

# Knowledge Graph Embedding

## A Geometrical Perspective

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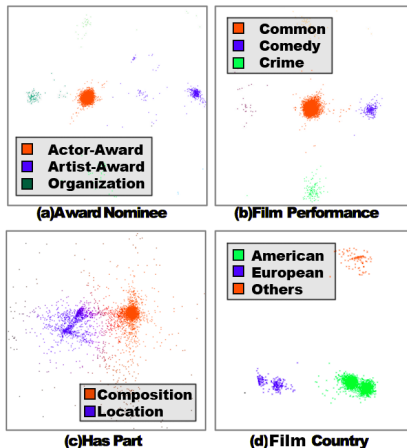
November 21, 2016

# Knowledge Graph Embedding: A Geometrical Perspective

1. From the geometric perspective of **DATA**, we propose *TransG* to model multiple relation semantics.
2. From the geometric perspective of **MODEL**, we propose *ManifoldE* to achieve an algebraic well-posed system and a flexible geometric form.
3. From the geometric perspective of **INTERACTION** between texts and triples, we propose *SSP* to utilize textual descriptions.

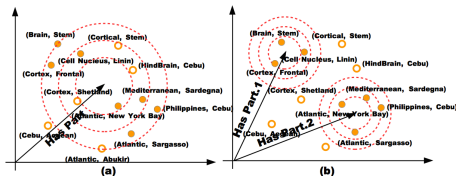
# TransG: A Generative Embedding Model

- **An Interesting Observation.** There are many entity-pair clusters in a relation-specific embedding space, representing various semantics, called **Multiple Relation Semantic**.



# TransG: A Generative Embedding Model

- ▶ **Multiple Relation Semantic:** A relation may have multiple meanings revealed by the entity pairs associated with the corresponding triples.
  - ▶ Composition Related: (*Table*, *HasPart*, *Leg*)
  - ▶ Location Related: (*Atlantics*, *HasPart*, *NewYorkBay*)
- ▶ **Reasons.**
  - ▶ Artificial Simplification.
  - ▶ Nature Of Knowledge.
- ▶ **Motivation.** Traditional methods such as TransE, could hardly model this phenomenon, incurring much noise.



# TransG: A Generative Embedding Model

- ▶ **Methodology.** TransG leverages a mixture of semantic component vectors for a specific relation. Each component represents a specific latent meaning. By this way, TransG could distinguish multiple relation semantics.
- ▶ **Generative Process.**
  1. For an entity  $e \in E$ :
    - 1.1 Draw each entity embedding mean vector from a standard normal distribution as a prior:  $\mathbf{u}_e \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ .
  2. For a triple  $(h, r, t) \in \Delta$ :
    - 2.1 Draw a semantic component from Chinese Restaurant Process for this relation:  $\pi_{r,m} \sim CRP(\beta)$ .
    - 2.2 Draw a head entity embedding vector from a normal distribution:  $\mathbf{h} \sim \mathcal{N}(\mathbf{u}_h, \sigma_h^2 \mathbf{E})$ .
    - 2.3 Draw a tail entity embedding vector from a normal distribution:  $\mathbf{t} \sim \mathcal{N}(\mathbf{u}_t, \sigma_t^2 \mathbf{E})$ .
    - 2.4 Draw a relation embedding vector for this semantics:  $\mathbf{u}_{r,m} = \mathbf{t} - \mathbf{h} \sim \mathcal{N}(\mathbf{u}_t - \mathbf{u}_h, (\sigma_h^2 + \sigma_t^2) \mathbf{E})$ .

# TransG: A Generative Embedding Model

- ▶ **Score Function:** the probability for generating the triple.

$$\mathbb{P}\{(h, r, t)\} \propto \sum_{m=1}^{M_r} \pi_{r,m} \mathbb{P}(\mathbf{u}_{r,m} | h, t) = \sum_{m=1}^{M_r} \pi_{r,m} e^{-\frac{\|\mathbf{u}_h + \mathbf{u}_{r,m} - \mathbf{u}_t\|_2^2}{\sigma_h^2 + \sigma_t^2}}$$

- ▶ **Geometrical Perspective.**

- ▶ TransG generalizes this geometric principle of translation from  $\mathbf{h} + \mathbf{r} = \mathbf{t}$  to the selective translation:

$$m_{(h,r,t)}^* = \arg \max_{m=1 \dots M_r} \left( \pi_{r,m} e^{-\frac{\|\mathbf{u}_h + \mathbf{u}_{r,m} - \mathbf{u}_t\|_2^2}{\sigma_h^2 + \sigma_t^2}} \right)$$
$$\mathbf{h} + \mathbf{u}_{r,m_{(h,r,t)}^*} \approx \mathbf{t}$$

- ▶ Previous studies make translation identically for all the triples of the same relation, but TransG automatically selects the best translation vector according to the specific semantics of a triple.

