Evaluating the Effectiveness of Multiple Hyperparameters and Constraints when Learning Embedding Representation for Categorised Knowledge Graphs

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Abstract. Learning knowledge representation is an increasingly important technology that supports a variety of machine learning related applications. However, the choice of hyperparameters is seldom justified and relies on exhaustive search. Understanding the effect of hyperparameter combinations on embedding quality is crucial to avoid the inefficient process and enhance practicality of vector representation methods. In this study, we evaluate the effects of distinct hyperparameters and learning constraints focused on translational embedding representation models for multi-relational categorised knowledge graphs. We assess the influence of multiple hyperparameters and constraints regarding the quality of embedding models by contrasting traditional link prediction task accuracy against a classification task. Our findings show that some hyperparameter choices follow more indistinct patterns, improving both knowledge completion and classification tasks, whereas some learning constraints can oppositely improve one task while worsen the other. Finally, we provide strong evidence that the link prediction does not directly reflect the effectiveness of using the resulting vector representation in a subsequent classification tasks, the correlation between link prediction and classification accuracy is a weak metric to represent the quality of resulting embedding approaches, which supports previous reported results.

Supplementary Material

The following tables provide supporting data to our research work.

Table 1. Examples of embedding scoring functions and their specific definitions.

Method	Scoring function $f_r(h,t)$	Specific definitions
TransE [2]	$\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|_{l_{1/2}}$	–
HEXTRATO [13]	$\|\mathbf{h}_{c_h}+\mathbf{r}-\mathbf{t}_{c_t}\|_2$	–
UM [1]	$\|\mathbf{h}-\mathbf{t}\|_{l_{1/2}}$	–
TransH [14]	$\|\mathbf{h}_\perp+\mathbf{r}-\mathbf{t}_\perp\|_2^2$	$\mathbf{h}_\perp=\mathbf{h}-\mathbf{w}_r^\top\mathbf{h}\mathbf{w}_r,\quad \mathbf{t}_\perp=\mathbf{t}-\mathbf{w}_r^\top\mathbf{t}\mathbf{w}_r$
TransR [10]	$\|\mathbf{h}_\perp+\mathbf{r}-\mathbf{t}_\perp\|_2^2$	$\mathbf{h}_\perp=\mathbf{M}_r\mathbf{h},\quad \mathbf{t}_\perp=\mathbf{M}_r\mathbf{t}$
TransD [8]	$\|\mathbf{h}_\perp+\mathbf{r}-\mathbf{t}_\perp\|_2^2$	$\mathbf{h}_\perp=\mathbf{M}_{r,h}\mathbf{h},\quad \mathbf{t}_\perp=\mathbf{M}_{r,t}\mathbf{t}$ $\mathbf{M}_{r,h}=\mathbf{w}_r\mathbf{w}_h^\top+\mathbf{I}$ $\mathbf{M}_{r,t}=\mathbf{w}_r\mathbf{w}_t^\top+\mathbf{I}$
SE [3]	$\|\mathbf{h}_\perp-\mathbf{t}_\perp\|_1$	$\mathbf{h}_\perp=\mathbf{M}_{r,h}\mathbf{h},\quad \mathbf{t}_\perp=\mathbf{M}_{r,t}\mathbf{t}$
STransE [12]	$\|\mathbf{h}_\perp+\mathbf{r}-\mathbf{t}_\perp\|_{l_{1/2}}$	$\mathbf{h}_\perp=\mathbf{M}_{r,h}\mathbf{h},\quad \mathbf{t}_\perp=\mathbf{M}_{r,t}\mathbf{t}$
