

Recommendation System Based on Knowledge Graph Completion with Imbalanced Relation Types

The Avengers

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Abstract

In this paper, we propose an effective and robust approach for alleviating the impacts of imbalanced relation types in the training and evaluation of recommendation systems based on knowledge graph completion methods. The adjusted loss function with focal loss was proven to be able to alleviate the bias towards dominant relations in the knowledge graph across model architectures. The success of our method can be attributed to the fact that, by down-weighting the abundant relations, the models are forced to pay extra attention to the scarce relations. As a result, the trained models are less biased towards abundant relations and more capable of detecting the scarce relations. We believe that this is a valuable property for a model to have in a knowledge graph based recommendation system, where the target relation is often a minority.

Introduction

The recommendation system seeks to infer customers' preferences to deliver a personalized experience by predicting a list of entities (e.g., products or other users) that likely results in a positive interaction, such as a conversion event. An effective recommendation system facilitates users seeking information and benefits content providers with more potential to make profits. Therefore, the applications of recommendation systems have been widely demonstrated in e-commerce websites like Amazon and Alibaba, streaming services like Netflix, Spotify, Pandora, and social networks like Facebook and LinkedIn. Consequentially, recommendation systems are prevalent in today's world.

Most studies of recommendation systems focus on developing machine learning models to fit user behavior data, without considering the potential impact of unbalanced data. This can lead to serious issues, so it is important to explore ways to eliminate the impacts of unbalanced data on the effectiveness of these models.

The representative types of implementations of recommendation systems:

1. Matrix completion is a popular approach to personalized recommendations that identifies similarities among users from their collective historical choices. This approach has yielded successful results, but it is acknowledged that attributes of entities may fail to reveal underlying preferences of customers beyond historical, collective user-item interactions.

2. Graph neural networks can be used to learn user and item embedding from the topological structure of a bipartite graph, in order to predict interactions between users and items. This is seen as a generalization of the matrix completion approach, since it allows for multi-hop message propagation across nodes.

3. The Knowledge Graph Completion approach expands on the bipartite graph approach by adding additional entities and relations to depict user-item interactions. This additional information provides a richer data representation of the users and the items, which can be valuable to the performance of the recommendation system. Recent developments of the graph neural network approach on knowledge graph include KGAT [19], KGNN [7], and CompGCN [15] building on the established line of shallow knowledge graph embedding models (TransE [2], ComplEx [14], TransR [8]) have shown promises in improving the state of the art results on drug-drug interaction problem, node classification, and link prediction problems.

In the knowledge graphs designed for recommendation system models, for every (user,item) pair, there are various relations to expand and enrich the information. See sample relation graph of Amazon Beauty Product as an example (Figure 1). As shown in the Figure 2, the target relation "like" (orange) only amounts to less than 5% of all observations in the data. This poses a relation imbalance problem to model training. Inspired by [6], we derive focal loss functions for each model to assign more weights

as highlight our approaches to the challenges that we encountered during the process.

Data Pipeline

Data Source The raw data is obtained from the Amazon product review dataset released by Ni et al. in 2019 [4].¹ The database includes two data collections: the "**meta**" collection stores product attributes across 39 main categories, and the "**review**" collection includes product review rating, corpus, and review summaries for each product in the meta database. Product items are identified by the Amazon Standard Identification Number (ASIN) in both data collections, while reviewers are identified by an anonymous user ID in "reviews". To conclude, for each product category, we are able to observe product attributes, as well as customer-item interactions in terms of written reviews. Note that we only observe purchase activities in which the customer wrote a product review for their purchase.² Here are excerpts from example documents of a meta and a review raw data:

```
{
  "price": "$9.99",
  "main_cat": "All Beauty",
  "category": [
    "Clothing, Shoes & Jewelry",
    "Costumes & Accessories",
    "Women",
    "Wigs"
  ],
  "asin": "B0002483KI",
  "brand": "Topbuti",
  ...
}

{
  "overall": 5.0,
  "verified": true,
  "reviewTime": "05 25, 2016",
  "reviewerID": "A0969754FZ",
  "asin": "B0002483KI",
  "reviewText": "With the low price of this wig,
    ↪ I was very impressed.",
  "summary": "Five Stars",
  ...
}
```

