between modalities while retaining unique information about each modality. However, these multimodal KG embedding methods are mainly designed for triple facts, under either entity-centric or relation-guided fusion schemes, and fail to integrate the multimodal information with the rich context of the hyper-relational fact consisting of multiple entities and relations. In this paper, we propose HyperFM following a fact-centric design capturing the intricate interactions between different modalities while accommodating the hyper-relational structure of the KG.

3 Preliminaries

In this section, we introduce key concepts about the Multimodal Hyper-relational Knowledge Graph (MHKG), including the definition of MHKGs and the link prediction task over MHKGs.

Definition 3.1. **Multimodal Hyper-Relational Knowledge Graph**. An MHKG consists of multimodal hyper-relational facts, where a hyper-relational fact is represented as $\{(h, r, t), \{(k_i, v_i)\}_{i=1}^{n} | h, t, v_i \in \mathcal{E}, r, k_i \in \mathcal{R}\}$, where (h, r, t) denotes the base triplet and (k_i, v_i) refers to an additional key-value pair. Here, $\mathcal{E}$ and $\mathcal{R}$ indicate the entity and relation sets, respectively. In a multimodal hyper-relational fact, each entity contains multiple features of different modalities. We denote the multimodality by $\mathcal{M} = \{m_s, m_v, m_t\}$, representing the structural, visual, and textual modalities, respectively. Accordingly, for an entity $e \in \mathcal{E}$, its multimodal information is represented by $(e_{m_s}, e_{m_v}, e_{m_t})$.

Definition 3.2. **Link Prediction over MHKGs**. The link prediction task aims to predict any missing element in a hyper-relational fact. The missing element could be an entity from $\{h, t, v_1, \ldots, v_n\}$ or a relation from $\{r, k_1, \ldots, k_n\}$.

4 HyperFM

The overall architecture of our Hyper-relational Fact-centric Multimodal Fusion (HyperFM) is shown in Figure 2. Specifically, it consists of three modules: 1) a series of modal encoders that extract the initial features of each modality for subsequent multimodal fusion; 2) a multimodal fusion module that integrates features from diverse modalities and captures their interactions; and 3) a link prediction module that resolves the link prediction tasks.

4.1 Modal Encoder

We design modal encoders similar to (Li et al., 2023; Lee et al., 2023), utilizing pre-trained VGG16 and BERT as the visual and textual encoders, respectively. For the structural encoder, we employ learnable embeddings to refine entity and relation representations during the multimodal fu-

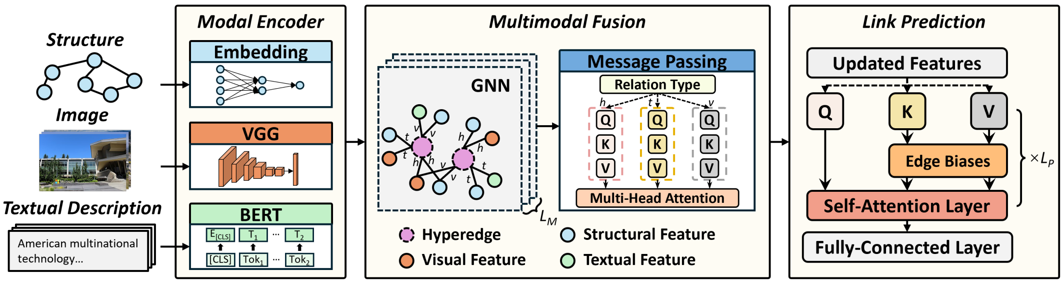


Figure 2: The overall architecture of HyperFM for link prediction over MHKGs.

sion process. Detailed descriptions of the modal encoders are provided in Appendix A. Note that our HyperFM can flexibly adopt any modal encoders as plug-and-play components. In the following, we focus on the design of the multimodal fusion process, which is our core contribution.

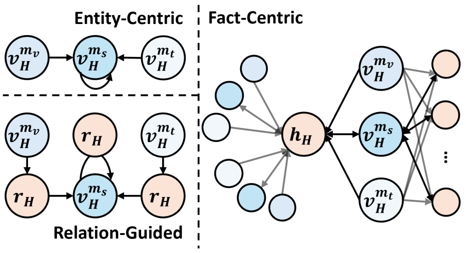


Figure 3: Comparison of the three fusion schemes 1) the entity-centric scheme fuses information of other modalities directly to entities (the structural modality); 2) the relation-guided scheme fuse information of other modalities to entities under the guidance of the relation of the given triplet r_H; 3) our fact-centric scheme fuses information of different modality to a hyper-relational fact (hyperedge), which can flexibly accommodate multimodality and hyper-relationality at the same time.

4.2 Multimodal Fusion

The multimodal fusion module captures the interactions between different modalities and learns multimodal representations that enhance link prediction performance. Most current multimodal KG embedding methods fuse multimodal information without considering the rich context of a hyper-relational fact, which consists of multiple entities and relations. To this end, we propose a Hypergraph Transformer that integrates multimodal information on the basis of the hyper-relationality of the KG.

