

# A shallow neural model for relation prediction

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**Abstract**—Knowledge graph completion refers to predicting missing triples. Most approaches achieve this goal by predicting entities, given an entity and a relation. We predict missing triples via the relation prediction. To this end, we frame the relation prediction problem as a multi-label classification problem and propose a shallow neural model (SHALLOM) that accurately infers missing relations from entities. SHALLOM is analogous to C-BOW as both approaches predict a central token ( $p$ ) given surrounding tokens ( $(s, o)$ ). Our experiments indicate that SHALLOM outperforms state-of-the-art approaches on the FB15K-237 and WN18RR with margins of up to 3% and 8% (absolute), respectively, while requiring a maximum training time of 8 minutes on these datasets. We ensure the reproducibility of our results by providing an open-source implementation including training and evaluation scripts at <https://github.com/dice-group/Shallom>.

## I. INTRODUCTION

Knowledge Graphs (KGs) represent structured collections of facts describing the world in the form of typed relationships between entities [1]. These collections of facts have been applied to diverse tasks, including machine translation and collaborative filtering [2], [3]. However, most KGs on the Web suffer from incompleteness [4]. For instance, the birth place of 71% of the persons in Freebase and 66% of the persons in DBpedia is not to be found in the respective KGs. In addition, more than 58% of the scientists in DBpedia are not linked to the predicate that describes what they are known for [5]. The identification of such missing information is called knowledge graph completion [6] that is addressed in predicting missing entities or relations. Knowledge graph embedding approaches have been particularly successful at the knowledge graph completion task, among many others [7], [2], [8].

We investigate the use of a shallow Neural Networks (NNs) for predicting missing triples. The motivation thereof lies in the following consideration: Several early works have shown that NNs (even with a single hidden layer) are universal approximators [9]. This means that shallow NNs with numerous non-polynomial activation functions approximate any continuous function on a complex domain. However, these theorems do not impose a constraint on the number of units in the hidden layer [10]. In addition, deep NNs seem to perform better than shallow NNs when the target function is expected to be a hierarchical composition of functions [11]. Still, training deep NNs requires more extensive hyperparameter optimization than training shallow NNs to alleviate the overfitting problem and

the choice of initialization technique plays a more important role for deep NN in their applications [10]. Moreover, deep NNs necessitate more computational resources, have higher energy consumption, and consequently lead to substantially higher  $CO_2$  emissions [12]. The essay of the hardware lottery [13] highlighted the impact of available hardware system in determining which research ideas succeed (and fail). It is therein emphasized how the hardware lottery can delay research progress by casting successful ideas as failures. Importantly, findings of Ruffinelli et al. [14] have shown that the relative performance differences between various KGE approaches often shrinks and sometimes even reverses when compared to prior results provided that approaches are optimized properly. With this consideration, we propose a shallow neural model, SHALLOM, for relation prediction that relies on two affine transformations. By virtue of this architecture, SHALLOM is analogous to C-BOW [15], as both approaches predict a central token ( $p$ ) given surrounding tokens ( $s, o$ ).

We evaluate our approach against many state-of-the-art approaches on the WN18, WN18RR, FB15K, FB15K-237, and YAGO3-10 benchmark datasets. Overall, our results suggest that SHALLOM outperforms the state-of-the-art in terms of Hits at N (Hits@N) and has a more efficient runtime. In particular, SHALLOM yields state-of-the-art performance with a training time of under ten minutes on a knowledge graph containing more than  $10^6$  triples.

