Neighborhood Mixture Model for Knowledge Base Completion

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Introduction

- Knowledge bases (KBs) of real-world triple facts (head entity, relation, tail entity) are useful resources for NLP tasks
- **Issue**: large KBs are still far from complete
- So it is useful to perform *link prediction in KBs* or *knowledge base completion* (KBC): predict which triples not in a knowledge base are likely to be true

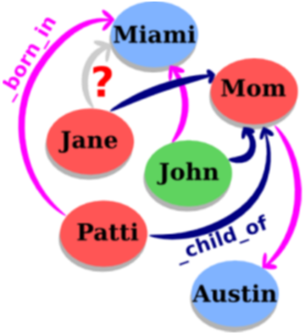


Figure extracted from "Jason Weston and Antoine Bordes. 2014. Embedding Methods for NLP. *EMNLP 2014 tutorial*."

Introduction

- Embedding models for KBC:
  - Associate entities and/or relations with dense feature vectors or matrices
  - Obtain SOTA performance and generalize to large KBs
- Most embedding models for KBC learn only from triples
- Recent works show that the relation paths between entities in KBs provide useful information and improve KBC

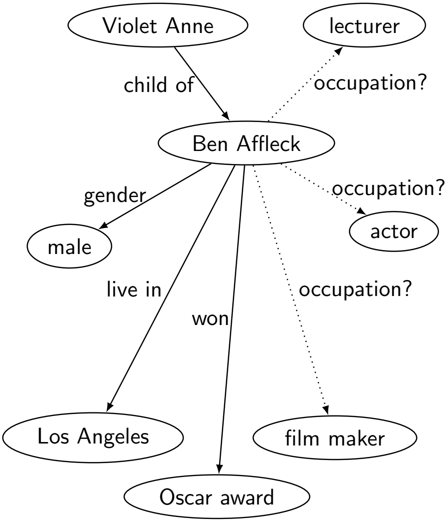
$$
\begin{aligned}
&(\text{Harrison Ford}, \textbf{born\_in\_hospital}/\mathrm{r}_1, \text{Swedish Covenant Hospital})\\
\Rightarrow&(\text{Swedish Covenant Hospital}, \textbf{located\_in\_city}/\mathrm{r}_2, \text{Chicago})\\
\Rightarrow&(\text{Chicago}, \textbf{city\_in\_country}/\mathrm{r}_3, \text{United States})
\end{aligned}
$$

Relation path $\mathrm{p} = \{\mathrm{r}_1, \mathrm{r}_2, \mathrm{r}_3\}$ is useful for predicting the relationship "*nationality*" between **Harrison Ford** and **United States**

Introduction

- **Our motivation**: neighborhoods could provide lots of useful information for predicting the relationship between the entities

$$
\begin{aligned}
&\text{Ben\_Affleck} \\
&= \omega_{r,1}(\text{Violet\_Anne}, \text{child\_of}) \\
&\quad + \omega_{r,2}(\text{male}, \text{gender}^{-1}) \\
&\quad + \omega_{r,3}(\text{Los\_Angeles}, \text{live\_in}^{-1}) \\
&\quad + \omega_{r,4}(\text{Oscar\_award}, \text{won}^{-1})
\end{aligned}
$$



Our approach: Neighbor-based entity representation

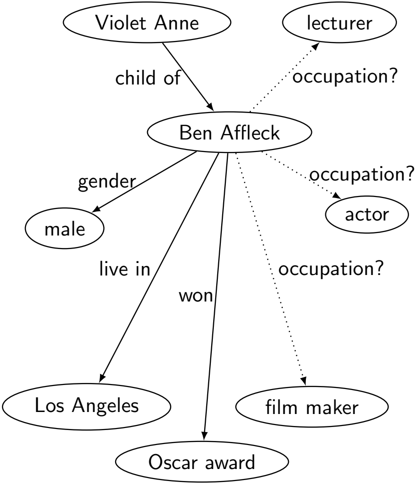
$\mathcal{E} = \{\text{Ben\_Affleck}, \text{Los\_Angeles}, \ldots\}$