Hypergraph construction for MHKG. To effectively integrate multimodal data in the KG, we consider the inherent hypergraph nature of MHKGs as the basis, and then aggregate multimodal features through message passing on the graph. Specifically, a multimodal hyper-relational fact involves more than two entities, with each containing up to three modalities; the entire MHKG forms a hypergraph. To effectively represent the MHKG, inspired by the incidence graph representation of a hypergraph (Antelmi et al., 2023), we propose a novel hypergraph construction strategy. The hypergraph of the MHKG is represented by $\mathcal{G}_H = \{\mathcal{E}_H, \mathcal{H}_H, \mathcal{I}_H\}$. Here, $\mathcal{H}_H$ is the hyperedge set, with each hyperedge corresponding to a multimodal hyper-relational fact and the entities of the fact being an incident of the hyperedge. The node set $\mathcal{E}_H = \{\mathcal{E}_H^{m_s}, \mathcal{E}_H^{m_v}, \mathcal{E}_H^{m_t}\}$, where $\mathcal{E}_H^{m_s}$, $\mathcal{E}_H^{m_v}$, and $\mathcal{E}_H^{m_t}$ denote the node sets of structural, visual, and textual modalities, respectively. $\mathcal{I}_H \in \mathbb{R}^{|\mathcal{E}_H|\times|\mathcal{H}_H|}$ is an incidence matrix defined by:

$$\begin{aligned} \mathcal{I}_H(v_H, h_H) &= 1, \text{ if } v_H \in h_H, \\ \mathcal{I}_H(v_H, h_H) &= 0, \text{ if } v_H \notin h_H. \end{aligned} \tag{1}$$

where $v_H \in \mathcal{E}_H$ and $h_H \in \mathcal{H}_H$. If v_H belongs to the hyperedge (fact) h_H, then $v_H \in h_H$; otherwise, $v_H \notin h_H$. The constructed hypergraph serves as the basis for achieving fact-centric multimodal fusion. Figure 3 compares our fact-centric scheme against the existing entity-centric (Li et al., 2023; Lee et al., 2023; Zhang et al., 2024b) and relation-guided (Zhao et al., 2022b; Zhang et al., 2024a) fusion schemes.

Hypergraph Transformer layer. Based on the built hypergraph, we model the interactions between multimodal features by propagating information between nodes and hyperedges using a GNN. For informative message passing, we incorporate the multi-head attention mechanism into the GNN, where each head corresponds to a relation type, discriminating the different positions of modalities within a fact. The *aggregation function* and *update function* in the GNN are designed as follows:

1) Aggregation function: The aggregation process is a bi-directional operation, including node-to-hyperedge (N-H) and hyperedge-to-node (H-N) steps. To apply multi-head attention, we first define the relation type between hyperedges and nodes as (here, $v_H \in h_H$):

$$r(h_H, v_H) = \begin{cases} r_h, & \text{if } p_{h_H}(v_H) = \text{head} \\ r_t, & \text{if } p_{h_H}(v_H) = \text{tail} \\ r_v, & \text{if } p_{h_H}(v_H) = \text{value} \end{cases} \tag{2}$$

where $p_{h_H}(v_H)$ denotes the position of v_H in h_H. There are three possible positions of a node: head, tail, and value. Accordingly, r_h, r_t, and r_v represent the three relation types between hyperedges and nodes. Notably, relation types are independent of relation direction, meaning that $r(h_H, v_H) = r(v_H, h_H)$. We denote the embeddings of h_H and v_H by $\mathbf{h}_H$ and $\mathbf{v}_H$, respectively. Notably, the input to the first layer consists of the initialized embeddings of hyperedges and the embeddings of nodes, which are obtained from the output of the modal encoders.

For N-H aggregation, we denote the embeddings of nodes connecting to the hyperedge h_H with relation type r_j by $\mathbf{V}_H^j$. Then the attention score of this specific relation type for h_H is computed by:

$$\mathbf{a}_j = \varphi_{\text{Softmax}}\left(\frac{\mathbf{q}_j \mathbf{K}_j}{\sqrt{d}}\right) \tag{3}$$

where $\mathbf{q}_j = \mathbf{h}_H \mathbf{W}_{Q_j}$ and $\mathbf{K}_j = \mathbf{V}_H^j \mathbf{W}_{K_j}$. $\mathbf{W}_{Q_j}$ and $\mathbf{W}_{K_j}$ are the query and key transformation matrices for relation type r_j, respectively. $\varphi_{\text{Softmax}}(\cdot)$ refers to the Softmax function and d is the dimension of embeddings incorporated for numerical stability. Subsequently, the attention score becomes relation type-aware, accounting for the heterogeneous relationships among elements within a fact. Afterward, the aggregated node embedding of relation type r_j for h_H is obtained by:

$$\hat{\mathbf{v}}_H^j = \mathbf{V}_H^j \mathbf{a}_j \tag{4}$$

We implement multi-head attention and gain a set of aggregated embeddings $\left\{\hat{\mathbf{v}}_H^j \mid j \in [1, n_r]\right\}$, where n_r denotes the number of relation types for h_H. These aggregated embeddings can be further integrated by:

$$\hat{\mathbf{v}}_H = \varphi_{\text{MLP}}\left(\varphi_{\text{Concat}}\left(\left\{\hat{\mathbf{v}}_H^j \mid j \in [1, n_r]\right\}\right)\right) \tag{5}$$

where $\varphi_{\text{MLP}}(\cdot)$ and $\varphi_{\text{Concat}}(\cdot)$ denote the MLP and concatenation operations, respectively.