## II. PRELIMINARIES AND NOTATION

### A. Knowledge Graph and Completion

Let  $\mathcal{E}$  and  $\mathcal{R}$  represent the set of entities and relations, respectively. Then, a KG  $\mathcal{G} = \{(s, p, o) \in \mathcal{E} \times \mathcal{R} \times \mathcal{E}\}$  can be formalised as a set of triples where each triple contains two entities  $s, o \in \mathcal{E}$  and a relation  $r \in \mathcal{R}$ . Knowledge Graph Completion (KGC) refers to predicting missing triples on a given  $\mathcal{G}$ . Most approaches learn a scoring function  $\psi$  that is often formalised as  $\psi : \mathcal{E} \times \mathcal{R} \times \mathcal{E} \mapsto \mathbb{R}$  [7]. In contrast, the scoring function of approaches solely addressing the relation prediction task is often defined as  $\psi : \mathcal{E} \times \mathcal{E} \mapsto \mathbb{R}^{|\mathcal{R}|}$  [16]. Both formalizations allow computing a score for any triple  $(s, p, o)$  either directly (i.e., by computing  $\psi(s, p, o)$ ) in the case of the entity prediction or indirectly (i.e., by looking up the value for  $p$  in  $\psi(s, o)$ ) for the relation prediction. Ergo, KGC approaches differ primarily in their scoring function  $\psi$  while sharing the same goal: given an  $(s, p, o)$ , its score is expected to be

proportional to the likelihood of such a triple being contained  $(s, p, o) \in \mathcal{G}$  [7]. To learn such function, most KGC approaches generate corrupted/negative examples [17], [4]. In this setting, each  $(s, p, o) \in \mathcal{G}$  is considered as a positive example, whilst all  $(x, y, z) \notin \mathcal{G}$  with  $x, z \in \mathcal{E}$  and  $y \in \mathcal{R}$  are considered to be candidates for negative examples [4]. Ergo, such approaches presuppose that the absence of a relationship between two entities implies that the corresponding triple is **false** if such triple is sampled as a corrupted triple otherwise **unknown**. Such a schema creates a **trichotomy** (positive, negative and unknown triples) and disregards the *open world assumption*, which suggests that non-existing triples are to be interpreted as unknown, not false [4]. SHALLOM complies with the open world assumption since the learning problem is formulated as a multi-label classification problem where a dichotomy between triples is created.

### III. SHALLOM

In this section, we formally elucidate SHALLOM that is defined as

$$\psi(s, o) = \sigma(\mathbf{W} \cdot \text{ReLU}(\mathbf{H} \cdot \Psi(s, o) + \mathbf{b}_1) + \mathbf{b}_2), \quad (1)$$

where  $\Psi(s, o) \in \mathbb{R}^{2d}$ ,  $\mathbf{H} \in \mathbb{R}^{k \times 2d}$ ,  $\mathbf{W} \in \mathbb{R}^{|\mathcal{R}| \times k}$ ,  $\mathbf{b}_1 \in \mathbb{R}^k$ , and  $\mathbf{b}_2 \in \mathbb{R}^{|\mathcal{R}|}$ .  $\sigma(\cdot)$ ,  $\text{ReLU}(\cdot)$  and  $\Psi(\cdot, \cdot)$  denote the sigmoid, the rectified linear unit and the vector concatenation functions, respectively. Given  $(s, o)$ ,  $\Psi(s, o)$  returns concatenated embeddings of  $(s, o)$ . Thereafter, we perform two affine transformations with the ReLU and the sigmoid function to obtain predicted probabilities for relation ( $\hat{y} \in \mathbb{R}^{|\mathcal{R}|}$ ). Finally, the incurred loss is computed by the binary cross-entropy function:

$$\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = - \sum_i^{|\mathcal{R}|} \left( (y_i \cdot \log(\hat{y}_i)) + (1 - y_i) \cdot \log(1 - \hat{y}_i) \right) \quad (2)$$

where  $\hat{\mathbf{y}}$  is the vector of predicted probabilities and  $\mathbf{y}$  is a binary vector of indicating multi labels.

Figure 1 shows the architecture of SHALLOM. To obtain a composite representation of  $(s, o)$ , we concatenate embeddings of entities as opposed to averaging them, since averaging embeddings loses the order of the input (as in the standard bag-of-words representation [18]). Retaining order of embeddings avoids possible loss of information. As concatenation does not consider any interaction between the latent features, the first affine transformation is applied with the ReLU activation function. Thereafter, the second affine transformation is applied with the sigmoid function to generate probabilities for relations.