To see how a knowledge graph is built from the raw data and to present the list of relations we kept, we extracted a snippet of our data illustrated in Figure 1: here products "*B0070WVEWE*" (the black wig), "*B00KXVY7M8*" (the green wig), and "*B00CQGUT3E*" (the red wig) are three most popular wigs in the dataset. Customers "*A...O3E*" (cus-

tomers A) and "*A...3KR*" (customer B) are two customers who purchased these three popular products as well as some other closely related products, including wigs of other colors and combs. There are some other relations, specifically, a product can be linked to a brand via the "brand" relation; to a category via the "is_an_instance_of" relation; to a price via the "price" relation; to other products via the "also_view" or "also_buy" relation, indicating that customers who purchased the product also viewed or bought some other products. Similarly, a customer can be linked to a product via "wrote_summary" relation, when they gave a review to the product, or "ranked_number" relation, with which the number stands for the number of stars that the customer has given to the product. Since the purpose of the recommendation system is to recommend products to customers that they might like, ranks above 4 are considered as liked, and the rest are classified as disliked. In this sense, the knowledge graph extends the collaborative filtering approach by featuring more types of user-item interactions. In the example, customer B has ranked 5 to the red wig, and the red wig has a "also_buy" relation to product "*BO1LZTOFTN*" (comb). Customer A, who bought the green wig as customer B did, has ranked 5 (like) to the comb, therefore, presumably, we would expect a system to recommend the comb to customer B.

A comprehensive visualization for the constructed knowledge graph around the same three products with actual observed number of nodes and edges is included in the Appendix.

Data Selection We select the subset products that belong to the "Beauty" category, one of the smaller datasets. This is mainly driven by storage and computational resource concerns. For model training purposes, we also filter on users and items with at least 5 interactions. As for the train-test split, our training set includes all relations and our test set includes only positive rankings (the like relation) as this is the only relation relevant to a recommender system. Implication of the induced relation class imbalanced will be discussed and addressed in the next section. The recommender systems we considered are transductive in nature, so users and items that appear in the validation and test sets must have appeared in the training set.

Data Format To streamline model training, the raw data needs to be transformed and parsed as a knowledge graph in a tensor format that can be readily loaded and read by machine learning modules such as the pytorch DataLoader class.

To elaborate on the data transformation, we invoke a definition of a knowledge graph data point

¹Data repository at: <https://nijianmo.github.io/amazon>

²Non-purchasers are not qualified to write product reviews on Amazon.

proposed in [3]: A knowledge is defined by an ontology using resource description framework (RDF). Let E and R denote the sets of entities and relations in the knowledge. The RDF representation of the knowledge graph data base consists data points in terms of triples. Each triple (s, p, o) is an ordered set of the following RDF terms: a subject $s \in E$, a predicate $p \in R$, and an object $o \in E$.

For instance, the RDF representation of the raw "meta" and "review" raw data regarding the item B0002483KI is:

```
{ #subject, predicate, object
  ["B0002483KI", "price", "$9.99"],
  ["B0002483KI", "main_cat", "All Beauty"],
  ["B0002483KI", "instance_of", "Wigs"],
  ["B0002483KI", "brand", "Topbuti"],
  ["A0969754FZ", "rank_5", "B0002483KI"],
  ["A0969754FZ", "wrote_summary", "Five Stars"],
  ...
}
```

The RDF data representation is essentially tabular. Therefore, it would suffice to assign an integer lookup ID for each entity and relation so they can be presented to computational module in terms of a pytorch Long tensor.