TransF [4]	$\|\mathbf{h}_\perp+\mathbf{r}-\mathbf{t}_\perp\|_2^2$	$\mathbf{h}_\perp=\mathbf{M}_{r,h}\mathbf{h},\quad \mathbf{t}_\perp=\mathbf{M}_{r,t}\mathbf{t}$ $\mathbf{M}_{r,h}=\sum_{i=1}^s\alpha_r^{(i)}\mathbf{U}^{(i)}+\mathbf{I}$ $\mathbf{M}_{r,t}=\sum_{i=1}^s\beta_r^{(i)}\mathbf{V}^{(i)}+\mathbf{I}$
TransM [5]	$\theta_r\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|_{l_{1/2}}$	–
ManifoldE [16]	$\|\mathcal{M}(h,r,t)-D_r^2\|^2$	linear kernel hyper-spheres: $\mathcal{M}(h,r,t)=\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|_2^2$ hyperplanes: $\mathcal{M}(h,r,t)=(\mathbf{h}+\mathbf{r}_h)^\top(\mathbf{t}+\mathbf{r}_t)$
TransE-FT [6]	$(\mathbf{h}+\mathbf{r})^\top\mathbf{t}+(\mathbf{t}-\mathbf{r})^\top\mathbf{h}$	–
TransA(Xiao) [15]	$(\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|)^\top\mathbf{M}_r(\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|)$	–
KG2E [7]	symmetric: $\frac{1}{2}\{\boldsymbol{\mu}^\top\boldsymbol{\Sigma}_r^{-1}\boldsymbol{\mu}+\ln(\det(\boldsymbol{\Sigma}))\}$ asymmetric: $\frac{1}{2}\{\mathrm{tr}(\boldsymbol{\Sigma}_\mathrm{r}^{-1}(\boldsymbol{\Sigma}_\mathrm{h}+\boldsymbol{\Sigma}_\mathrm{t}))+$ $\boldsymbol{\mu}^\top\boldsymbol{\Sigma}_r^{-1}\boldsymbol{\mu}-\ln\frac{\det(\boldsymbol{\Sigma}_h+\boldsymbol{\Sigma}_t)}{\det(\boldsymbol{\Sigma}_r)}\}$	$\mathbf{h}\sim\mathcal{N}(\boldsymbol{\mu}_h,\boldsymbol{\Sigma}_h),\quad \mathbf{t}\sim\mathcal{N}(\boldsymbol{\mu}_t,\boldsymbol{\Sigma}_t),$ $\mathbf{r}\sim\mathcal{N}(\boldsymbol{\mu}_r,\boldsymbol{\Sigma}_r)$ $\mathbf{h}-\mathbf{t}\sim\mathcal{N}(\boldsymbol{\mu}_h-\boldsymbol{\mu}_t,\boldsymbol{\Sigma}_t+\boldsymbol{\Sigma}_h)$ $\boldsymbol{\mu}=\boldsymbol{\mu}_h-\boldsymbol{\mu}_r-\boldsymbol{\mu}_t$ $\boldsymbol{\Sigma}=\boldsymbol{\Sigma}_h+\boldsymbol{\Sigma}_r+\boldsymbol{\Sigma}_t$
TKRL [18]	$\|\mathbf{h}_\perp+\mathbf{r}-\mathbf{t}_\perp\|$	$\mathbf{h}_\perp=\mathbf{M}_{r,h}\mathbf{h},\quad \mathbf{t}_\perp=\mathbf{M}_{r,t}\mathbf{t}$ $\mathbf{M}_{r,h}=\frac{\sum_{i=1}^n\alpha_i\mathbf{M}_{c_i}}{\sum_{i=1}^n\alpha_i},\quad \alpha_i=\begin{cases}1, c_i\in C_{r_h}\\0, c_i\notin C_{r_h}\end{cases}$ $\mathbf{M}_{r,t}=\frac{\sum_{i=1}^n\alpha_i\mathbf{M}_{c_i}}{\sum_{i=1}^n\alpha_i},\quad \alpha_i=\begin{cases}1, c_i\in C_{r_t}\\0, c_i\notin C_{r_t}\end{cases}$ recursive: $\mathbf{M}_c=\prod_{i=1}^m\mathbf{M}_{c^{(i)}}$ weighted: $\mathbf{M}_c=\sum_{i=1}^m\beta_i\mathbf{M}_{c^{(i)}},$ $\beta_i:\beta_{i+1}=(1-\eta):\eta,\quad \sum_{i=1}^m\beta_i=1$
TransT [11]	$\begin{cases}-\ln p(h\|r,t,true)+\\ \quad\ln p(h'\|r,t,true), \quad h'\neq h\\-\ln p(t\|h,r,true)+\\ \quad\ln p(t'\|h,r,true), \quad t'\neq t\\-\ln p(r\|h,t,true)+\\ \quad\ln p(r'\|h,t,true), \quad r'\neq r\end{cases}$	$p(t\|h,r,true)=$ $\begin{cases}\frac{p(true\|h,r,t)p(t\|h,r)}{p(true\|h,r)}, & p(t\|h,r)\neq 0\\0 & p(t\|h,r)=0\end{cases}$

Table 2. Link prediction scores for WN18 and FB15k reported in multiple translational models.

