OpticE: A Coherence Theory-Based Model for Link Prediction

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Abstract
Knowledge representation learning is a key step required for link prediction tasks with knowledge graphs (KGs). During the learning process, the semantics of each entity are embedded by a vector or a point in a feature space. The distance between these points is a measure of semantic similarity. However, in a KG, while two entities may have similar semantics in some relations, they have different semantics in others. It is ambiguous to assign a fixed distance to depict the variant semantic similarity of entities. To alleviate the semantic ambiguity in KGs, we design a new embedding approach named OpticE, which is derived from the well-known physical phenomenon of optical interference. It is a lightweight and relation-adaptive model based on coherence theory, in which each entity’s semantics vary automatically regarding different relations. In addition, a unique negative sampling method is proposed to combine the multimapping properties and self-adversarial learning during the training process. The experimental results obtained on practical KG benchmarks show that the OpticE model, with elegant structures, can compete with existing link prediction methods.

1 Introduction
Knowledge graphs (KGs) consist of sets of triplets that can represent real-world concepts, common sense information or facts. Each triplet \((h, r, t)\) indicates a directional relation \(r\) from the head entity \(h\) to the tail entity \(t\). WordNet (Miller, 1995), Freebase (Bollacker et al., 2008) and Wikidata (Vrandečić and Krötzsch, 2014) are the most well-known KGs with tremendous numbers of entities and relations. These KGs play important roles in a range of areas, such as natural language processing tasks (Cao et al., 2021), question answering applications (Bosselut et al., 2021) and recommendation systems (Shao et al., 2021). Research on KGs is thriving in both academic and industrial communities.

Link prediction is a fundamental problem when addressing KGs. To learn the hidden patterns from the observed triplets, extensive investigations have been performed to embed entities and relations into a continuous semantic space; this is known as KG embedding learning (Rossi et al., 2021). Among these embedding models, from a mathematical perspective, TransE (Bordes et al., 2013), TransH (Wang et al., 2014) and TransR (Lin et al., 2015) are translation-based models that use translation transformations to characterize the existence of triplets. Other methods (e.g., RESCAL (Nickel et al., 2011) and DistMult (Yang et al., 2015)) tackle this problem with matrix or tensor multiplication. Recently, the embedding problem has been discussed in the complex domain (e.g., ComplEx (Trouillon et al., 2016), RotatE (Sun et al., 2019) and HAKE (Zhang et al., 2020)). These methods have achieved great performance on related tasks. While our models are discussed in the complex domain, they are designed under an interference framework.

The semantic ambiguity caused by multimapping relations was ignored in most previous methods. As illustrated in Figure 1 (a), the semantics of New York and Washington D.C. are similar under the relation Located_in, while they are quite different under the relation Capital_of because New York is not a capital. Previous methods such as TransE and RotatE suffer from this ambiguity problem. As shown in Figure 1 (b), it is difficult to disambiguate New York from Washington D.C. for the relation Capital_of in RotatE. To alleviate this problem, TransH utilizes a hyperplane to project entities into independent semantic space. RatE (Huang et al., 2020) integrates a semantic matching method with an extra relation-adaptive matrix. Instead of relying on extra settings, we tackle this problem by the intrinsic attribute of the
rotational semantic space.

We are motivated by the optical interference phenomenon (bright or dark fringes appear after the superposition of two beams of light), because (i) it is intuitive to simulate positive cases and negative cases utilizing distinct dark and bright fringes; and (ii) since coherence theory in the complex field is sufficiently sophisticated, it can play a theoretical guiding role. As OpticE is one type of rotation-based model, it can be illustrated with the rotation transformation shown in Figure 1 (c). The entities New York and Washington D.C. are mapped into different relation-adaptive orbits with the same phase difference. The two entities are close to each other in the orbit of Located_in, while in the orbit of relation Capital_of they no longer overlap. By embedding entities into orbits with different semantic densities, OpticE can take control of the similarity of entities regarding specific relations. Generally, multimapping relations map entities into small-radius orbits in dense semantic space, while one-to-one relations rely on large-radius orbits in sparse semantic space to distinguish entities. This will be verified in our experiments.