### IV. EXPERIMENTS

We compared SHALLOM against many state-of-the-art approaches and Uniform Random Classifier (URC) in the relation prediction task on benchmark datasets [7].

#### A. Evaluation Protocol

We applied Hits@N to evaluate the prediction performances. Given a test triple  $(s, p, o) \in \mathcal{G}^{\text{Test}}$ , we computed  $|\mathcal{R}|$  number

of scores and obtained  $I_{\text{relation}} = [(p', \text{score}) : \text{score} = \psi(s, p', o) \wedge p' \in \mathcal{R}]$ . Then, we sorted the  $I_{\text{relation}}$  in descending order of assigned scores and we computed Hits@N as follows:

$$\text{Hits@N} = \frac{1}{|\mathcal{G}^{\text{Test}}|} \sum_{(s, p, o) \in \mathcal{G}^{\text{Test}}} f(I_{\text{relation}}, p, N), \quad (3)$$

where  $f$  returns 1 if  $p$  is contained in the top  $N$  ranked tuples, otherwise 0 [6]. To evaluate runtime performances, we measured the elapsed runtime during the training phase. Ergo, we ignored the elapsed time during the data preprocessing since the training setup for SHALLOM is done on the fly while some approaches, including RDF2Vec, require additional computations such as applying the random walk technique. All approaches were trained four times on datasets. The reported runtimes (RT) of approaches are in seconds and the mean of the last three runs.

#### B. Hyperparameter Optimization

We selected the hyperparameters of SHALLOM via grid search according to the Hits@1 on the validation set of each dataset. The hyperparameter ranges for the grid search were set as follows: embedding size  $d = [30, 50, 100, 200]$ , epochs =  $[30, 50, 100]$ , the width of the hidden layer  $k = [.5d, d, 3d]$ , batch size =  $[256, 1000]$ , dropout rate =  $[.0, .2, .5]$  and  $L_2$ -normalizer =  $[.0, .1]$ . Initially, we used the default hyperparameters for all competing approaches provided in [19]. However, RESCAL, ComplEx, CP and DistMult did not terminate within three hours of computation. The long runtimes are corroborated by [19]. We hence optimized the hyperparameters of RESCAL, CP, TransE, DistMult and ComplEx via a grid search according to the Hits@1 on the validation set of each dataset. The hyperparameter ranges for the grid search were as follows: epochs =  $[100, 200]$ , negative ratio per valid triple =  $[1, 5, 10, 50]$ , and batch size =  $[256, 512, |\mathcal{G}^{\text{Train}}|/100]$ . We omitted  $d$ , regularization term and learning rate from grid-search and used the parameter settings provided in [19]. We selected the hyperparameters of RDF2Vec via grid search according to the Hits@1 on the validation set of each dataset. The hyperparameter ranges of RDF2Vec for the grid search were set as follows: embedding size  $d = [50, 100]$ , epochs =  $[100]$ , number of negatives for W2V =  $[25, 100]$  and random walk depth =  $[3, 5, 7]$ . After the embedding vectors are generated, we train the same scoring function defined in Equation (1) (look-up operation performed on RDF2Vec embeddings), by following the same optimization schema as our approach.

### V. RESULTS

Table I, Table II and Table III report the HitsN relation prediction results on the five benchmark datasets. Overall, SHALLOM outperforms many state-of-the-art approaches while maintaining a superior runtime performance. The slightly superior (.018 absolute) performance of ProjE on the FB15K comes with the cost of more than 3 hours of computation. SHALLOM is significantly more time-efficient; it requires only 8 minutes, on average, a commodity computer. Since we could not reproduce

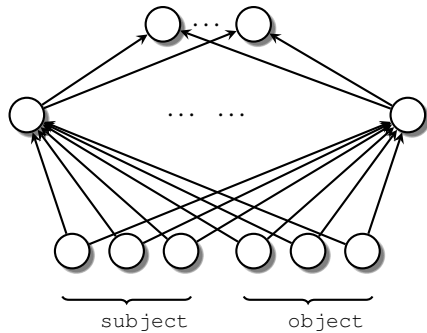


Fig. 1. Visualization of SHALLOM.