Embedding Method	**WN18**						**FB15K**					
	MR		**MRR**		**Hits@10**		**MR**		**MRR**		**Hits@10**	
	Raw	Filter	Raw	Filter	Raw	Filter	Raw	Filter	Raw	Filter	Raw	Filter
TransE [2]	263	251	–	–	75.4	89.2	243	125	–	–	34.9	47.1
HEXTRATO [13]	–	–	–	–	–	–	116	–	–	–	53.5	–
TransH [14]	401	388	–	–	73.0	82.3	212	87	–	–	45.7	64.4
TransR [10]	238	225	–	–	79.8	79.4	198	77	–	–	48.2	68.7
CTransR [10]	231	218	–	–	79.4	92.3	199	75	–	–	48.4	70.2
TransD [8]	224	212	–	–	79.6	92.2	194	91	–	–	53.4	77.3
TranSparse [9] (shr, S)	237	224	–	–	80.4	93.6	194	88	–	–	53.4	77.7
TranSparse [9] (shr, US)	233	221	–	–	80.5	93.9	191	86	–	–	53.5	78.3
TranSparse [9] (sep, S)	224	221	–	–	79.8	92.8	187	82	–	–	53.3	79.5
TranSparse [9] (sep, US)	223	211	–	–	80.1	93.2	190	82	–	–	53.7	79.9
STransE [12]	217	206	0.469	0.657	80.9	93.4	219	69	0.252	0.543	51.6	79.7
TransF [4]	–	198	–	0.856	–	95.3	–	62	–	0.564	–	82.3
TransM [5]	293	281	–	–	75.7	85.4	197	94	–	–	44.6	55.2
ManifoldE [16] (sphere)	–	–	–	–	80.7	92.8	–	–	–	–	55.7	86.2
ManifoldE [16] (hyperplane)	–	–	–	–	84.2	94.9	–	–	–	–	55.2	88.1
TransA(Xiao) [15]	405	392	–	–	82.3	94.3	155	74	–	–	56.1	80.4
TransA(Jia) [19]	165	153	–	–	–	–	164	58	–	–	–	–
KG2E [7]	342	331	–	–	80.2	92.8	174	59	–	–	48.9	74.0
TransG [17]	357	345	–	–	84.5	94.9	152	50	–	–	55.9	88.2
UM [1]	315	304	–	–	35.3	38.2	1074	979	–	–	4.5	6.3
SE [3]	1011	985	–	–	68.5	80.5	273	162	–	–	28.8	39.8
TKRL [18]	–	–	–	–	–	–	184	68	–	–	49.2	69.4
TransT [11]	137	130	–	–	92.7	97.4	199	46	–	–	53.3	85.4

Table 3. Optimal hyperparameters reported in multiple translational KG embedding models for the link prediction task on WN18 and FB15K benchmark datasets (η: learning rate; γ: learning margin; K: dimensions).

Embedding Method	WN18			FB15K		
	η	γ	K	η	γ	K
TransE [2]	0.01	2.0	20	0.01	1.0	50
TransH [14]	0.01	1.0	50	0.005	0.25	100
TransR [10]	0.001	4.0	50	0.001	1.0	50
CTransR [10]	0.001	4.0	50	0.001	1.0	50
TransD [8]	*	1.0	50	*	2.0	100
TranSparse [9]	0.01	3.5	50	0.001	1.5	100
STransE [12]	0.0005	5.0	50	0.0001	1.0	100
TransF [4]	0.001	4.0	50	0.001	2.0	150
TransM [5]	0.01	2.0	20	0.01	1.0	50
ManifoldE [16] (sphere)	0.001	3.0	100	0.0005	1.0	800
ManifoldE [16] (hyperplane)	0.01	0.2	800	0.01	0.2	1000
TransA(Xiao) [15]	0.001	2.0	50	0.002	3.2	300
TransA(Jia) [19]	0.001	*	100	0.001	*	50
KG2E [7]	0.01	4.0	50	0.001	1.0	50
TransG [17]	0.001	2.5	100	0.0015	3.0	400
TransT [11]	0.001	3.0	50	0.00025	3.5	300
HEXTRATO [13]	–	–	–	0.01	2.0	32

* variable and/or adapted during training

Table 4. Link Prediction (MRR) improvement (%) when varying hyperparameters and embedding constraints.