To optimize OpticE effectively, we optimize self-adversarial sampling (Sun et al., 2019) by integrating a Bernoulli filtering process. The proposed method can leverage the high efficiency of self-adversarial sampling and reduce the performance loss caused by false negative labels. Tested on WN18, FB15k, WN18RR and FB15k-237, the widely recognized benchmark datasets for link prediction, the lightweight OpticE model is comparable to the previous rotation-based models. OpticE’s ability to adapt to multimapping relations is also verified in our experiments. Our contributions can be summarized as follows:

- **Coherence theory** is introduced into the KG reasoning task for the first time to make the embeddings of KGs in a complex field more intuitive and understandable.

- **A relation-adaptive amplitude modulation technique**, which is simple, effective and lightweight, is developed to alleviate the multimapping problem in KGs.

- **A novel negative sampling method** is provided to train our model precisely and effectively; this approach can be generally applied to other models.

2 Related Work

All the typical related works are listed in Table 1 with their model realizations and complexities in terms of the number of utilized parameters. They are divided into two groups according to whether they are calculated in a real or complex number field.

Real number field models. The most important and influential model is TransE (Bordes et al., 2013), which takes relations as translation transformation by simply assuming that \( h + r = t \). However, its expressiveness is limited, especially when representing a multimapping relation. TransH (Wang et al., 2014) exploits an extra projection transformation and manages to eliminate the ambiguity in TransE. DistMult (Yang et al., 2015) uses a semantic matching method while ignoring the directionality of the relations.

Complex field models. ComplEx (Trouillon et al., 2016) utilizes complex numbers in KG embeddings and achieves great performance. It can be considered a complex version of DistMult, but it overcomes the shortcomings of DistMult via tail conjugation. RotatE (Sun et al., 2019) surpasses all the previous models by rotation transformation; similar to TransE, the model assumes that \( h\text{or} = t \) and suffers from the same ambiguity problem. Based on RotatE, RatE (Huang et al., 2020) defines a relation-specific weight \( W_r \) with an extra 8 parameters per relation to solve the ambiguity problem. HAKE (Zhang et al., 2020) employs a hierarchical structure simulated by a modulus, but the model is complicated and difficult to train.

OpticE (ours) belongs to the category of complex field models and provides a novel way to solve the semantic ambiguity problem in RotatE. Like RatE and TransH, it has a relation-adaptive strategy that can retrieve each entity’s different semantics. However, our strategy is much simpler due to the use of a relation-modulated amplitude. In the aspect of negative sampling, we adopt multiple negative sampling (Trouillon et al., 2016) and self-adversarial strategy (Sun et al., 2019) in our model, but optimize the process with a Bernoulli distribution (Wang et al., 2014) according to the multimapping relations.

3 The Coherence Theory-Based Model

In this part, we briefly introduce coherence theory in §3.1. In §3.2, we provide three ways to modulate an interference model and demonstrate the ad-
Figure 1: Illustration of OpticE. (a) A toy example is given. (b) RotatE is unable to disambiguate New York from Washington D.C. for the relation Capital_of. (c) The entities New York and Washington D.C. are mapped into different relation-adaptive orbits with the same phase difference.

Table 1: KG embedding models and their storage complexities of parameters, where ◦ denotes the Hadamard product, \(\| \cdot \|_{1/2}\) denotes the L1 or L2 norm, and ◦ denotes a specific weighted product defined in RatE. \(k\) is the dimensionality. \(N_c\) and \(N_r\) are the numbers of entities and relations.

| Model      | Score function                                                                 | Parameters                                                                 | Complexity                          |
|------------|--------------------------------------------------------------------------------|---------------------------------------------------------------------------|-------------------------------------|
| TransE     | \(-\|h + r - t\|_{1/2}\)                                                      | \(h, r, t \in \mathbb{R}^k\)                                             | \(O(N_c k + N_r k)\)                |
| TransH     | \(-\|\langle h - w_r, hw_r \rangle + d_r - (t - w_t, tw_t) \rangle\|_2^2\)       | \(h, t, d_r, w_r \in \mathbb{R}^k\)                                     | \(O(N_c k + 2N_r k)\)               |
| DistMult   | \(h \cdot \text{diag}(t)\)                                                    | \(h, r, t \in \mathbb{R}^k\)                                             | \(O(N_c k + N_r k)\)                |
| ComplEx    | \(Re(h^\dagger \text{diag}(r)t)\)                                             | \(h, r, t \in \mathbb{C}^k\)                                             | \(O(2N_c k + 2N_r k)\)              |
| RotatE     | \(-\|h \circ Ow_{g(r)} \circ r - t\|_1\)                                      | \(h, r, t \in \mathbb{C}^k, |r_i| = 1\)                                 | \(O(2N_c k + N_r k)\)               |
| RatE       | \(-\|h_o \circ w_{m(r)} \circ r_m - t_m \|_2\)                               | \(h, r, t \in \mathbb{C}^{k_i}, W \in \mathbb{R}^{2 \times 4}\)        | \(O(2N_c k + N_r (k + 8))\)         |
| HAKE       | \(-\|h_m \circ r_m - t_m \|_2 - \lambda \|\sin((h_p + r_p - t_p)/2)\|_1\)     | \(h_m, r_m, t_m, h_p, r_p, t_p \in \mathbb{R}^k\)                       | \(O(2N_c k + 2N_r k)\)              |
| OpticE     | \(-\|(M_r(h), M_r(t))\|_1\)                                                  | \(h\) and \(t\) are light sources, \(M_r(\cdot)\) is modulator          | \(O(N_c k + 3N_r k)\)               |