$\mathcal{R} = \{\text{live\_in}, \text{won}, \text{child\_of}, \text{gender}, \ldots\}$

$$\mathcal{G} = \{(\text{Violet\_Anne}, \text{child\_of}, \text{Ben\_Affleck}),\\ (\text{Ben\_Affleck}, \text{won}, \text{Oscar\_award}),\\ (\text{Ben\_Affleck}, \text{live\_in}, \text{Los\_Angeles}), \ldots\}$$

$\mathcal{N}_e$ is the set of all entity and relation pairs that are neighbors for entity e

$$\mathcal{N}_{\text{Ben\_Affleck}} = \{(\text{Violet\_Anne}, \text{child\_of}),\\ (\text{male}, \text{gender}^{-1}),\\ (\text{Los\_Angeles}, \text{live\_in}^{-1}),\\ (\text{Oscar\_award}, \text{won}^{-1})\}$$



Our approach: Neighbor-based entity representation

- $\boldsymbol{v}_e \in \mathbb{R}^k$: k-dimensional base vector associated with entity e
- $\boldsymbol{u}_{e,r} \in \mathbb{R}^k$: relation-specific entity vector, $e \in \mathcal{E},\ r \in \mathcal{R} \cup \mathcal{R}^{-1}$
- The neighborhood-based entity representation $\boldsymbol{\vartheta}_{e,r}$ for an entity e for predicting the relation r is defined as follows:

$$\boldsymbol{\vartheta}_{e,r} = a_e \boldsymbol{v}_e + \sum_{(e',r') \in \mathcal{N}_e} b_{r,r'} \boldsymbol{u}_{e',r'} \tag{1}$$

a_e and $b_{r,r'}$ are the mixture weights that are constrained to sum to 1:

$$a_e \propto \delta + \exp \alpha_e \tag{2}$$

$$b_{r,r'} \propto \exp \beta_{r,r'} \tag{3}$$

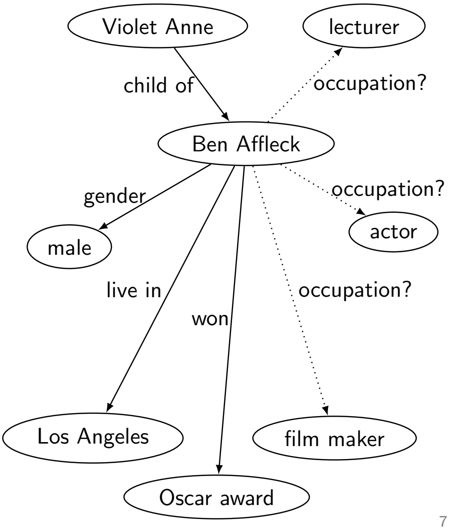
$\delta \geqslant 0$: hyper-parameter

α_e, $\beta_{r,r'}$: learnable exponential mixture parameters

Our approach: Neighbor-based entity representation

$$\boldsymbol{\vartheta}_{e,r} = a_e \boldsymbol{v}_e + \sum_{(e',r')\in\mathcal{N}_e} b_{r,r'} \boldsymbol{u}_{e',r'}$$

$$\begin{aligned} e &= \text{Ben\_Affleck} \\ r &= \text{occupation} \\ \mathcal{N}_e &= \{(\text{Violet\_Anne}, \text{child\_of}), \\ &\quad (\text{male}, \text{gender}^{-1}), \\ &\quad (\text{Los\_Angeles}, \text{live\_in}^{-1}), \\ &\quad (\text{Oscar\_award}, \text{won}^{-1})\} \end{aligned}$$



Our approach: Applying neighborhood mixtures to TransE

- Embedding models define for each triple $(h, r, t) \in \mathcal{G}$, a *score function* $f(h, r, t)$ that measures its implausibility
- **Goal**: choose f such that the score $f(h, r, t)$ of a plausible triple (h, r, t) is smaller than the score $f(h', r', t')$ of an implausible triple (h', r', t').
- Entity e and relation r are represented with vectors $\boldsymbol{v}_e \in \mathbb{R}^k$ and $\boldsymbol{v}_r \in \mathbb{R}^k$

$$f(h, r, t)_{\text{TransE}} = \|\boldsymbol{v}_h + \boldsymbol{v}_r - \boldsymbol{v}_t\|_{\ell_{1/2}}$$