TABLE I  
HITS@1 RELATION PREDICTION RESULTS ON FB15K AND WN18.  
RESULTS ARE TAKEN FROM CORRESPONDING PAPERS.

Method	FB15K	WN18
TransE [6]	.651	.736
TransR [20]	.702	.713
ProjE-listwise [6]	<b>.758</b>	-
PTransE (ADD, len-2 path) [6]	.695	-
DKLR(CNN) [20]	.698	-
TKRL (RHE) [21]	.711	-
RDFDNN [22]	.691	.770
KGML [16]	.725	<b>.975</b>
SSP [23]	.709	-
SHALLOM	.734	.970

the reported relation prediction results [6], we could neither re-evaluate ProjE on FB15K nor include it on the other benchmark datasets. Approaches perform significantly better on WN18 than on FB15K. This may stem from the fact that WN18 contains (1) significantly fewer relations and (2) entity pairs having multiple relations than FB15K. More specifically, FB15K and WN18 datasets contain 63.856 and 277 number entity pairs, respectively, that occurred with multiple relations in the training splits. Table II shows that SHALLOM outperforms all state-of-the-art approaches on the WN18RR and FB15K-237 datasets while maintaining an overall superior runtime performance. Note that the RT solely denotes the elapse training runtime (see section IV-A for details.) Initially, we trained RESCAL, TransE, ComplEx, CP and DistMult with hyperparameters provided in [24]. However, models other than TransE did not terminate within 3 hours of computation. Consequently, we selected the hyperparameters of approaches via grid search as explained in Section IV-B. TransE and DistMult yield a surprisingly better performance on WN18RR and FB15K-237 than on WN18 and FB15K. This may stem from (1) the hyperparameter optimization and (2) the fact that fewer numbers of entity pairs have multiple relations on training and testing datasets. The hyperparameters of TransE were not optimized in [6], [22], [16] where the Hit@1 performances of TransE were taken. CP performed poorly on the WN18RR due to the small number of relations as observed in [19]. During the training phase, the batch size was set to 32 in KGML

and RDFDNN [16], [22]. Although training models with a small-batch regime seemed to alleviate a possible degradation in the generalization performances of models [25], it came with the cost of increased runtime. By virtue of being a shallow NN, the error propagation was computationally more efficient in SHALLOM than KGML. Importantly, KGML and RDFDNN do not optimize the width of the hidden layers. Conversely, we optimized the width of SHALLOM, as per the suggestion in [26]—that optimizing the width of the network has an impact on the generalization performance. RDFDNN erroneously assumes one-to-one mapping between entity pairs to relations and possibly suffers from the hyperbolic tangent saturation as the hyperbolic tangent is applied in the hidden layer [27]. RDF2Vec outperforms RESCAL, TransE, CP and DistMult w.r.t. Hits@3 and Hits@5 on WN18RR.

To confirm the performance of SHALLOM, we compared it with some of the best approaches in terms of runtime requirement and Hits@1 on a large benchmark dataset. Table III shows that SHALLOM reaches close to 1.0 Hits@5 and requires less than 10 minutes on the YAGO3-10. We could not evaluate KGML on YAGO3-10 due to its high memory consumption requiring more than 16 GB RAM.