3.2 The Proposed Models

Based on the coherence theory, we take the entities as a series of light sources and the relations as a type of modulation performed on their phases and the amplitudes. Then, the existence of triplets can be indicated by the intensity of the lights after superposition.

To be more intuitive, we modify Equation (2) as

\[ I = A_1^2 + A_2^2 - 2A_1A_2 \cos(\varphi_1 - \varphi_2). \]  

Then, the total destructive interference condition becomes \(A_1 = A_2\) and \(\varphi_1 = \varphi_2\). Given a triplet \((h, r, t) \in \mathcal{G}\), each entity consists of \(k\) \((k\) is the dimensionality) light sources. By extending Equation (1), the head entity can be represented as \(h = [E_h^1, E_h^2, \ldots, E_h^k]\), and the tail entity is represented as \(t = [E_t^1, E_t^2, \ldots, E_t^k]\). The score function is

\[ f_r(h, t) = -\|\langle M_r(h), M_r(t) \rangle\|_1, \]

where \(M_r(\cdot)\) is the modulation operates on the head or the tail, and \(\langle M_r(h), M_r(t) \rangle\) is a list of

vantage of the proposed OpticE. In §3.3, the model training process is introduced with the proposed Bernoulli self-adversarial sampling method.

3.1 Interference under Coherence Theory

Optical interference is a common phenomenon in physics that can be interpreted formally by the superposition of waves in coherence theory. We briefly introduce this theory. More details can be found in (Hecht, 2016).

Monochromatic harmonic light can be represented as a point in the complex field as

\[ E = A \exp[i\varphi], \]  

where \(\varphi\) is the phase and \(A\) is the amplitude (or modulus). The intensity of the light synthesized by \(E_1\) and \(E_2\) can be defined as

\[ I = \langle E_1, E_2 \rangle = A_1^2 + A_2^2 + 2A_1A_2 \cos(\varphi_1 - \varphi_2). \]  

If and only if \(A_1 = A_2\) and phase difference is \(\pi\), the intensity tends to be 0, which is called total destructive interference. In our models, we utilize this state to indicate positive triplets in KGs.
Algorithm 1 Bernoulli self-adversarial sampling

Require: A KG \( G \), the given true triplet \((h, r, t) \in G\), the number of negative samples \( n \). For each relation in KG, we first get the statistics about \( hpt \) and \( tph \) (\( hpt \) is the average number of head entities per tail entity; \( tph \) is the average number of tail entities per head entity).

Ensure: The negative sample set \( S \) and \( p(h', t, t') \).

1: \( p = \frac{n_{pt} \pm n_{tp}}{n} \) // probability to corrupt the tail
2: \( \epsilon \leftarrow U(0, 1) \) // \( \epsilon \) uniformly generated from \((0, 1]\)
3: if \( \epsilon < p \) then
4: \( S \leftarrow S \cup (h, r, t') \) // to corrupt the tail
5: end while
6: else
7: \( S \leftarrow S \cup (h', r, t) \) // to corrupt the head
8: end while
9: end if
10: for the \( i \)-th sample \((h', r, t') \in S\),
11: its weight \( p(h', r, t') \) can be obtained from
12: Equation (4).

Similar to other rotation-based models, our models can infer symmetric, anti-symmetric, inversion and composition relations because all these models rely on the modulated phase difference \((\varphi_h + \varphi_r - \varphi_t)\).