For H-N aggregation, we apply a similar procedure as in N-H aggregation and obtain the refined aggregated embedding for v_H by:

$$\hat{\mathbf{h}}_H = \varphi_{\text{MLP}}\left(\varphi_{\text{Concat}}\left(\left\{\hat{\mathbf{h}}_H^j \mid j \in [1, n_r]\right\}\right)\right) \tag{6}$$

where $\left\{\hat{\mathbf{h}}_H^j \mid j \in [1, n_r]\right\}$ denotes the set of aggregated embeddings of hyperedges that connect to v_H through different relation types.

2) Update function: We use a Feed-Forward Network (FFN) to update the aggregated embeddings:

$$\widetilde{\mathbf{h}}_H = \varphi_{\text{LN}}\left(\varphi_{\text{FFN}}\left(\hat{\mathbf{v}}_H\right) + \mathbf{h}_H\right) \tag{7}$$

$$\widetilde{\mathbf{v}}_H = \varphi_{\text{LN}}\left(\varphi_{\text{FFN}}\left(\hat{\mathbf{h}}_H\right) + \mathbf{v}_H\right) \tag{8}$$

Note that we employ Layer Normalization $\varphi_{\text{LN}}(\cdot)$ (Ba et al., 2016) for training stability.

By stacking multiple Hypergraph Transformer layers, high-order multimodal interactions with relation type-aware semantics are extracted. The updated features of the structural modality are then read out from the final layer L_M for link prediction:

$$\mathbf{X}_e = \left\{\mathbf{v}_H^{(L_M)} | v_H \in \mathcal{E}_H^{m_s}\right\} \tag{9}$$

In summary, our multimodal fusion module first builds a fact-centric hypergraph that flexibly accommodates multimodality and hyper-relationality at the same time, and then designs the Hypergraph Transformer applying multi-head attention to aggregate multimodal information while discriminating the different positions of modalities in a fact.

4.3 Link Prediction

The link prediction module aims at predicting the missing element in a hyper-relational fact, where the missing element is represented by a learnable [MASK] token. We use an edge-biased self-attention layer to make predictions.

Edge-biased self-attention layer. Through the previous module, a hyper-relational fact $\{(h, r, t), \{(k_i, v_i)\}_{i=1}^n\}$ is encoded into $\left\{(\mathbf{x}_h, \mathbf{x}_r, \mathbf{x}_t), \{(\mathbf{x}_{k_i}, \mathbf{x}_{v_i})\}_{i=1}^n\right\}$, where $\{\mathbf{x}_h, \mathbf{x}_t, \mathbf{x}_{v_i}\} \in \mathbf{X}_e$ denote the updated entity features and $\{\mathbf{x}_r, \mathbf{x}_{k_i}\}$ denote the initialized relation features. For an element $\mathbf{x}_i$ in the fact, its features can be further updated by the self-attention

Dataset	Entities	Entities with images	Entities with text	Relations	Training	Test	Facts (Hyper%)	Arity
WikiPeople	34,839	33,265	34,839	178	294,439	37,712	332,151 (2.6%)	2-7
WD50K	47,156	43,823	47,156	532	166,435	46,159	212,594 (13.6%)	2-67

Table 1: Dataset statistics. The columns (from left to right) denote the number of entities, entities with images, entities with textual descriptions, relations, training facts, test facts, all facts (the ratio of hyper-relational facts), and the range of arity.

mechanism:

$$\alpha_{ij} = \frac{\left(\mathbf{W}_Q^{LP}\mathbf{x}_i + \mathbf{b}_{ij}^{Q}\right)^\top \left(\mathbf{W}_K^{LP}\mathbf{x}_j + \mathbf{b}_{ij}^{K}\right)}{\sqrt{d}} \tag{10}$$

$$\bar{\mathbf{x}}_i = \sum_{j=1}^{2n+2} \frac{\exp\left(\alpha_{ij}\right)}{\sum_{k=1}^{2n+2} \exp\left(\alpha_{ik}\right)} \left(\mathbf{W}_V^{LP}\mathbf{x}_j + \mathbf{b}_{ij}^{V}\right) + \mathbf{x}_i \tag{11}$$