- The score function of our new model TransE-NMM is defined as follows:

$$f(h, r, t) = \|\boldsymbol{\vartheta}_{h,r} + \boldsymbol{v}_r - \boldsymbol{\vartheta}_{t,r^{-1}}\|_{\ell_{1/2}} \tag{4}$$

$$\boldsymbol{\vartheta}_{e,r} = a_e \boldsymbol{v}_e + \sum_{(e',r') \in \mathcal{N}_e} b_{r,r'} \boldsymbol{u}_{e',r'}$$

$$\boldsymbol{u}_{e,r} = \boldsymbol{v}_e + \boldsymbol{v}_r \tag{5}$$

$$\boldsymbol{v}_{r^{-1}} = -\boldsymbol{v}_r \tag{6}$$

Our approach: Parameter optimization

- Model parameters:
  - Entity vectors $\boldsymbol{v}_e$
  - Relation type vectors $\boldsymbol{v}_r$
  - $\boldsymbol{\alpha} = \{\alpha_e | e \in \mathcal{E}\}$: entity-specific weights
  - $\boldsymbol{\beta} = \{\beta_{r,r'} | r, r' \in \mathcal{R} \cup \mathcal{R}^{-1}\}$: relation-specific weights
- Minimize the L_2-regularized margin-based objective function:

$$\mathcal{L} = \sum_{\substack{(h,r,t)\in\mathcal{G} \\ (h',r,t')\in\mathcal{G}'_{(h,r,t)}}} [\gamma + f(h,r,t) - f(h',r,t')]_+ + \frac{\lambda}{2}\left(\|\boldsymbol{\alpha}\|_2^2 + \|\boldsymbol{\beta}\|_2^2\right)$$

$$\begin{aligned}\mathcal{G}'_{(h,r,t)} = &\{(h',r,t) \mid h' \in \mathcal{E}, (h',r,t) \notin \mathcal{G}\} \\ &\cup \{(h,r,t') \mid t' \in \mathcal{E}, (h,r,t') \notin \mathcal{G}\}\end{aligned}$$

  - $[x]_+ = \max(0, x)$
  - γ: the margin hyper-parameter
  - λ: the L_2 regularization parameter
  - Impose constraints during training with RMSProp: $\|\boldsymbol{v}_e\|_2 \leqslant 1$, $\|\boldsymbol{v}_r\|_2 \leqslant 1$