(ii) aOpticE with additional entity-adaptive amplitudes. The amplitudes of the sources are determined by the specific entities themselves. Then, we obtain

\[
\begin{align*}
M_h(h) &= A_h \exp [i(\varphi_h + \varphi_r)] \\
M_t(t) &= A_t \exp [i(\varphi_t)].
\end{align*}
\]

Similar to RotatE, the amplitudes of the entities in aOpticE remain unalterable under different relations.

(iii) OpticE with relation-adaptive amplitude modulation. The amplitudes of the sources are determined by the entities and relations, simultaneously. We have

\[
\begin{align*}
M_h(h) &= A_{r,h} \exp [i(\varphi_h + \varphi_r)] \\
M_t(t) &= A_{r,t} \exp [i(\varphi_t)],
\end{align*}
\]

in which \( A_{r,h} \) and \( A_{r,t} \) are the amplitudes of the entities modulated by the relations. In this paper, we provide a specific format of \( A_{r,h} \) and \( A_{r,t} \) to map the entities into relation-adaptive rotational orbits with different semantic density:

\[
\begin{align*}
A_{r,h} &= 1 + \lambda \cos(\varphi_h + \phi_r) \\
A_{r,t} &= 1 + \lambda \cos(\varphi_t + \phi_t),
\end{align*}
\]

where \( \lambda \in (0, 1) \) is the coefficient. For OpticE, the amplitudes, which fluctuate between \([1-\lambda, 1+\lambda]\), are controlled by different relations through the extra parameters \( \phi_r \) and \( \phi_t \).

OpticE is a lightweight model with high storage efficiency, as demonstrated in Table 1. By reusing phase parameters \( \varphi_h \) and \( \varphi_t \) in \( A_{r,h} \) and \( A_{r,t} \), only \( 2N_r \times k \) (\( N_r \) is the number of relations) extra parameters are needed. However, for other rotation-based models like aOpticE, we need \( N_e \times k \) (\( N_e \) is the number of entities) parameters to represent the amplitudes. The number of parameters is reduced by \((N_e - 2N_r) \times k\), where \( N_r \ll N_e \) in KGs.

3.3 Training

Negative sampling is essential to train the models well. This approach is an effective method derived from word embedding (Mikolov et al., 2013) and has been proven powerful for KG embedding.
Table 2: Statistics of the datasets. The last column is the number of the observed triplets in each test, validation and training set.

| Dataset   | N_h | N_r | # Te./Val./Tr. |
|-----------|-----|-----|----------------|
| FB15k     | 14,951 | 1,345 | 50k / 50k / 483k |
| WN18      | 40,943 | 18 | 5k / 5k / 141k |
| FB15k-237 | 14,541 | 237 | 20k / 18k / 272k |
| WN18RR    | 40,943 | 11 | 3k / 3k / 87k |

(Huang et al., 2020; Krompaß et al., 2015; Sun et al., 2019). Similar to (Sun et al., 2019), the self-adversarial sampling method is used:

\[
\mathcal{L} = - \log \sigma(\gamma + f_r(h, t)) - \sum_{i=1}^{n} p(h_i', r, t_i') \log \sigma(-f_r(h_i', t_i') - \gamma),
\]

where \((h_i', r, t_i')\) is the \(i\)-th negative sample of the true triplet \((h, r, t)\), \(\gamma\) is a fixed margin and \(\sigma\) is the sigmoid function. In OpticE and pOpticE, \(f_r(h, t)\) need to be reduced by a proper times to fit the value of \(\gamma\). Furthermore,

\[
p(h_i', r, t_i') = \frac{\exp \alpha f_r(h_i', t_i')}{\sum_j \exp \alpha f_r(h_j', t_j')}
\]

(4)

is the weight of the \(i\)-th negative sample, where \(\alpha\) is the adversarial temperature. According to Equation (4), negative samples with higher scores are assigned with higher weights during the training phase. This is an effective way to filter out high-scoring negative samples and lower their scores efficiently. Apparently, this technique is better than assigning the same average weight to each sample.