where $\mathbf{W}_Q^{LP}$, $\mathbf{W}_K^{LP}$, and $\mathbf{W}_V^{LP}$ are linear transformation matrices of query, key, and value, respectively. $2n+2$ is the total number of input elements excluding $\mathbf{x}_i$. α_{ij} refers to the importance of $\mathbf{x}_j$ to $\mathbf{x}_i$. $\mathbf{b}_{ij}^{Q}$, $\mathbf{b}_{ij}^{K}$, and $\mathbf{b}_{ij}^{V}$ are edge biases used to accommodate the heterogeneous connections between different elements in the fact. We design five categories of edge biases based on the edge heterogeneity: $(\mathbf{x}_h, \mathbf{x}_r)$, $(\mathbf{x}_t, \mathbf{x}_r)$, $(\mathbf{x}_r, \mathbf{x}_{k_i})$, $(\mathbf{x}_{k_i}, \mathbf{x}_{v_i})$, and others not included in the above categories. Note that the edge biases are independent of edge direction; the edge biases of $(\mathbf{x}_h, \mathbf{x}_r)$ and $(\mathbf{x}_r, \mathbf{x}_h)$ are thus the same. With an L_P-layer edge-biased self-attention network, an informative feature of the [MASK] token is generated, providing a rich context for predicting the missing element.

Fully-connected decoder. We denote the final output embedding of the [MASK] token by $\bar{\mathbf{x}}_M$. A fully-connected layer with Softmax function is then employed to produce the link prediction results:

$$\mathbf{p} = \varphi_{\text{Softmax}}\left(\mathbf{W}_M \bar{\mathbf{x}}_M + \mathbf{b}_M\right) \tag{12}$$

where $\mathbf{W}_M$ is the weight matrix of the MLP in the structural encoder, and $\mathbf{b}_M$ denotes the learnable entity bias. The prediction outcome $\mathbf{p}$ is a probability distribution over the entity set $\mathcal{E}$, indicating the likelihood of each entity being the actual missing element. Notably when predicting missing relations, $\mathbf{W}_M$ and $\mathbf{b}_M$ are the weight matrix of the initial embedding layer and the learnable relation bias, respectively.

Our model training process optimizes the cross-entropy loss in the link prediction tasks using Adam optimizer (Kingma, 2014):

$$\mathcal{L} = \sum_{i=1}^{|\mathcal{E}|} \mathbf{y}_i \log \mathbf{p}_i \tag{13}$$

where $\mathbf{y}_i$ is the ground-truth label for i-th entry. The code of HyperFM is publicly available online[1].

5 Experiments

5.1 Experimental Setup

Datasets. The experiments are conducted on two widely-used hyper-relational KG datasets, **WikiPeople** (Guan et al., 2019) and **WD50K** (Galkin et al., 2020), with pre-defined data splits provided for fair comparison. Since these datasets do not include multimodal information, we crawl images and textual descriptions of entities from their data source Wikidata. Specifically, we extract the image for each entity through the "image" property and obtain the textual description from the "description" label. The detailed statistics of both datasets are presented in Table 1.

Baselines. We compare our HyperFM with a wide range of state-of-the-art baselines, which are divided into two categories. The first category includes hyper-relational KG (HKG) embedding methods: **m-TransH** (Wen et al., 2016); **RAE** (Zhang et al., 2018); **NaLP** (Guan et al., 2019); **NeuInfer** (Guan et al., 2020); **HINGE** (Rosso et al., 2020); **ShrinkE** (Xiong et al., 2023); **HyConvE** (Wang et al., 2023a); **HJE** (Li et al., 2024); **GRAN** (Wang et al., 2021); **MSeaHKG** (Di and Chen, 2021); **HyNT** (Chung et al., 2023); **HyperFormer** (Hu et al., 2023); **StarE** (Galkin et al., 2020); **Hy-Transformer** (Yu and Yang, 2021); **QUAD** (Shomer et al., 2022); **HAHE** (Luo et al., 2023). The second category consists of multimodal KG (MKG) embedding methods: **IMF** (Li et al., 2023); **VISTA** (Lee et al., 2023); **NativE** (Zhang et al., 2024a); **MoSE** (Zhao et al., 2022b); **AdaMF** (Zhang et al., 2024b). The detailed descriptions of baselines are in Appendix B.