Related work

Model	Score function $f(h, r, t)$
STransE	$\lVert \mathbf{W}_{r,1}\boldsymbol{v}_h + \boldsymbol{v}_r - \mathbf{W}_{r,2}\boldsymbol{v}_t \rVert_{\ell_{1/2}}$; $\mathbf{W}_{r,1}$, $\mathbf{W}_{r,2} \in \mathbb{R}^{k\times k}$; $\boldsymbol{v}_r \in \mathbb{R}^k$
TransE	$\lVert \boldsymbol{v}_h + \boldsymbol{v}_r - \boldsymbol{v}_t \rVert_{\ell_{1/2}}$; $\boldsymbol{v}_r \in \mathbb{R}^k$
TransH	$\lVert (\mathbf{I} - \boldsymbol{r}_p\boldsymbol{r}_p^\top)\boldsymbol{v}_h + \boldsymbol{v}_r - (\mathbf{I} - \boldsymbol{r}_p\boldsymbol{r}_p^\top)\boldsymbol{v}_t \rVert_{\ell_{1/2}}$ $\boldsymbol{r}_p$, $\boldsymbol{v}_r \in \mathbb{R}^k$; $\mathbf{I}$: Identity matrix size $k \times k$
TransD	$\lVert (\mathbf{I} + \boldsymbol{r}_p\boldsymbol{h}_p^\top)\boldsymbol{v}_h + \boldsymbol{v}_r - (\mathbf{I} + \boldsymbol{r}_p\boldsymbol{t}_p^\top)\boldsymbol{v}_t \rVert_{\ell_{1/2}}$ $\boldsymbol{r}_p$, $\boldsymbol{v}_r \in \mathbb{R}^n$; $\boldsymbol{h}_p, \boldsymbol{t}_p \in \mathbb{R}^k$; $\mathbf{I}$: Identity matrix size $n \times k$
TransR	$\lVert \mathbf{W}_r\boldsymbol{v}_h + \boldsymbol{v}_r - \mathbf{W}_r\boldsymbol{v}_t \rVert_{\ell_{1/2}}$; $\mathbf{W}_r \in \mathbb{R}^{n\times k}$; $\boldsymbol{v}_r \in \mathbb{R}^n$
NTN	$\boldsymbol{v}_r^\top \mathit{tanh}(\boldsymbol{v}_h^\top \mathbf{M}_r \boldsymbol{v}_t + \mathbf{W}_{r,1}\boldsymbol{v}_h + \mathbf{W}_{r,2}\boldsymbol{v}_t + \mathbf{b}_r)$ $\boldsymbol{v}_r$, $\mathbf{b}_r \in \mathbb{R}^n$; $\mathbf{M}_r \in \mathbb{R}^{k\times k\times n}$; $\mathbf{W}_{r,1}$, $\mathbf{W}_{r,2} \in \mathbb{R}^{n\times k}$
DISTMULT	$\boldsymbol{v}_h^\top \mathbf{W}_r \boldsymbol{v}_t$; $\mathbf{W}_r$ is a diagonal matrix $\in \mathbb{R}^{k\times k}$
Bilinear-COMP	$\boldsymbol{v}_h^\top \mathbf{W}_{r_1}\mathbf{W}_{r_2}...\mathbf{W}_{r_m}\boldsymbol{v}_t$; $\mathbf{W}_{r_1}, \mathbf{W}_{r_2}, ..., \mathbf{W}_{r_m} \in \mathbb{R}^{k\times k}$
TransE-COMP	$\lVert \boldsymbol{v}_h + \boldsymbol{v}_{r_1} + \boldsymbol{v}_{r_2} + ... + \boldsymbol{v}_{r_m} - \boldsymbol{v}_t \rVert_{\ell_{1/2}}$; $\boldsymbol{v}_{r_1}, \boldsymbol{v}_{r_2}, ..., \boldsymbol{v}_{r_m} \in \mathbb{R}^k$
TransE-NMM	$\lVert \boldsymbol{\vartheta}_{h,r} + \boldsymbol{v}_r - \boldsymbol{\vartheta}_{t,r^{-1}} \rVert_{\ell_{1/2}}$

Evaluation: experimental setup

Dataset:	WN11	FB13	NELL186
#R	11	13	186
#E	38,696	75,043	14,463
#Train	112,581	316,232	31,134
#Valid	2,609	5,908	5,000
#Test	10,544	23,733	5,000

- #E: number of entities
- #R: number of relation types
- #Train, #Valid and #Test are the numbers of correct triples in the training, validation, and test sets, respectively
- Each validation and test set also contains the same number of incorrect triples as the number of correct triples

Triple classification task:

- Predict whether a triple (h, r, t) is correct or not
- Set a relation-specific threshold θ_r for each relation type r
- For an unseen test triple (h, r, t), if $f(h, r, t)$ is smaller than θ_r then the triple will be classified as correct, otherwise incorrect
- The relation-specific thresholds are determined by maximizing the micro-averaged accuracy on the validation set

Evaluation: experimental setup

- **Entity prediction task**:
  - Predict h given $(?, r, t)$ or predict t given $(h, r, ?)$ where ? denotes the missing element
  - Corrupt each correct test triple (h, r, t) by replacing either h or t by each of the possible entities in turn
  - Rank these candidates in ascending order of their implausibility value computed by the score function
  - "Raw" and "Filtered" setting protocols in which "Filtered" setting is to filter out before ranking any corrupted triples that appear in the KB
  - Metrics: mean rank (MR), mean reciprocal rank (MRR) and Hits@10 (H10)
- **Relation prediction task**:
  - Predict r given $(h, ?, t)$ where ? denotes the missing element
  - Corrupt each correct test triple (h, r, t) by replacing r by each of the possible relations in turn