However, there are obvious defects in the self-adversarial sampling methods above. During the sampling process, those missing true triplets to be predicted will inevitably suffer from a severe penalty if they are sampled, which will undermine the prediction accuracy. Here, we take advantage of the Bernoulli sampling strategy described in (Wang et al., 2014) to reduce the chance of sampling false negative samples. Instead of replacing the head and tail uniformly, we use a Bernoulli distribution to decide whether to corrupt the head or the tail. For example, given a triplet \((Biden, nationality, the U.S.)\), since nationality is a many-to-one relation, it is safer to change the entity the U.S. to obtain a negative sample than altering entity Biden. In Algorithm 1, the process of the Bernoulli self-adversarial sampling method is clarified.

4 Experiments

In this part, the experimental conditions are elaborated, and the performance of the proposed models is compared. Different negative sampling methods are tested. Finally, we examine the effects of the amplitude of OpticE. All the experiments are conducted on an NVIDIA-v100 GPU. The code for this paper is available on https://github.com/guixiangyu1/OpticE.

4.1 Experimental Settings

Four widely used datasets, FB15k (Bordes et al., 2013), WN18 (Bordes et al., 2013), FB15k-237 (Toutanova and Chen, 2015) and WN18RR (Dettmers et al., 2018), are benchmark datasets in our experiments. All these datasets contain plenty of multimapping instances. The statistics of these datasets are presented in Table 2. The models are trained on the training set and tested on the test set.

- **FB15k** contains tremendous entities and multimapping relations from real-world settings and is extracted from Freebase (Bollacker et al., 2008).
- **WN18** is extracted from WordNet (Miller, 1995) and is designed to manipulate the semantic relations between words and phrases.
- **FB15k-237** is a subset of FB15k. To avoid the data leakage problem in FB15k, duplicate triplets and direct links are removed in FB15k-237.
- **WN18RR** is a subset of WN18. WN18RR follows the same processes as FB15k-237.

**Hyperparameters.** During the training process, Adam (Kingma and Ba, 2014) is used to optimize OpticE. Grid search is used and the range of hyperparameters is set as follows: the batch size \(b \in [512, 1024, 2048]\), the number of embedding dimensions \(k \in [500, 1000, 1500, 2000]\), the temperature for Bernoulli self-adversarial sampling \(\alpha \in [0.5, 1.0]\), the negative sample size \(n \in [50, 100, 200, 256]\) and the margin \(\gamma \in [6, 9, 12, 15]\). All amplitudes and phases are initialized uniformly. The range of the phases is \([0, 2\pi]\).

**Evaluation.** All the models are tested their link prediction performance with three standard evaluation metrics: the mean reciprocal rank (MRR), mean rank (MR) and hits at N (Hits@N). Given a true test triplet, its head entity or tail entity is
Table 3: Link prediction results on FB15k and WN18. We take TransE results from (Nickel et al., 2016), and DistMult results from (Kadlec et al., 2017). Other results are extracted as benchmarks from the corresponding original papers.

| Method  | FB15k |               | WN18 |               |
|---------|-------|---------------|------|---------------|
|         | MR    | MRR           | Hits@1 | Hits@3 | Hits@10 | MR    | MRR           | Hits@1 | Hits@3 | Hits@10 |
| TransE  | -     | .463          | .297  | .578  | .749    | -     | .495          | .113   | .888  | .943    |
| DistMult| 42    | .798          | -     | -     | .893    | 655   | .797          | -      | -     | .946    |
| HolE    | -     | .524          | .402  | .613  | .739    | -     | .938          | .930   | .945  | .949    |
| ComplEx | 51    | .657          | .558  | .723  | .831    | 374   | .943          | .935   | .946  | .956    |
| RotatE  | 40    | .797          | .746  | .830  | .884    | 309   | .949          | .944   | .952  | .959    |
| RatE    | 24    | .810          | .724  | .859  | .898    | 180   | .950          | .944   | .953  | .962    |
| pOpticE | 42    | .792          | .742  | .823  | .881    | 290   | .948          | .940   | .952  | .960    |
| aOpticE | 45    | .788          | .736  | .822  | .879    | 362   | .946          | .940   | .952  | .958    |
| OpticE  | 39    | .804          | .756  | .837  | .889    | 261   | .951          | .946   | .955  | .961    |

Table 4: Link prediction results on FB15k-237 and WN18RR. The results of [1] are taken from (Dettmers et al., 2018). Other results are extracted as benchmarks from the corresponding original papers.