[1] https://github.com/UM-Data-Intelligence-Lab/HyperFM

Method Type	Method	WikiPeople						WD50K					
		All entities			Head/Tail			All entities			Head/Tail		
		MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10
HKG Embedding	m-TransH	0.167	0.162	0.354	0.081	0.079	0.321	0.074	0.072	0.198	0.058	0.057	0.298
	RAE	0.193	0.175	0.388	0.073	0.073	0.305	0.132	0.118	0.243	0.062	0.061	0.325
	NaLP	0.327	0.265	0.449	0.401	0.327	0.535	0.223	0.162	0.337	0.135	0.134	0.368
	NeuInfer	0.349	0.281	0.506	0.483	0.416	0.581	0.235	0.178	0.355	0.257	0.181	0.396
	HINGE	0.367	0.305	0.488	0.447	0.381	0.567	0.245	0.181	0.362	0.243	0.169	0.392
	ShrinkE		N/A		0.489	0.419	0.594		N/A		0.321	0.237	0.462
	HyConvE	0.277	0.172	0.467	0.275	0.171	0.465	0.244	0.171	0.382	0.226	0.154	0.365
	HJE	0.472	0.387	0.609	0.471	0.387	0.608	0.345	0.274	0.477	0.322	0.252	0.455
	GRAN	0.494	0.423	0.617	0.492	0.420	0.616	0.361	0.287	0.504	0.327	0.252	0.473
	MSeaHKG	0.393	0.301	0.562	0.456	0.392	0.607	0.324	0.239	0.481	0.287	0.204	0.416
	HyNT	0.457	0.376	0.597	0.459	0.377	0.597	0.337	0.271	0.464	0.308	0.240	0.439
	HyperFormer		N/A		0.473	0.378	0.626		N/A		0.332	0.249	0.479
	StarE		N/A		0.394	0.290	0.593		N/A		0.315	0.240	0.458
	Hy-Transformer		N/A		0.399	0.298	0.588		N/A		0.314	0.241	0.453
	QUAD		N/A		0.379	0.272	0.583		N/A		0.316	0.245	0.451
	HAHE	0.495	0.421	0.623	0.492	0.418	0.620	0.379	0.305	0.521	0.345	0.269	0.491
MKG Embedding	IMF		N/A		0.462	0.393	0.605		N/A		0.298	0.212	0.429
	VISTA		N/A		0.457	0.389	0.593		N/A		0.251	0.174	0.408
	NativE		N/A		0.458	0.391	0.582		N/A		0.252	0.173	0.388
	MoSE		N/A		0.412	0.349	0.557		N/A		0.227	0.151	0.346
	AdaMF		N/A		0.407	0.331	0.559		N/A		0.214	0.136	0.342
MHKG Embedding	HyperFM	**0.515**	**0.448**	**0.645**	**0.514**	**0.446**	**0.643**	**0.408**	**0.337**	**0.546**	**0.375**	**0.302**	**0.523**

Table 2: Overall link prediction performance (*All entities* and *Head/Tail entities*). “N/A” indicates tasks that the method cannot be applied to (specifically, ShrinkE, HyperFormer, StarE, Hy-Transformer, QUAD, IMF, VISTA, NativE, MoSE, and AdaMF can only predict head/tail entities).

Evaluation metrics. In the link prediction task, a ranking list of entities is generated for the missing entity in a test fact. We then apply the filtered setting to remove any potential true entities other than the ground-truth entity. The prediction results are evaluated using Mean Reciprocal Rank (MRR), Hits@1, and Hits@10. We report both results on all entities and on head/tail entities only (because some baselines can only predict head/tail entities).

Hyperparameters and environment. Our HyperFM is trained for 300 epochs using the early stopping strategy on our benchmark hardware (Intel Xeon 6416H@2.20GHz, NVIDIA GeForce RTX4090 24GB, Ubuntu 22.04). Three key hyperparameters for HyperFM are the number of Hypergraph Transformer layers L_M, the number of edge-biased self-attention layers L_P, and the embedding dimension d. The optimal hyperparameter settings ($L_M = 2$, $L_P = 12$, $d = 256$) on both datasets are identified by grid search (more details in Appendix C).

Efficiency of Hypergraph Construction. As hyper-relational facts inherently form a hypergraph structure, there is no need to manually design a specific hypergraph for hyper-relational facts. As a result, the cost of constructing the hypergraph in the context of HKG embedding is negligible, because they are ready-to-use. For reference, the whole graph indexing process for HyperFM takes only 46.2 seconds on the WikiPeople dataset and 57.6 seconds on the WD50K dataset. In comparison, the total training time on the WikiPeople and WD50K datasets is 18.6 hours and 14.3 hours, respectively. Thus, the time required for graph indexing is negligible relative to the overall training process.

5.2 Overall Performance

Table 2 presents the link prediction performance on both datasets. The best results are highlighted in bold, while the second-best results are underlined. We observe that HyperFM consistently outperforms all baselines, achieving 6.0% and 6.8% improvements on average over the best-performing baselines in predicting all entities and head/tail entities, respectively.

Note that HyperFM performs better on WD50K than on WikiPeople, due to the larger ratio of hyper-relational facts in WD50K, as HyperFM is specifically designed for learning from such facts. We also find that three MKG embedding methods achieve performance comparable to HKG embedding methods in predicting head/tail entities, even without utilizing key-value pair information. This suggests that multimodal information is indeed helpful in link prediction. These observa-

Method	WikiPeople						WD50K					
	All entities			Head/Tail			All entities			Head/Tail		
	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10
HyperFM	**0.515**	**0.448**	**0.645**	**0.514**	**0.446**	**0.643**	**0.408**	**0.337**	**0.546**	**0.375**	**0.302**	**0.523**
w/o multi	0.496	0.422	0.625	0.493	0.418	0.623	0.379	0.306	0.522	0.346	0.271	0.495
w/o visual	0.499	0.424	0.630	0.497	0.420	0.625	0.385	0.312	0.530	0.356	0.273	0.508
w/o textual	0.504	0.431	0.637	0.502	0.430	0.633	0.392	0.318	0.538	0.362	0.280	0.513
w/ EC	0.497	0.420	0.631	0.495	0.415	0.630	0.382	0.302	0.533	0.358	0.283	0.499
w/ RG	0.498	0.420	0.631	0.495	0.417	0.625	0.377	0.295	0.531	0.356	0.282	0.490
w/o FC	0.503	0.430	0.629	0.500	0.424	0.631	0.389	0.313	0.534	0.361	0.281	0.505
w/o biases	0.509	0.441	0.643	0.510	0.443	0.642	0.402	0.334	0.541	0.369	0.298	0.521

Table 3: Ablation study of HyperFM with five variants.

tions further support the design principle of our HyperFM, which incorporates features from different *modalities* and integrates them through a *hypergraph* structure. We also report the results on relation prediction in Appendix D.

