# Novel Embedding Model for Knowledge Base Completion Based on Convolutional Neural Network

#### Vikram Bhatt Kapil Pathak

Department of Computational and Data Sciences Department of Computer Science and Automation

November 15, 2018

- Neural Link Prediction Model
- 2 Datasets
- 3 Baseline Implementation
- 4 Futher Directions....

- Neural Link Prediction Model
- 2 Datasets
- 3 Baseline Implementation
- 4 Futher Directions....

#### Motivation

- Previous works[TWR<sup>+</sup>16] [YYH<sup>+</sup>14] [BGWB14] [BUGD<sup>+</sup>13] on link prediction focused on shallow,fast models which can scale to large knowledge graphs.
- These models learn less expressive features than deep multilayers models which potentially limits it's performance.

#### Motivation

- Previous works[TWR<sup>+</sup>16] [YYH<sup>+</sup>14] [BGWB14] [BUGD<sup>+</sup>13] on link prediction focused on shallow,fast models which can scale to large knowledge graphs.
- These models learn less expressive features than deep multilayers models which potentially limits it's performance.
- A novel embedding model ConvKB[NNNP17] employs Convolutional Neural networks for knowledge base completion task.
- Captures global relationships and transitional characteristics between entities and relations.

### ConvKB Model

- Embedding of each triple (h, r, t) defined by  $(v_h, v_r, v_t)$  stacked in matrix  $A = [v_h, v_r, v_t] \in \mathbb{R}^k$ 
  - $A = [v_h, v_r, v_t] \in \mathbb{R}^n$ We use a filter  $w \in \mathbb{R}^n$
- We use a filter  $\omega \in \mathbb{R}^{1\times 3}$  operated on convolutional layer.
- Filter aims to capture global relationships + generalize transistional charectersitics as in other models.

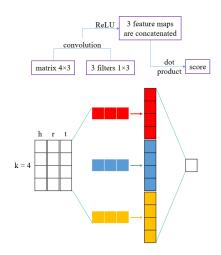


Figure 1: Process involved in ConvKB with embedding size k = 4 and number of filters  $\tau = 3$ 

### ConvKB Model

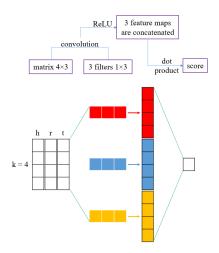


Figure 2: Process involved in ConvKB with embedding size k = 4 and number of filters  $\tau = 3$ 

- Apply  $\omega$  repeatedly over all rows and concatenate feature maps  $\mathbf{v} = [v_1, v_2, \dots, v_k] \in \mathbb{R}^k$
- $v_i = g(\omega.A_{i,:} + b)$  where b is bias and g is non-linear activation function.
- We use  $\tau$  different filters and these  $\tau$  feature maps concated into single vector  $\chi \in \mathbb{R}^{\tau k \times 1}$

#### ConvKB Model

- Score function  $f(h, r, t) = concat(g([v_h, v_r, v_t] * \omega)).w$
- $\Omega$ (set of all filters) and w are shared parameters and \* denotes convolution operation.

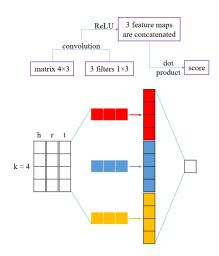


Figure 3: Process involved in ConvKB with embedding size k = 4 and number of filters  $\tau = 3$ 

### Loss function

$$L = \sum_{(h,r,t) \in \mathbb{G} \cup \mathbb{G}'} \log_e(1 + exp(l_{(h,r,t)}.f(h,r,t)))) + \frac{\lambda}{2} ||w||^2$$

$$l_{(h,r,t)} = \begin{cases} 1 \text{ for } (h,r,t) \in \mathbb{G} \\ -1 \text{ for } (h,r,t) \in \mathbb{G}' \end{cases}$$

 $\mathbb G$  is collection of valid triples in knowledge base.

 $\mathbb{G}'$  is collection of invalid triples generated by corrupting triples in  $\mathbb{G}$ 

### Loss function

$$L = \sum_{(h,r,t) \in \mathbb{G} \cup \mathbb{G}'} \log_e (1 + exp(l_{(h,r,t)}.f(h,r,t)))) + \frac{\lambda}{2} ||w||^2$$

$$l_{(h,r,t)} = \begin{cases} 1 \text{ for } (h,r,t) \in \mathbb{G} \\ -1 \text{ for } (h,r,t) \in \mathbb{G}' \end{cases}$$

 $\mathbb{G}$  is collection of valid triples in knowledge base.

 $\mathbb{G}'$  is collection of invalid triples generated by corrupting triples in  $\mathbb{G}$ 

Given two entities (h, t) log-odd probability that (h, r, t) is true  $\sigma(f(h, r, t))$ , where  $\sigma$  is sigmoid unit link function[TWR<sup>+</sup>16].

- Neural Link Prediction Model
- 2 Datasets
- 3 Baseline Implementation
- 4 Futher Directions....

#### Datasets

DATASET	WN	FB15K-237
ENTITIES	40,943	14,951
RELATIONS	18	1,345
TRAIN EX.	141,442	483,142
TEST EX.	5,000	50,000
VALID EX.	5,000	59,071

Table 1: [YYH+14]Some statistics of datasets we initally used for training our model.