| Method  | FB15k-237 |               | WN18RR |               |
|---------|------------|---------------|--------|---------------|
|         | MR    | MRR           | Hits@1 | Hits@3 | Hits@10 | MR    | MRR           | Hits@1 | Hits@3 | Hits@10 |
| TransE  | 357   | .294          | -      | -      | .465    | 3384  | .226          | -      | -      | .501    |
| DistMult| 254   | .241          | .155   | .263   | .419    | 5110  | .43           | .39    | .44    | .49     |
| ComplEx | 339   | .247          | .158   | .275   | .428    | 5261  | .44           | .41    | .46    | .51     |
| ConvE   | 244   | .325          | .237   | .356   | .501    | 4187  | .43           | .40    | .44    | .52     |
| RotatE  | 177   | .338          | .241   | .375   | .533    | 3340  | .476          | .428   | .492   | .571    |
| RatE    | 172   | .344          | .261   | .382   | .541    | 2860  | .488          | .441   | .506   | .590    |
| pOpticE | 183   | .329          | .232   | .366   | .525    | 3182  | .477          | .435   | .491   | .559    |
| aOpticE | 186   | .340          | .244   | .377   | .536    | 3510  | .473          | .425   | .489   | .563    |
| OpticE  | 151   | .359          | .264   | .398   | .550    | 1930  | .497          | .453   | .512   | .585    |

4.2 Main Results

The existing state-of-the-art models are compared with ours in terms of link prediction. They are TransE (Bordes et al., 2013), DistMult (Yang et al., 2015), ComplEx (Trouillon et al., 2016), HolE (Nickel et al., 2016), ConvE (Dettmers et al., 2018), RotatE (Sun et al., 2019), HAKE (Zhang et al., 2020) and RatE (Huang et al., 2020).

In Tables 3 and 4, the main results obtained on the link prediction task are listed. RotatE surpasses all the previous models by simultaneously modeling different kinds of relations in KGs, including symmetry, antisymmetry, inversion and composition (Sun et al., 2019). HAKE, RatE and our OpticE can be considered members of the RotatE family because they all employ the rotation transformation approach and are capable of representing the four types of relations described above. By optimizing the hierarchy and ambiguity aspects, HAKE and RatE outperform RotatE to a large extent. According to the results, by mapping entities into different relation-adaptive semantic spaces, OpticE is comparable to these two models and even exceeds them in terms of most evaluation metrics.

The performances of different modulation styles are also compared. pOpticE (with only phase modulation) can complete the link prediction task well to some extent. By assigning trainable amplitudes decided by entities, aOpticE optimizes the corresponding outcomes. OpticE, with relation-adaptive modulated amplitude, greatly surpasses aOpticE in four datasets, which verifies that it is beneficial to use relation-adaptive amplitude modulation rather than entity-adaptive amplitude modulation.

4.3 Performance for Different Relation Types

We further investigate the performance of OpticE when processing prediction tasks with different relation types. According to the general classification method given by (Wang et al., 2014), the relations are classified into one-to-one, one-to-many,
Table 5: Performance on FB15k-237 for different relation types. TransE and RotatE are trained according to the code released by (Sun et al., 2019) with their best configurations.

| Relation Type | Head Prediction (MRR) | Tail Prediction (MRR) |
|---------------|------------------------|------------------------|
|               | 1-to-1  | 1-to-M  | M-to-1  | M-to-M  | 1-to-1  | 1-to-M  | M-to-1  | M-to-M  |
| TransE        | .491    | .453    | .085    | .255    | .481    | .074    | .741    | .361    |
| RotatE        | .501    | .472    | .092    | .261    | .488    | .075    | .748    | .368    |
| OpticE (ours) | .505    | .484    | .113    | .285    | .499    | .073    | .777    | .390    |

Table 6: Performance of RotatE and OpticE with different negative sampling methods. For FB15k-237, the negative sample size is set to 256. For WN18RR, the negative sample size is set to 100. Other conditions remain the same.

| Model          | FB15k-237 | WN18RR |
|----------------|-----------|--------|
|                | MR | MRR | Hits@1 | Hits@3 | Hits@10 | MR | MRR | Hits@1 | Hits@3 | Hits@10 |
| RotatE (uni.)  | 186 | .295 | .203    | .326    | .479    | 3226 | .471 | .425    | .487    | .564    |
| RotatE (adv.)  | 178 | .335 | .234    | .374    | .531    | 3338 | .477 | .429    | .493    | .574    |
| RotatE (badv.) | 179 | .337 | .241    | .374    | .531    | 3267 | .478 | .430    | .496    | .578    |
| OpticE (uni.)  | 152 | .348 | .254    | .385    | .537    | 2267 | .486 | .442    | .501    | .568    |
| OpticE (adv.)  | 168 | .354 | .260    | .390    | .541    | 2890 | .488 | .445    | .504    | .570    |
| OpticE (badv.) | 151 | .359 | .264    | .398    | .550    | 1930 | .497 | .453    | .512    | .585    |