Evaluation: quantitative results

Data	Method		Triple class.		Entity prediction			Relation prediction		
			Mic.	Mac.	MR	MRR	H@10	MR	MRR	H@10
WN11	R	TransE	85.21	82.53	4324	0.102	19.21	2.37	0.679	**99.93**
		TransE-NMM	**86.82**	**84.37**	**3466**	**0.123**	**20.59**	**2.14**	**0.687**	99.92
	F	TransE			4304	0.122	21.86	2.37	0.679	**99.93**
		TransE-NMM			**3447**	**0.137**	**23.03**	**2.14**	**0.687**	99.92
FB13	R	TransE	87.57	86.66	9037	0.204	35.39	1.01	0.996	99.99
		TransE-NMM	**88.58**	**87.99**	**8289**	**0.258**	**35.53**	1.01	0.996	**100.0**
	F	TransE			5600	0.213	36.28	1.01	0.996	99.99
		TransE-NMM			**5018**	**0.267**	**36.36**	1.01	0.996	**100.0**
NELL186	R	TransE	92.13	88.96	309	0.192	36.55	8.43	0.580	77.18
		TransE-NMM	**94.57**	**90.95**	**238**	**0.221**	**37.55**	**6.15**	**0.677**	**82.16**
	F	TransE			279	0.268	47.13	8.32	0.602	77.26
		TransE-NMM			**214**	**0.292**	**47.82**	**6.08**	**0.690**	**82.20**

- **Mic.**: Micro-averaged accuracy; **Mac.**: Macro-averaged accuracy
- "R" and "F" denote the "Raw" and "Filtered" settings used in the entity prediction and relation prediction tasks, respectively
- Better results are in **bold**

Evaluation: quantitative results

Method	**W11**	**F13**
TransR	85.9	82.5
CTransR	85.7	-
TransD	<u>86.4</u>	**89.1**
TranSparse-S	<u>86.4</u>	88.2
TranSparse-US	**86.8**	87.5
NTN	70.6	87.2
TransH	78.8	83.3
SLogAn	75.3	85.3
KG2E	85.4	85.3
Bilinear-COMP	77.6	86.1
TransE-COMP	80.3	87.6
TransE	85.2	87.6
TransE-NMM	**86.8**	<u>88.6</u>

Micro-averaged accuracy for triple classification on WN11 and FB13

Results on the NELL186 test set:

Method	**Triple class.**		**Entity pred.**	
	Mic.	Mac.	MR	H@10
TransE-LLE	90.08	84.50	535	20.02
SME-LLE	93.64	89.39	<u>253</u>	37.14
SE-LLE	<u>93.95</u>	88.54	447	31.55
TransE-SkipG	85.33	80.06	385	30.52
SME-SkipG	92.86	<u>89.65</u>	293	**39.70**
SE-SkipG	93.07	87.98	412	31.12
TransE	92.13	88.96	309	36.55
TransE-NMM	**94.57**	**90.95**	**238**	<u>37.55</u>

The entity prediction results are in the "Raw" setting

Evaluation: qualitative results

- Take the relation-specific mixture weights from the learned TransE-NMM
- Extract neighbor relations with the largest mixture weights given a relation

Relation	**Top 3-neighbor relations**
has_instance (WN11)	type_of subordinate_instance_of domain_topic
nationality (FB13)	place_of_birth place_of_death location
CEOof (NELL186)	WorksFor TopMemberOfOrganization PersonLeadsOrganization

Conclusions and future work

- We introduced a neighborhood mixture model for knowledge base completion by constructing neighbor-based vector representations for entities
- We demonstrated its effect by extending TransE with our neighborhood mixture model
- Our model significantly improves TransE and obtains better results than the other state-of-the-art embedding models on three evaluation tasks
- We plan to apply the neighborhood mixture model to the relation path models to combine the useful information from both relation paths and entity neighborhoods

Thank you for your attention!

$$\boldsymbol{\vartheta}_{e,r} = a_e \boldsymbol{v}_e + \sum_{(e',r') \in \mathcal{N}_e} b_{r,r'} \boldsymbol{u}_{e',r'}$$

$$\begin{aligned}
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r &= \text{occupation} \\
\mathcal{N}_e &= \{(\text{Violet_Anne}, \text{child_of}), \\
&\quad (\text{male}, \text{gender}^{-1}), \\
&\quad (\text{Los_Angeles}, \text{live_in}^{-1}), \\
&\quad (\text{Oscar_award}, \text{won}^{-1})\}
\end{aligned}$$