- Freebase(N-Triples RDF,22Gzip,1.9 billion triples)
- Contains too many redudancies, inverse realtions and noisy also.
- Requires lot of pre-processing.
- Eventually we want to scale up our model to the dataset.

- Neural Link Prediction Model
- 2 Datasets
- 3 Baseline Implementation
- 4 Futher Directions....

## Training Protocol

- Initial embeddings obtained from STransE[NNNP17] which are fed to CNN layer, available at https://github.com/datquocnguyen/STransE.
- Corrupted triples are sampled using Bernoulli trick ([WZFC14][dai13])
- We train our model parameters including entity and relation embeddings, filters and weight vector W

## Asynchronous SGD

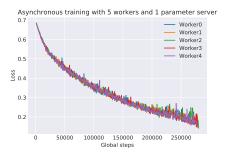


Figure 4: Learning curve for asynchronous SGD with 5 workers and 1 parameter server

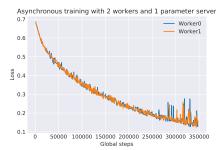


Figure 5: Learning curve for asynchronous SGD with 2 workers and 1 parameter server

## Racing Conditions in Asynchronous Training

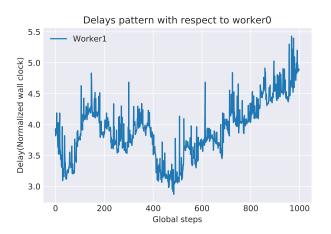
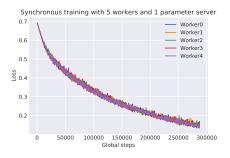


Figure 6: Intially both workers start at same point but eventually worker0 is straggling behind causing stale updates pushed at later steps during local gradient aggregation. Here I hand picked two workers to emphasize stark difference and increasing trend of lag after a certain point.

## Bulk Synchronous Parallel Training

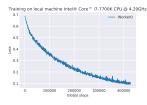


Synchronous training with 2 workers and 1 parameter server 0.7 Worker0 Worker1 0.6 0.5 S 0.4 0.3 0.2 0.1 0 100000 200000 300000 400000 Global steps

Figure 7: Learning curve for synchronous SGD with 5 workers and 1 parameter server

Figure 8: Learning curve for synchronous SGD with 2 workers and 1 parameter server

# Just for comparison.....



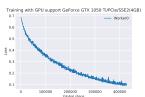


Figure 9: Learning curves in local machine( above Intel® Core<sup>TM</sup> i7-7700K CPU @ 4.20GHz) and below GPU GeForce GTX 1050 Ti/PCIe/SSE2

Train Setting	WallClock Time
GPU	$37 \mathrm{m}$
CPU	1hr 30min
1PS & 2W(Async)	4hr 23min
1PS & 5W(Async)	1hr 45min
1PS & 2W(Sync)	7hr 12min
1PS & 5W(Sync)	3hr

Table 2: Wallclock timings of our experiments took so far.

- Neural Link Prediction Model
- 2 Datasets
- 3 Baseline Implementation
- 4 Futher Directions....

#### Plans Ahead

- We need to implement and scale up the inference part(Not done yet).
- Need to understand and pre-process the entire Freebase dataset(quite messy!).
- A possible direction to explore is stale synchronous parallel training for more stable and faster convergence.
- Identify bottlenecks in training and inference phase.
- A trade off between a possible improved link prediction scores by implementing deeper model and scalability issues due to increasing computational complexity

#### References I

- Antoine Bordes, Xavier Glorot, Jason Weston, and Yoshua Bengio, A semantic matching energy function for learning with multi-relational data, Mach. Learn. 94 (2014), no. 2, 233–259.
- Antoine Bordes, Nicolas Usunier, Alberto Garcia-Durán, Jason Weston, and Oksana Yakhnenko, *Translating embeddings for modeling multi-relational data*, Proceedings of the 26th International Conference on Neural Information Processing Systems Volume 2 (USA), NIPS'13, Curran Associates Inc., 2013, pp. 2787–2795.
- daiquocnguyen, *Project title*, https://github.com/daiquocnguyen/ConvKB, 2013.

### References II

- Dai Quoc Nguyen, Tu Dinh Nguyen, Dat Quoc Nguyen, and Dinh Phung, A novel embedding model for knowledge base completion based on convolutional neural network, arXiv preprint arXiv:1712.02121 (2017).
- Théo Trouillon, Johannes Welbl, Sebastian Riedel, Éric Gaussier, and Guillaume Bouchard, Complex embeddings for simple link prediction, International Conference on Machine Learning, 2016, pp. 2071–2080.
- Zhen Wang, Jianwen Zhang, Jianlin Feng, and Zheng Chen, Knowledge graph embedding by translating on hyperplanes, Proceedings of the Twenty-Eighth AAAI Conference on Artificial Intelligence, AAAI'14, AAAI Press, 2014, pp. 1112–1119.

### References III



Bishan Yang, Wen-tau Yih, Xiaodong He, Jianfeng Gao, and Li Deng, Embedding entities and relations for learning and inference in knowledge bases, arXiv preprint arXiv:1412.6575 (2014).