Figure 2: Visualization of several entities on FB15k-237. The Mid of $h_1$ and $h_2$ are /m/04ztj and /m/07tg4; the Mid of $t_1$ and $t_2$ are /m/08mbj5d and /m/0bwfn.

many-to-one and many-to-many types. The results obtained by OpticE on the FB15k-237 dataset are given in Table 5 and compared with those of TransE and RotatE.

We can see that OpticE achieves improvements for almost all types of relations, except the one-to-many tail prediction relations for which all the methods obtain low MRR scores. It is difficult to predict the ‘many’ parts of one-to-many and many-to-one relations. This is in line with the common sense notion that ‘many’ indicates more uncertainty. By employing relation-adaptive amplitudes, OpticE alleviates this problem to some extent.

4.4 Analysis of Negative Sampling Methods

We apply different negative sampling methods to OpticE and RotatE and record the results in Table 6. Uniform sampling (uni.), self-adversarial sampling (adv.) and Bernoulli self-adversarial sampling (badv.) are alternated in the models during the test. These methods are evaluated based on the results in Table 6. During the sampling phase, Bernoulli sampling can decrease the chance of sampling false negative samples. As indicated in the table, compared with adv. and uni. sampling, models with badv. sampling achieve the best result. From the perspective of models, OpticE outperforms RotatE with the same negative sampling method, which proves the excellent representation ability of OpticE.
4.5 Analysis Regarding the Amplitude

To verify the effects of the amplitude, we monitor and visualize it in OpticE. We visualize the heads and tails on FB15k-237 with several relations, as shown in Figure 2. In Figure 3, we test the amplitude distribution of different kinds of relations.

Visualization of relation-adaptive amplitudes in OpticE. In Figure 2, all the entities are mapped into a 2D space with the data of their first 500 dimensions, based on a complex coordinate system. To make the property of the amplitude more obvious, we take the logarithm operation on the amplitudes. Since the amplitudes and moduli are less than 1, the smaller radii in the figure will actually indicate larger amplitudes or moduli. The numbers in the parentheses are \((hpt : tph)\) of the relations.

In Figure 2(a) and (b), (c) and (d), RotatE mixes entities in the same space while OpticE can distinguish them by different relations. The radii under one-to-one relations (Institution\textsubscript{2} and Campuses) are smaller in OpticE, which means the entities are mapped into sparse semantic space with larger amplitudes. In Figure 2(e) and Figure 2(f), although Yale is the head entity of both relations, entity Yale is mapped into sparse semantic space by relation Campuses (one-to-one) and dense semantic space by relation Student (many-to-one). A similar situation occurs with UMich on Institution\textsubscript{1} and Institution\textsubscript{2}. These visualizations prove that OpticE can tackle the semantic ambiguity problem with relation-adaptive amplitudes.

Distribution of amplitudes of different relations. The relation between the values of amplitudes and the multimapping properties of the relation is investigated. As illustrated in Figure 3, the amplitudes of injective (one-to-one) relations (Campuses and Institution\textsubscript{2}) are larger than those of noninjective relations (Student and Institution\textsubscript{1}). The reason is that for multimapping relations, the semantics of entities overlap with each other. Then with smaller amplitudes in a dense semantic space, similar semantics are more convenient to express. For the one-to-one relations, entities are exclusive and there are semantic gaps between them. With larger amplitudes in a sparse semantic space, each entity can disambiguate with each other more easily. These attributes are also demonstrated in Figure 2, showing that multimapping relations have smaller radii (red points) and one-to-one relations with larger ones (blue points).