Implementation

Several knowledge graph completion models were used to approach the user-item prediction problem, including two shallow embedding approaches (TransE [2] and ComplEx [14]), and two graph neural network models (CompGCN [15] and KGAT [19]).

In our data, the target relation is "like": a user s is identified to "like" an item o if, s left a rating of at least 4 stars on the product page of o . Ultimately, for each user s in the test set, we want to find items o such that (s, like, o) .

Given an RDF triplet (s, p, o) we want to train an encoder model to learn a representation/embedding for each of the entities s, o and the relation p in the d -dimensional vector space, $e_s, e_p, e_o \in \mathbb{R}^d$ such that the relation likelihood can be evaluated using a score function of tuple $\phi(e_s, e_p, e_o)$. A loss function L is then constructed to optimize the model weights.

At the end, fine-tuned models decode ϕ and output a score for each (user, item) pair, indicative of how likely the user will like the item. The scores are then ranked to give K recommendations for each test user. We will discuss performance metrics in the next section.

Shallow Knowledge Graph Embedding (KGE) Approach: TransE and ComplEx In [12], it was noted that some of the older shallow knowledge graph embedding (KGE hereafter) models, when

trained and tuned properly, can provide very satisfactory results, even matching state-of-the-art results in knowledge graph completion. We also note that KGE models are much less computational expensive than deep graph networks. So, we start our implementation with two popular KGE approach and will compare performances to see if they provide simpler, but faster and more economic performances than the deep learning counterparts.

In TransE [2], an embedding representation $e_s, e_p, e_o \in \mathbb{R}^d$ is learned for each (s, p, o) . The score ϕ of triplet (s, p, o) is simply the vector norm $\|e_s + e_p - e_o\|$, which the model learns to minimize.³ The intuition for the scoring function is to consider a relation as a translation operator that moves entities in a given direction. This simple setup turns out to be scalable and compatible with a lot of real world relations⁴ and makes TransE the state-of-the-art knowledge graph embedder at its time. Nevertheless, we do not anticipate TransE to perform particularly well in recommender systems because the target relation that we seek to predict - positive rating - is essentially one-to-many. For a given customer embedding, e_s , the positive rating embedding e_o learned by a TransE model will always map the customer to the same entity $e_s + e_o$. ComplEx [14] is another shallow knowledge graph embedding model that learns such one-to-many relations.

In ComplEx, the embeddings (e_s, e_p, e_o) learned are in the complex vector space \mathbb{C}^d . The score function for the ComplEx encoder is $\phi(s, p, o) = \text{Re}(\langle e_p, e_s, \bar{e}_o \rangle)$, such that the odds of observing the triplet (s, p, o) is given by the sigmoid-activated scores. One can easily see that given an user embedding there can be multiple item embeddings that yield similar scores ϕ . Like TransE, ComplEx also utilizes a contrastive loss with negative sampling.

We implement both TransE and ComplEx on our data using the LibKGE package.⁵

Deep Graph Neural Network Approach: CompGCN and KGAT: We refer to TransE and ComplEx as "shallow" embedding methods as they do not involve deep neural networks. Graph neural networks presented below are deep learning extensions of KGE methods that are more expressive and powerful in fitting network patterns arising from multi-hop interactions. We implement two deep learning models for knowledge graph completion:

³The loss function here corresponds to the original form given in [2]. When implemented, we apply a sigmoid activation in a pairwise logistic loss formulation for smoothness. Please see appendix.

⁴For example, we can enforce logical constraints such as symmetry to enhance performance

⁵Repository at: <https://github.com/uma-pi1/kge/>

CompGCN [15] and KGAT [19]. The former is an extension of GCN [5] that learns multiple relations, and latter is an extension of GAT [16] with the explicit goal of modeling user-item interactions. We view both models as extensions of KGE approaches because both models use elements of established KGE models to learn embedded layer that propagate in the networks. Because KGE models only apply to seen entities in a fixed graph, this implies that all the models we have considered in this project are transductive in nature - that they cannot generalize to new, unseen nodes or edge types. We acknowledge that scaling and inductive learning in knowledge graph completion poses real business importance and there is a line of work about this topic ([17], [9], [18], [20]); but that would be out of the scope for this project.