The superior performance of SHALLOM stems from: (1) it being a shallow neural model, (2) optimizing the width of the hidden layer, (3) the task and evaluation measures used. By virtue of being a shallow NN, SHALLOM requires only 562 seconds to train on  $|\mathcal{G}| > 10^6$  on a commodity computer. NNs are required to be wide enough (larger than the input dimension) to learn disconnected decision regions [26]. Lastly, given the example (Obama, Hawaii), SHALLOM assigns high scores for BirthPlace and low scores for SpouseOf. This stems from the fact that input  $\mathcal{G}$  does not involve triples such as (SpouseOf, Hawaii), while it involves many triples (BirthPlace, Hawaii). SHALLOM assigns presumably a high score (Obama, BirthPlace, Paderborn) although such a triple is not contained in  $\mathcal{G}$ . Since the test splits of the benchmark datasets do not involve such false triples, the Hit@N metric quantifies merely the performances of the relation prediction approaches on the valid triples. Ergo, the idea of corrupted triples is not necessary for relation prediction as each entity pair found in the test split is linked with a relation.

TABLE II  
THE MEAN OF HITS@N RELATION PREDICTION AND RUNTIME RESULTS ON WN18RR AND FB15K-237.

	WN18RR				FB15K-237			
	RT	Hits			RT	Hits		
		@1	@3	@5		@1	@3	@5
RESCAL	1860±6	.331	.529	.734	5160±4	.115	.327	.456
TransE	960±11	.507	.761	.864	540±10	.774	.899	.918
Complex	2160±15	.515	.652	.758	5880±30	.153	.300	.378
CP	840±15	.332	.518	.659	8040±39	.467	.609	.675
DistMult	780±13	.497	.677	.799	1140±8	.092	.176	.428
KGML	840±15	.868	.954	.975	1080±10	.921	.960	.976
RDFDNN	540±8	.819	.967	.985	720±10	.913	.934	.953
RDF2VecSkip-Gram	310±5	.534	.815	.940	482±6	.518	.600	.677
RDF2VecCBOW	337±10	.451	.785	.932	472±8	.522	.608	.687
URC		.095	.265	.446		.003	.013	.020
SHALLOM	610±13	<b>.874</b>	<b>.982</b>	<b>.995</b>	404±8	<b>.948</b>	<b>.993</b>	<b>.997</b>

TABLE III  
THE MEAN OF HITS@N RELATION PREDICTION AND RUNTIME RESULTS ON YAGO3-10.

	YAGO3-10			
	RT	Hits		
		@1	@3	@5
RDF2VecSkip-Gram	593±11	.487	.796	.875
RDF2VecCBOW	625±12	.491	.803	.873
SHALLOM	562±19	<b>.630</b>	<b>.983</b>	<b>.996</b>

## VI. RELATED WORK

A wide range of works have investigated the KGC problem [4], [28]. DistMult [29] can be seen as an efficient extension of RESCAL with a diagonal matrix per relation. ComplEx [24] extends DistMult into a complex vector space. RDFDNN [22] considers the relation prediction task as a multi-class classification problem. Embeddings of entities are learned disjointly. Relations are predicted through the softmax function. KGML [16] implements a multi-layer neural model for relation prediction. Experimental results show that KGML outperforms TransE, TransR, PTransE and RDFDNN in the relation prediction task. After an embedding layer, KGML concatenates embeddings of subject and object with the element-wise product of embeddings. This is followed by two inner product layers with fixed decreasing width. SHALLOM differs from KGML by: (1) concatenating embeddings of entities without including a multiplication step, (2) having solely one inner product layer and omitting dynamic weighted binary cross entropy loss. RDF2Vec [30] employs Word2Vec [15] for unsupervised feature extraction from sequences of words, and adapts them to RDF graphs.

## VII. CONCLUSION

We presented a shallow neural model effectively predicts missing triples without disregarding the *open world assumption*. SHALLOM retains a linear space complexity in the number of entities. Experiments showed that training SHALLOM on

benchmark datasets is completed within a few minutes. This is an important result, as it means that our approach can be applied on large knowledge graphs without requiring high-performance hardware. This also implies that winning the hardware lottery is not necessary to tackle the link prediction problem [13]. In future work, we plan to investigate extending SHALLOM into temporal knowledge graphs and learning complex-valued valued embeddings via SHALLOM [31], [32].

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