5 Conclusion

We embed KGs with a novel optic interference perspective to tackle the link prediction problem. Guided by coherence theory, we explore three kinds of modulation methods and analyze their properties theoretically. With our proposed negative sampling method, OpticE achieves the best score in comparison with other translation- and rotation-based models. Its ability to disambiguate entities in multiple mapping relations is verified experimentally. The results suggest that we can alleviate semantic ambiguity in rotation-based models by mapping entities into relation-adaptive orbits with different semantic densities.
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The final intensity is

\[ I = \|E\|^2 = (A_1 \cos \varphi_1 + A_2 \cos \varphi_2)^2 + (A_1 \sin \varphi_1 + A_2 \sin \varphi_2)^2 = A_1^2 + A_2^2 + 2A_1A_2 \cos(\varphi_1 - \varphi_2). \]

The final intensity is \( I = \frac{1}{2} \|E\|^2 \). For convenience, the coefficient \( \frac{1}{2} \) is ignored. The synthetic light intensity of two coherent lights can be noted as

\[ I = A_1^2 + A_2^2 + 2A_1A_2 \cos(\varphi_1 - \varphi_2). \]

To be more intuitive, we modify the intensity as

\[ I = \|E_1 - E_2\|^2 = A_1^2 + A_2^2 - 2A_1A_2 \cos(\varphi_1 - \varphi_2). \]

Then, the phase difference between \( \varphi_1 \) and \( \varphi_2 \) is important during the process (\( k \in \mathbb{Z} \)):

\[ I = \begin{cases} 
(A_1 + A_2)^2, & \varphi_1 - \varphi_2 = (2k + 1)\pi, \\
A_1^2 + A_2^2, & \varphi_1 - \varphi_2 = \left(\frac{1}{2} + k\right)\pi, \\
(A_1 - A_2)^2, & \varphi_1 - \varphi_2 = 2k\pi.
\end{cases} \]

When \( \cos(\varphi_1 - \varphi_2) = 1 \), the intensity reaches its maximum as \((A_1 + A_2)^2\). When \( \cos(\varphi_1 - \varphi_2) = 0 \), the interference effect disappears, and intensity is the sum of the individual intensities as \(A_1^2 + A_2^2\). The extreme case is total destructive interference, in which the waves tend to cancel, and the intensity tends to be zero. This extreme case occurs only if \( A_1 = A_2 \) and \( \varphi_1 = \varphi_2 \) (suppose \( \varphi_1, \varphi_2 \in (0, 2\pi) \)).

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**A More Details about Coherence Theory**

Given \( E_1 = A_1e^{i\varphi_1} \) and \( E_2 = A_2e^{i\varphi_2} \), after the superposition of the two light waves, the formed synthetic light is

\[ E = A_1e^{i\varphi_1} + A_2e^{i\varphi_2} = A_1 \cos \varphi_1 + A_2 \cos \varphi_2 + i(A_1 \sin \varphi_1 + A_2 \sin \varphi_2). \]

Then, we have

\[ \|E\|^2 = (A_1 \cos \varphi_1 + A_2 \cos \varphi_2)^2 + (A_1 \sin \varphi_1 + A_2 \sin \varphi_2)^2 = A_1^2 + A_2^2 + 2A_1A_2 \cos(\varphi_1 - \varphi_2). \]

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**B Reasoning in Symmetric Relations**

OpticE can infer symmetric, anti-symmetric, inversion and composition relations. We give the proof for symmetric relations here, and others are omitted in this paper.

For a symmetric relation \( r \) with two positive cases, \((h, r, t)\) and \((t, r, h)\), to satisfy the coherence condition of phase matching,

\[ \varphi_h + \varphi_r - \varphi_t = 2k_1\pi \]
\[ \varphi_t + \varphi_r - \varphi_h = 2k_2\pi, \]

where \( k_1 \) and \( k_2 \in \mathbb{Z} \). By adding the formulas above, we can obtain

\[ \varphi_r = (k_1 + k_2)\pi = k\pi, \]

in which \( k \in \mathbb{Z} \). Specifically, \( \varphi_r = \pm \pi \) and 0 in OpticE.

The phase properties inherited from the rotation models are tested. Compared with translation models, e.g., TransE, rotation transformation models are able to represent symmetric relations. For instance, when \((h, r, t)\) and \((t, r, h)\) are both positive cases, it is trivial for TransE to set \( r \) to 0. However, for OpticE, the period of the phase takes effect with a phase \( \varphi_r = k\pi \). This is verified in Figure 4, in which the phase of the symmetric relation _similar_to and spouse is distributed around \( \pm \pi \) and 0.

![Distribution histogram of the phases of _similar_to in WN18RR and spouse in FB15k-237.](image)

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