CompGCN is a graph convolutional network that learns relations between entities in the graph. The model is a generalization of GCN [5] that can learn to combine multiple relations in the graph. Unlike KGAT, CompGCN does not rely on pre-learned KGE models. In CompGCN a score ϕ is computed for the embedded nodes and relations (the authors considered KGE scoring functions from TransE, DistMult, ConvE) and then is propagated across layers. Like GCN [5], the computation graph for a node in each layer is given by its one-hot neighbor. At the end, a sigmoid activation layer is applied to the embedding output of the final layer to represent the likelihood of an observe/corrupt triplet.

KGAT attempts to learn two aspects of the data: a collaborative filtering component and a knowledge graph completion component. The first concerns whether interactions should exist given similarity of historical behavior in the data, to be learned by a GAT [16] instance. The latter concerns message propagation across entities for all observed relations, which is learned by a TransR [8] KGE. Embedding and model weights are trained to optimize an additive composite loss: the collaborative filtering (CF) cross entropy loss for edge prediction (for the target relation class), and a knowledge graph (KG) loss implied by the TransR [8] scoring function $\phi(s, p, o) = \|W_p e_s + e_p - W_p e_o\|^2$.

Both models utilize negative sampling. We implement them using the CompGCN⁶ and KGAT-pytorch⁷ modules.

Challenges

As we applied the workflow to train models on our data, we encountered the following empirical challenges:

1. **Users with little activities:** We observe that more than 95% of users present in the review database only wrote one review among all Beauty products. The sparseness of these users would make it difficult for the models to learn their embeddings with adequate statistical confidence. We filtered our training and test data to include users and products with at least 5 interactions.
2. **Memory space and time limitations:** Even with the filter above, the data size is still rather large to train and takes a long time to fine-tune. Another problem that comes with data size is having to train larger models, since graph model scales up as number of nodes and edges increase. A few instances of our attempt to fit the full data could not fit in the GPU memory. In light of the timeline and resources available of this project, we made the following compromises:
 - i Further filtered the data to manageable size,
 - ii Searched over larger learning rates,
 - iii Reduced max epochs limits,
 - iv Decreased model sizes in terms of embedding dimension,
 - v Reduced training time memory requirement by reducing batch sizes.
3. **Hyper-parameter Search:** There are a large number of hyper-parameters to be tuned for each model. Also, the evaluation metrics vary greatly across combinations. To facilitate tuning, we employ Bayesian hyper-parameter optimization techniques (implemented from with Ax through LibKGE and optuna) to effectively search the hyper-parameter space. We documented results across our hyperparameter trials in [ML Flow server](#).⁸
4. **Gradient Explosion:** When the focal loss parameter γ is close to 1, gradients can become very large in magnitude and result in NaN values in training loss. To solve the problem, we applied clipping of focal weights - constraining them to lie in $[\varepsilon, 1 - \varepsilon]$ - to stabilize learning.⁹

Experiments & Results

Experiments

After configuring the experiment environment stated as above, experiments were carried out in two stages: 1. to set baseline for each model, each of TransE, ComplEx, CompGCN, and KGAT were fitted with the same training data and validated with validation dataset. many iterations of hyper-parameters tuning were performed to achieve representative results for each model. Finally, evaluated each tuned

⁶Repo at: <https://github.com/malllabiisc/CompGCN>

⁷Repo at: <https://github.com/LunaBlack/KGAT-pytorch>

⁸<http://52.53.202.9:5000>

⁹We take ε to be 10^{-6} .

model with test set as baseline. 2. to compare our proposed method, we adjusted loss functions of all TransE, ComplEx, CompGCN, and KGAT models, then proceeded to tuning hyper-parameters for the adjusted model algorithms with the same manner performed in the first stage. Finally, evaluated these new models with the same test set for comparison.