5.3 Ablation Study

To systematically validate the design choices of our HyperFM, we conduct a series of ablation studies to evaluate the effectiveness of the visual and textual modalities, our fact-centric fusion scheme, and the edge-biased mechanism.

Impact of multimodality. We consider three variants of HyperFM: 1) *w/o multi* removes both visual and textual modalities, 2) *w/o visual* removes the visual modality, and 3) *w/o textual* removes the textual modality. As shown in Table 3, we observe that both modalities contribute to performance improvement. Moreover, removing the visual modality shows a larger performance drop (4.5-4.9%) than removing the textual modality, showing that the visual modality provides more information to distinguish the subtle differences between entities than the textual modality.

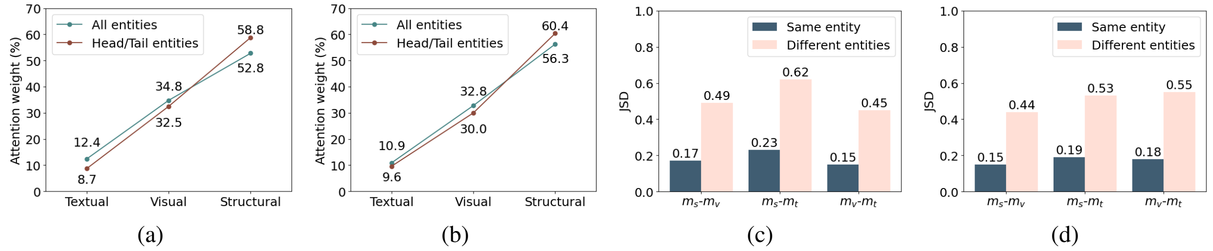
Impact of the multimodal fusion scheme. We first design two variants, *w/ EC* and *w/ RG*, to evaluate the superiority of our fact-centric fusion over the Entity-Centric (EC) and Relation-Guided (RG) fusion schemes, respectively. Specifically, in the *w/ EC* variant, bi-directional aggregation is performed between the structural modality and the structural, visual, and textual modalities. The *w/ RG* variant follows a similar pipeline to *w/ EC*, with the key difference being that, prior to the N-H aggregation, the representations of the three modalities are transformed by the primary relation-specific matrix. A detailed explanation of both fusion schemes is provided in Figure 3. The results of the two variants are presented in Table 3. We see that both *w/ EC* and *w/ RG* variants significantly underperform HyperFM, highlighting the superiority of our fact-centric fusion scheme over the entity-centric and relation-guided fusion strategies. In addition, we introduce a variant *w/o FC* that replaces the fact-centric hypergraph with a fully connected graph, to demonstrate the effectiveness of the proposed Hypergraph Transformer. As shown in Table 3, the results of *w/o FC* demonstrate that the Hypergraph Transformer boosts the link prediction performance with an average improvement of 4.0-4.1% across different datasets. This indicates that capturing interactions between diverse modalities while incorporating the hyper-relational structure of the fact is vital for link prediction tasks.

Impact of the edge biases. We verify the utility of edge biases by designing a variant *w/o biases*, which removes edge biases from the self-attention network. Results show that edge biases can also improve the link prediction performance and yield consistent improvements across different datasets.

5.4 Insights on the Multimodal Fusion Process

To further understand our fact-centric multimodal fusion process, we extract attention weights between hyperedges and nodes from the final layer of the Hypergraph Transformer and conduct in-depth analyses as follows.

Importance of different modalities. We compute the attention weights assigned to each modality averaged over all facts. We analyze the averaged attention weights on 1) all entities and 2) head/tail entities only. Figure 4a-4b shows the results on WikiPeople and WD50K datasets, respectively. We observe that the structural modality maintains the highest importance (weights) across different entity positions in a fact. This implies the primary role of the graph structure in multimodal fusion, aligning with our design of incorporating the hyper-relationality of the KG. Moreover, the Hypergraph Transformer can also learn to adjust the attention



(a) (b) (c) (d)

Figure 4: Insights on the multimodal fusion process. (a)-(b) show the average attention weights of different modalities on WikiPeople and WD50K datasets, respectively. (c)-(d) show the distributional difference of attention weights over facts between different modalities on WikiPeople and WD50K datasets, respectively.

weights for different positions, as evidenced by the different attention weights of the structural modality between all entities and head/tail entities.