Parameter Changed	**Global Improv**	**K**			**η**			**γ**			**Onto**				**Norm**		**Proj**			**Reg**	
		16	**32**	**64**	**0.1**	**0.01**	**0.001**	**1**	**2**	**4**	**T**	**TI**	**TID**	**TIDF**	**No**	**Yes**	**L0**	**L1**	**L2**	**Spc**	**Srf**
Dimensions (K)																					
16 $\Rightarrow$ 32	**3.0**	-	-	-	2.2	3.7	3.1	0.6	4.0	4.3	2.2	1.7	2.8	5.2	4.3	2.6	3.4	3.0	2.5	3.3	2.6
32 $\Rightarrow$ 64	**0.2**	-	-	-	0.7	-0.1	0.0	0.5	0.2	-0.2	0.2	0.1	0.2	0.0	0.1	0.2	-0.2	0.3	0.4	0.1	0.2
Learning Rate (η)																					
0.1 $\Rightarrow$ 0.01	**11.7**	7.3	8.9	19.4	-	-	-	8.9	12.4	13.9	11.6	9.5	11.0	14.8	16.4	16.2	9.5	12.8	12.9	15.4	8.1
0.01 $\Rightarrow$ 0.001	**2.0**	2.8	2.2	0.9	-	-	-	-0.1	2.0	4.0	0.8	1.2	2.9	3.2	-1.8	-0.4	1.7	2.9	1.2	2.2	1.8
Learning Margin (γ)																					
1 $\Rightarrow$ 2	**-1.1**	-4.2	-1.0	2.1	-3.7	-0.8	1.3	-	-	-	1.1	-0.4	-2.3	-2.8	-1.3	-2.0	-2.2	-0.8	-0.1	-1.4	-0.8
2 $\Rightarrow$ 4	**-5.1**	-6.7	-6.5	-2.0	-6.4	-5.3	-3.7	-	-	-	-4.6	-4.3	-5.0	-6.7	-7.8	-8.1	-7.0	-4.5	-3.8	-5.3	-4.9
Ontology Constraint (Onto)																					
T $\Rightarrow$ TI	**-4.1**	-4.1	-4.5	-3.7	-3.2	-4.8	-4.4	-3.3	-4.6	-4.4	-	-	-	-	-9.0	1.8	-1.4	-5.4	-5.6	-4.0	-4.2
TI $\Rightarrow$ TID	**4.2**	3.5	4.7	4.5	2.4	4.1	6.0	5.8	3.8	3.1	-	-	-	-	0.5	4.6	4.3	3.9	4.5	5.3	3.1
TID $\Rightarrow$ TIDF	**0.1**	-1.7	0.6	3.1	-2.3	1.1	1.5	0.9	0.4	-1.0	-	-	-	-	5.4	-1.2	2.2	-2.0	-0.3	-0.3	0.5
Normalized Relations (Norm)																					
No $\Rightarrow$ Yes	**7.4**	8.9	7.0	6.4	6.8	7.0	8.5	8.1	7.1	6.9	-3.1	9.8	14.7	9.3	-	-	1.0	11.0	10.2	6.9	7.9
Embedding Approach (Proj)																					
L0 $\Rightarrow$ L1	**1.1**	3.1	2.6	-2.5	-0.8	1.5	2.5	-0.8	0.6	3.4	5.7	1.1	0.6	-3.4	-3.0	5.2	-	-	-	1.5	0.6
L1 $\Rightarrow$ L2	**0.1**	0.4	0.0	-0.2	0.1	0.8	-0.6	-0.6	0.1	0.8	-0.5	-0.8	-0.2	1.9	-1.5	-2.5	-	-	-	0.3	-0.1
Regularization Constraint (Reg)																					
Spc $\Rightarrow$ Srf	**0.0**	0.7	0.1	-1.0	4.6	-2.2	-2.5	-0.6	0.1	0.4	1.0	0.7	-1.3	-0.5	0.1	0.8	0.8	-0.2	-0.7	-	-

Table 5. Classifier accuracy improvement (%) when varying hyperparameters and embedding constraints.