Hyperparameter search over the candidate grid points was facilitated using Bayesian optimization techniques [1]. The sets of grid points for tuned hyperparameters for each model are presented in the Appendix. We use mean reciprocal rank (MRR) as the validation metric and criterion for model selection.

Results

We present the results from models fine-tuned with automatic hyper-parameter search algorithm¹⁰ for each knowledge graph embedding methods. For each method, the model with best validation set result are selected, and test set results with selected models are recorded below (better performances are in bold font).

	Loss Function	Metric ¹ @5	Metric @10	Metric @100
TransE	Original	0.000	0.000	0.090
ComplEx		0.060	0.075	0.383
CompGCN		0.128	0.162	0.451
KGAT		0.129	0.188	0.771
TransE	Focal	0.004	0.004	0.117
ComplEx		0.048	0.094	0.447
CompGCN		0.132	0.192	0.519
KGAT		0.115	0.239	0.692

¹ TransE, ComplEx, CompGCN: Hits@X, KGAT: Recall@X

Table 1: Evaluation metrics for models fitting with original loss function and loss function adjusted with focal.

Overall, deep learning models, including CompGCN and KGAT surpass the distance translation method TransE, and the shallow semantic learning method ComplEx by a significant margin. This is not surprising to us because deep learning models are more expressive than shallow embedding models. On the other hand, as we had anticipated, ComplEx performs better than TransE as the latter is known to have a shortcoming of fitting one-to-many relations. Finally, we observe improvements in at least one of the metrics from applying focal loss for each of the models.

As a robustness check of our focal weight approach, we conduct a separate run on the bench-

mark knowledge graph dataset amazon-book with KGAT, using the best hyperparameter set mentioned in the paper[19], to compare the original model and the focal-adjusted model. The results are presented in Table 2.

	Recall @3	Recall @5	Recall @10	Recall @100
Original	0.043	0.061	0.094	0.307
Focal	0.044	0.062	0.097	0.310

Table 2: Evaluation metrics for KGAT models fitted with original loss function and focal-adjusted loss function

Summary and Future Extension

We propose an effective and robust approach for alleviating the impacts of imbalanced relation types in the training and evaluation of recommendation systems based on knowledge graph completion methods. The adjusted loss function with focal loss was proven to be able to alleviate the bias towards dominant relations in the knowledge graph across model architectures. The success of our method can be attributed to the fact that, by down-weighting the abundant relations, the models are forced to pay extra attention to the scarce relations. As a result, the trained models are less biased towards abundant relations and more capable of detecting the scarce relations. We believe that this is a valuable property for a model to have when used in a knowledge graph based recommender system, where the target relation is often a minority.

Beyond our achievements, various other factors may also affect the prediction of minority relations, such as possible data leakage among train, valid, and test sets. Substitute and complementary relations among products, or more broadly the diverse specifications of knowledge graph ontology that we did not explore, plus the potential to fusion with knowledge bases [10] like WikiData,¹¹ NELL.¹² Further investigation of the impacts of all the above factors is worth exploring in the future. Additionally, we could explore different ways of weighting the relations in the knowledge graph, such as explicit weighting, to see if this leads to improved performance. Finally, we could investigate the differences between the errors produced by the original loss function and the focal loss adjusted loss function to see if there are any patterns that could be exploited to improve the performance of our method.

¹¹<https://www.wikidata.org/>

¹²<http://rtw.ml.cmu.edu/rtw/kbbrowser/>

¹⁰Implemented with optuna and ax (through LibKGE)

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Appendices

Focal Weights Formulation

In binary classification, given a predicted probability for $y_i = 1$, the loss function is $L = \sum_i (y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i))$. As in [6], the focal weight for example i is p_i^γ if y_i is 1, and $(1 - p_i)^\gamma$ if y_i is 0. That is, the focal weight is taken to be the predicted mis-classified probability. This is very intuitive - when the model is largely predicting an incorrect outcome, we would like the example weight to increase.