Varying relationship between modalities of different entities. We further analyze the importance of different modalities of entities by measuring their variations across different facts. To this end, we compute the Jensen–Shannon divergence (JSD) between the attention weight distributions (over facts) of two different modalities of two entities, and we compare the cases of the two entities being 1) *different entities* and 2) the *same entity* (as a reference). We report the results on each pair of modalities $m_s - m_v$, $m_s - m_t$, and $m_v - m_t$. As shown in Figure 4c-4d, we see that the JSD between the modalities of different entities (>0.45 in most cases) is much larger than that of the same entity (<0.2 in most cases). This implies that the relative importance of different modalities of different entities indeed varies across facts. Our fact-centric fusion scheme can model such variation through the incidence graph representation of MHKG, where multimodal nodes of entities of a fact are directly connected to the fact hyperedge, as shown in Figure 3.

6 Conclusion

In this study, we propose HyperFM, a Hyper-relational Fact-centric Multimodal Fusion technique, which can directly learn from multimodal hyper-relational facts by capturing intricate interactions between diverse modalities while at the same time accommodating the hyper-relational structure using our designed Hypergraph Transformer. Experiments on two real-world multimodal KG datasets show the superiority of HyperFM in link prediction tasks, outperforming a sizeable collection of state-of-the-art baselines with an average improvement of 6.0-6.8%. Furthermore, ablation studies systematically validate the fact-centric fusion scheme of our HyperFM.

Our future work will study multimodal link prediction tasks for images/text using large vision/language models. We also identify multi-hop reasoning over HKGs as a promising direction for addressing complex query scenarios. To this end, we will explore the incorporation of multimodal information to enhance the effectiveness and interpretability of multi-hop reasoning on HKGs.

7 Limitations

In this study, we focus on the link prediction task for entities and relations, combining multimodal information of images and text for each entity. However, images and text in real-world KGs also face missing data challenges. Therefore, we plan to extend our model beyond traditional link prediction to address image and text prediction using advanced large vision and language models.

8 Ethics Statement

This paper investigates the problem of knowledge graph link prediction, aiming at hyper-relational knowledge graph completion with multimodal information to empower a wide range of web applications, such as question answering, recommender systems, and query expansion. The multimodal KG datasets used in this paper are all publicly available. Therefore, we believe it does not raise any ethical issues.

Acknowledgments

This project has received funding from the Science and Technology Development Fund, Macau SAR (0047/2022/A1, 001/2024/SKL), Jiangyin Hi-tech Industrial Development Zone under the Taihu Innovation Scheme (EF2025-00003-SKL-IOTSC). This work was performed in part at SICC which is supported by SKL-IOTSC, University of Macau.

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Appendix

A Modal Encoder

This section introduces the three modal encoders used to extract specific modal features.

Structural encoder. Traditionally, the structural features of entities are extracted using pre-trained KG embedding models, and the obtained features are fed in parallel with extracted visual and textual features into the subsequent multimodal fusion module (Li et al., 2023; Lee et al., 2023). However, this design overlooks the fact-level information for link prediction and thus impairs the essential information preserved by the graph structure. Therefore, we propose to directly use randomly initialized learnable embeddings as structural features, thus allowing for the multimodal fusion process to flexibly learn the intricate structural information by

Method	WikiPeople			WD50K		
	L_M	L_P	d	L_M	L_P	d
HyperFM	2	12	256	2	12	256
w/o multi	2	10	256	2	10	256
w/o visual	2	12	256	2	12	256
w/o textual	2	12	256	2	12	256
w/o FC	2	10	256	2	10	256
w/o biases	2	12	256	2	10	256

Table 4: The optimal hyperparameter settings for HyperFM and its variants.

fusing information from other modalities (more detail below) in the training process.

Visual encoder. Visual information encoded in the entity images characterizes additional information about entities beyond the KG structures. Following (Li et al., 2023; Lee et al., 2023), we utilize pre-trained VGG16 (Liu et al., 2019) as the visual encoder to derive visual embeddings for the corresponding entities. Specifically, for each image fed into VGG16, we get embeddings from the last hidden layer before the Softmax function as the visual features for the corresponding entity.

Textual encoder. Textual descriptions populate and enrich semantic information for entities. To extract textual features, we resort to pre-trained BERT (Devlin et al., 2018), which can comprehensively represent textual descriptions and convert them into semantically enriched embeddings. Specifically, for each textual description fed to BERT, we get the pooled outputs of BERT as the textual features for the corresponding entity.

It should be noted that the pre-trained visual or textual models (VGG16 and BERT respectively) are not fine-tuned during the training stage but are employed as fixed feature extractors. In addition, our HyperFM is designed to be flexible, allowing for any of these pre-trained models to be replaced with other pre-trained visual or textual models if necessary.