Param Changed	**Global Improv**	**K**			η			γ			**Onto**				**Norm**		**Proj**			**Reg**	
		16	**32**	**64**	**0.1**	**0.01**	**0.001**	**1**	**2**	**4**	**T**	**TI**	**TID**	**TIDF**	**No**	**Yes**	**L0**	**L1**	**L2**	**Spc**	**Srf**
Dimensions (K)																					
16 ⇒ 32	**7.1**	-	-	-	3.5	5.5	12.2	2.9	4.0	14.3	5.4	11.9	3.9	7.1	5.1	4.8	5.0	4.8	11.4	9.2	4.9
32 ⇒ 64	**0.3**	-	-	-	2.1	-0.8	-0.6	0.8	0.4	-0.5	0.1	0.2	0.5	0.2	0.6	0.5	-0.4	0.6	0.5	0.1	0.4
Learning Rate (η)																					
0.1 ⇒ 0.01	**24.4**	12.4	14.9	47.0	-	-	-	14.4	21.5	37.4	22.1	21.3	22.7	31.3	33.7	32.8	26.9	24.4	21.9	28.9	19.9
0.01 ⇒ 0.001	**-3.1**	-1.5	-2.8	-5.0	-	-	-	-6.3	-6.3	3.3	-7.5	-6.3	-5.3	7.7	4.8	5.6	-4.5	-0.7	-4.2	-3.0	-3.2
Learning Margin (γ)																					
1 ⇒ 2	**-1.7**	-3.1	-2.7	0.7	-5.5	0.0	0.2	-	-	-	-2.4	-1.7	-0.9	-2.1	-2.8	-2.2	-3.7	-0.9	-0.7	-3.3	-0.2
2 ⇒ 4	**-8.6**	-12.3	-9.3	-3.9	-16.5	-6.8	-2.4	-	-	-	-7.0	-7.1	-5.9	-14.8	-12.4	-13.1	-13.5	-6.0	-6.1	-9.3	-7.9
Ontology Constraint (Onto)																					
T ⇒ TI	**1.1**	2.0	1.2	0.0	1.1	0.3	1.8	0.4	1.4	1.5	-	-	-	-	1.6	1.5	3.9	0.0	-0.6	1.2	1.0
TI ⇒ TID	**0.2**	3.6	-0.5	-2.5	-1.2	-1.3	3.1	-1.5	-1.0	3.0	-	-	-	-	-0.1	0.5	0.4	-2.0	2.1	1.1	-0.7
TID ⇒ TIDF	**-2.8**	-3.6	-2.5	-2.3	-8.8	-3.5	3.9	0.0	-0.3	-8.4	-	-	-	-	-6.2	-6.0	2.8	-5.9	-5.8	-2.1	-3.6
Normalized Relations (Norm)																					
No ⇒ Yes	**0.0**	-0.1	-0.2	0.2	-0.2	-0.4	0.5	-0.1	0.4	-0.5	0.0	-0.4	0.1	0.1	-	-	-0.1	-0.2	0.1	-0.1	0.0
Embedding Approach (Proj)																					
L0 ⇒ L1	**8.2**	11.9	10.5	2.1	12.4	5.5	6.8	2.1	5.2	17.5	15.8	10.4	7.6	-1.3	7.9	8.9	-	-	-	8.2	8.3
L1 ⇒ L2	**-1.8**	-2.7	-1.9	-0.9	0.3	-1.7	-4.1	-1.7	-1.8	-2.0	-2.0	-2.6	-1.1	-1.5	-1.4	-0.8	-	-	-	-0.6	-3.1
Regularization Constraint (Reg)																					
Spc ⇒ Srf	**3.3**	6.4	2.5	0.8	6.7	-0.6	3.6	-1.1	2.5	8.4	2.1	6.4	2.9	1.6	2.0	1.9	2.1	3.1	4.5	-	-

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