In knowledge graph models we worked with, a pairwise logistic loss function is derived from contrastive learning using negative samples. In general terms, suppose the un-noramlized ("energy") score of a knowledge triplet is given by $\phi(\cdot)$. Let (s, p, o) be a positive example actually observed in the training set and (s', p, o') be a corrupt example negatively sampled from the set of entities and relation. The pairwise logistic loss for this pair is: $-\ln \sigma(\phi(s, p, o) - \phi(s', p, o'))$. Here σ is the sigmoid activation. Despite not having the interpretation of 1-P(ground truth) in binary cross entropy loss case, we propose to have similar formulation:

$$L^* = \sum_{(s,p,o),(s',p,o')} -\lambda^\gamma \ln \sigma(\phi(s, p, o) - \phi(s', p, o'))$$
$$\lambda = 1 - \sigma(\phi(s, p, o) - \phi(s', p, o'))$$

The intuition is that whenever score differential between the true and corrupt triplets, $\phi(s, p, o) - \phi(s', p, o')$ is low, it means that the model is not learning the contrast between true and corrupt interactions well. So we emphasize the example by assigning a (positive) weight loss decreasing in $\phi(s, p, o) - \phi(s', p, o')$. The sigmoid activation bounds the loss to within $[0, 1]$ and provides a convenient transformation: 1-sigmoid activated score. To prevent gradient explosion, we clip λ and restrict it lie in the interval $[\varepsilon, 1 - \varepsilon]$.

Hyperparameter Set

TransE and ComplEx:

```
{
  "num_trials": 200,
  "num_sobol_trials": 15,
  "batch_size": {64, 128, 256, 512},
  "learning_rate": (0.0003, 1.0),
  "lookup_embedder_dim": {64, 128, 256, 512, 1024
    ↪ },
  "lookup_embedder_dropout": (0.2, 0.8),
  "lookup_embedder_regularize_weight": (0.0, 0
    ↪ .1),
  "train_type": "negative_sampling",
  "max_epochs": 40,
  "loss": {"bce", "bce_focal"}
}
```

CompGCN:

```
{
  "score_func" : {"conve", "transe", "distmult"},
  "opn" : {"corr", "sub", "mult"},
  "batch" : (128, 600),
  "gamma" : (0, 44.0),
  "lr" : (0.005, 0.01),
  "lbl_smooth" : (0.01, 0.3),
  "gcn_dim" : (10, 200),
  "gcn_layer" : {1, 2},
  "gcn_drop" : (0.0, 0.3),
  "hid_drop" : (0.0, 0.3),
  "hid_drop2" : (0.0, 0.3),
  "feat_drop" : (0.0, 0.3),
  "k_w" : (5, 20),
  "k_h" : (5, 20),
  "num_filt" : (10, 200),
  "ker_sz" : (10, 30),
  "fc_loss_gamma" : {0, 0.9999},
}
```

KGAT:

```
{
  "kg_batch_size" : (1024, 2048),
  "laplacian_type" : {"random-walk",
    ↪ "symmetric"},
  "aggregation_type" : {"bi-interaction", "gcn",
    ↪ "graphsage"},
  "kg_l2loss_lambda" : (1e-5, 1e-2),
  "cf_l2loss_lambda" : (1e-5, 1e-2),
  "lr" : (0.0001, 0.01),
  "use_gamma": {0, 0.9999}
}
```