B Baseline Details

The first category includes hyper-relational KG embedding methods: **m-TransH** (Wen et al., 2016) captures the interactions among entities within an n-ary fact; **RAE** (Zhang et al., 2018) extends m-TransH by explicitly taking the pairwise correlation features between entities into account; **NaLP** (Guan et al., 2019) captures the interactions between relation-entity pairs using CNNs; **NeuInfer** (Guan et al., 2020) separately learns from the base triplet and its affiliated key-value pairs; **HINGE** (Rosso et al., 2020) repeatedly learns from triplets and affiliated key-value pairs using CNNs; **ShrinkE** (Xiong et al., 2023) models a base triplet as a spatio-functional transformation from the head entity to a relation-specific box; **HyConvE** (Wang et al., 2023a) leverages 3D convolution to capture the sophisticated interactions among entities and relations in a fact; **HJE** (Li et al., 2024) extends HyConvE to further capture the global semantics between facts; **GRAN** (Wang et al., 2021) incorporates edge biases to discriminate connections between elements in a fact and harnesses the self-attention mechanism to further capture the correlation; **MSeaHKG** (Di and Chen, 2021) employs neural architecture search to identify the most suitable graph encoder for hyper-relational facts; **HyNT** (Chung et al., 2023) develops a context Transformer to learn representations of the primary triplets and the qualifiers by exchanging information among them; **HyperFormer** (Hu et al., 2023) encodes the local-level semantics in hyper-relational facts using Transformers; **StarE** (Galkin et al., 2020) designs a directed heterogeneous graph encoder to capture the interactions among elements in a fact; **Hy-Transformer** (Yu and Yang, 2021) replaces the computation-heavy graph neural network module with light-weight entity/relation processing techniques; **QUAD** (Shomer et al., 2022) is another variant of StarE by designing two paralleled pipelines to learn from the triplets and key-value pairs, respectively; **HAHE** (Luo et al., 2023) employs a hypergraph attention mechanism to encode the global structure of a KG and leverages edge-biased self-attention networks to capture local semantics in a fact.

The second category includes multimodal KG embedding methods: **IMF** (Li et al., 2023) integrates multimodal information with bilinear functions; **VISTA** (Lee et al., 2023) models the correlation between structural and visual modalities via a relation-aware Transformer; **NativE** (Zhang et al., 2024a) balances the information of different modalities using a collaborative adversarial training approach; **MoSE** (Zhao et al., 2022b) learns modality-split relation embeddings for each modality instead of a single modality-shared one; **AdaMF** (Zhang et al., 2024b) achieves multimodal fusion with adaptive modality weights and generates adversarial samples for imbalanced modality information.

Method Type	Method	WikiPeople						WD50K					
		All relations			Primary relations			All relations			Primary relations		
		MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10
HKG Embedding	NaLP	0.875	0.838	0.929	0.854	0.817	0.929	0.775	0.702	0.896	0.748	0.685	0.853
	NeuInfer	0.906	0.852	0.954	0.853	0.824	0.901	0.816	0.759	0.924	0.802	0.738	0.886
	HINGE	0.935	0.895	0.976	0.927	0.875	0.951	0.878	0.812	0.963	0.850	0.796	0.928
	GRAN	0.959	0.944	0.976	0.957	0.937	0.983	0.945	0.917	0.983	0.929	0.891	0.970
	MSeaHKG	0.836	0.792	0.953	0.801	0.783	0.906	0.825	0.778	0.917	0.787	0.759	0.901
	HyNT	0.948	0.928	0.973	0.953	0.935	0.978	0.907	0.881	0.948	0.906	0.875	0.952
	HAHE	0.959	0.944	0.977	0.953	0.939	0.972	0.940	0.914	0.977	0.930	0.900	0.971
MKG Embedding	IMF	N/A			0.867	0.839	0.903	N/A			0.845	0.756	0.929
MHKG Embedding	HyperFM	**0.971**	**0.955**	**0.989**	**0.969**	**0.952**	**0.988**	**0.961**	**0.934**	**0.995**	**0.949**	**0.928**	**0.989**

Table 5: Overall relation prediction performance (*All relations* and *Primary relations*). "N/A" indicates tasks that the method cannot be applied to (specifically, IMF can only predict primary relations). All baselines are implemented in our environment using their original hyperparameter settings. Other baselines, including m-TransH, RAE, ShrinkE, HyConvE, HJE, HyperFormer, StarE, Hy-Transformer, QUAD, VISTA, NativE, MoSE, and AdaMF, cannot predict relations by design, and are thus excluded from the table.

C Hyperparameter Settings

Three key hyperparameters of HyperFM are the number of Hypergraph Transformer layers L_M, the number of edge-biased self-attention layers L_P, and the embedding dimension d. We employ the grid search strategy to identify the optimal hyperparameter setting. The range of candidate values for hyperparameters L_M, L_P, and d are {1, 2, 3, 4}, {6, 8, 10, 12}, and {64, 128, 256, 512}, respectively. Afterward, the optimal hyperparameter setting of a model is identified by comparing the link prediction performance under different hyperparameter combinations. The final hyperparameter settings for all models (HyperFM and its variants) are shown in Table 4.

D Experiments on Relation Prediction

Table 5 shows the relation prediction performance on the two datasets. We observe that the proposed HyperFM consistently outperforms all baselines, achieving average improvements of 1.4% and 1.7% over the best-performing baselines in predicting all relations and primary relations (namely the relation connecting head and tail entities), respectively. The slight improvements are due to the solution space for relations being much smaller than that for entities, resulting in a high benchmark in relation prediction for all methods.