Knowledge Graph Visualization

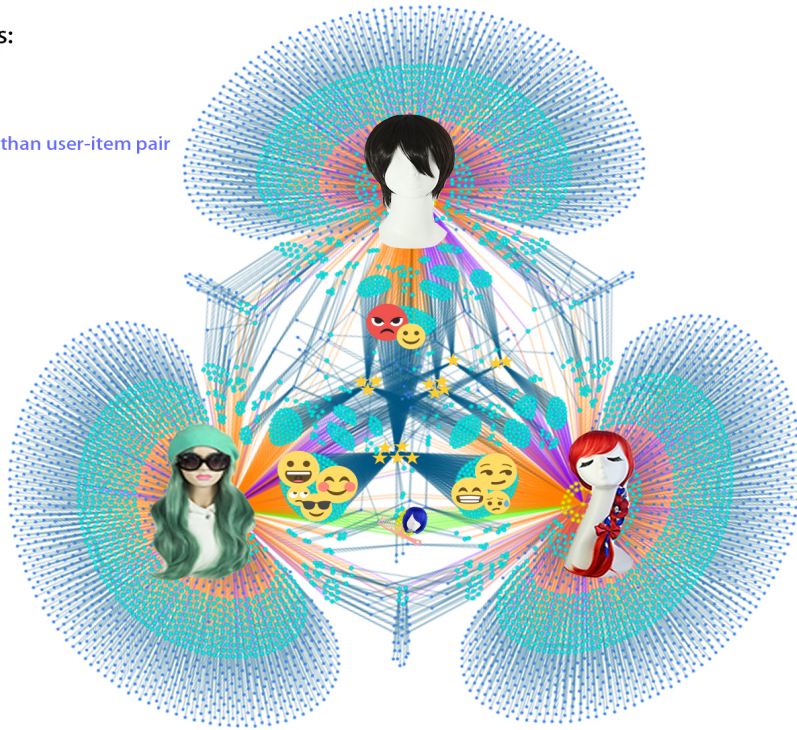
Figure 4 shows all edges and nodes connected to the three wig products featured in Figure 1. The products nodes are represented by the product images in the figure. There are 3,667 users (blue) who reviewed these products. Common user nodes that share review history between any two of the products are represented by emojis. There are 195 edges that represent non-interactions, such as price, brand, and category instances.

color of nodes:

---- reviewer

---- meta

---- entities other than user-item pair



color of relations:

---- has_written_summary

---- ranked_1 (dislike)

---- ranked_2 (dislike)

---- ranked_3 (dislike)

---- ranked_4 (like)

---- ranked_5 (like)

---- also_view

---- is_of_brand

---- also_buy

---- price

---- is_an_instance_of

---- is_discontinued

Figure 4: Knowledge Graph of Amazon Beauty Product Review (best viewed in color)

Work Distribution

Student	Contributed Aspects	Details
Hao Xu	research implement conduct experiments paper writing active discussion.	research and implementation on * KGAT Implement focal loss and debug on KGAT conduct research on Amazon datasets
Kin-ping Wong	research implement conduct experiments paper writing active discussion project planning activity coordination	research and implementation on * TransE * ComplEx * CompGCN * KGAT Clean, create, and transform training data Derive focal weight formulation Implemented KGE models Literature review Paper Writing and Editing
Ruhan Li	research implement conduct experiments paper writing active discussion data visualization	research and implementation on * TransE * ComplEx * KGAT Conducted research on benchmark datasets Generated datasets distributions for benchmark & Amazon product dataset Generated relation visualization for Amazon product dataset Tuned hyper-parameters for TransE Paper formating, writing and editing
Yongkang Zhao	research implement conduct experiments paper writing active discussion project planning activity coordination data visualization code-base setup database setup mlflow server setup	research and implementation on * CompGCN * KGAT Setup mongodb server, Import and index amazon-product review dataset Develop library to query from mongodb Setup github repository and codebase structure. Develop and run pipeline for: querying data, setup environment, tuning hyper-parameters, model statistics storage with mlflow initiatives to support data visualization tasks conduct preliminary research on the topic to set the direction.