# TransG: A Generative Embedding Model

## ► Training Procedure.

### ► CRP Part.

$$\mathbb{P}(m_{r,new}) = \frac{\beta e^{-\frac{\|h-t\|_2^2}{\sigma_h^2 + \sigma_t^2 + 2}}}{\beta e^{-\frac{\|h-t\|_2^2}{\sigma_h^2 + \sigma_t^2 + 2}} + \mathbb{P}\{(h, r, t)\}}$$

### ► Other Parts.

$$\begin{aligned} \min \quad & - \sum_{(h,r,t) \in \Delta} \ln \left( \sum_{m=1}^{M_r} \pi_{r,m} e^{-\frac{\|u_h + u_{r,m} - u_t\|_2^2}{\sigma_h^2 + \sigma_t^2}} \right) + \\ & \sum_{(h',r',t') \in \Delta'} \ln \left( \sum_{m=1}^{M_r} \pi_{r',m} e^{-\frac{\|u_{h'} + u_{r',m} - u_{t'}\|_2^2}{\sigma_{h'}^2 + \sigma_{t'}^2}} \right) \\ & + C \left( \sum_{r \in R} \sum_{m=1}^{M_r} \|u_{r,m}\|_2^2 + \sum_{e \in E} \|u_e\|_2^2 \right) \end{aligned}$$

# TransG: A Generative Embedding Model

## ► Experiments: Link Prediction.

Datasets	WN18				FB15K			
Metric	Mean Rank		HITS@10(%)		Mean Rank		HITS@10(%)	
	Raw	Filter	Raw	Filter	Raw	Filter	Raw	Filter
TransE	263	251	75.4	89.2	243	125	34.9	47.1
TransH	401	388	73.0	82.3	212	87	45.7	64.4
TransR	238	225	79.8	92.0	198	77	48.2	68.7
CTransR	<b>231</b>	<b>218</b>	79.4	92.3	199	75	48.4	70.2
PTransE	N/A	N/A	N/A	N/A	207	58	51.4	84.6
KG2E	362	348	80.5	93.2	183	69	47.5	71.5
TransG	357	345	<b>84.5</b>	<b>94.9</b>	<b>152</b>	<b>50</b>	<b>55.9</b>	<b>88.2</b>



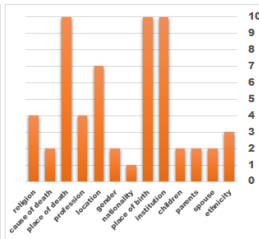
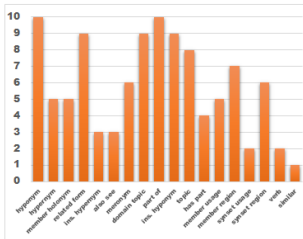
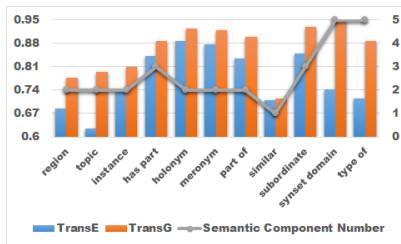
# TransG: A Generative Embedding Model

- **Experiments:** Triple Classification.

Methods	WN11	FB13	AVG.
NTN	70.4	87.1	78.8
TransE	75.9	81.5	78.7
TransH	78.8	83.3	81.1
TransR	85.9	82.5	84.2
CTransR	85.7	N/A	N/A
KG2E	85.4	85.3	85.4
TransG	<b>87.4</b>	<b>87.3</b>	<b>87.4</b>

# TransG: A Generative Embedding Model

## ► Experiments: Semantic Component Analysis.



# TransG: A Generative Embedding Model

- ▶ In this paper, we propose a generative Bayesian non-parametric infinite mixture embedding model, TransG, to address a new issue, multiple relation semantics, which can be commonly seen in knowledge graph.
- ▶ TransG can discover the latent semantics of a relation automatically and leverage a mixture of relation components for embedding.
- ▶ Extensive experiments show our method achieves substantial improvements against the state-of-the-art baselines.

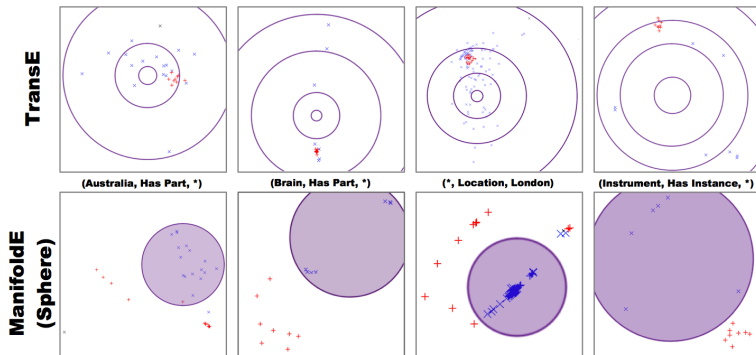
**Thanks.**

# Summaries

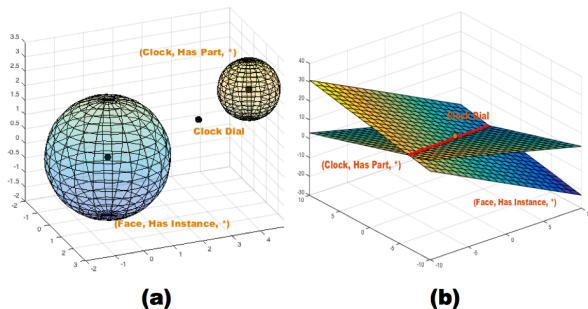
1. From the geometric perspective of **DATA**, we propose *TransG* to model multiple relation semantics.
2. From the geometric perspective of **MODEL**, we propose *ManifoldE* to achieve an algebraic well-posed system and a flexible geometric form.
3. From the geometric perspective of **INTERACTION** between texts and triples, we propose *SSP* to utilize textual descriptions.

# ManifoldE: From A Point To A Manifold

- ▶ **Precise Link Prediction** attempts to find the exact entity given another entity and the relation.
- ▶ **Motivations.**
  - ▶ Being *ill-posed algebraic system*.
    - ▶ There are  $Td$  equations ( $h_i + r_i = t_i$ ).
    - ▶ There are  $(E + R)d$  variables.
    - ▶ Since  $T \gg E + R$ , it is an *ill-posed algebraic system*.
  - ▶ Adopting *over-strict geometric form*.



# ManifoldE: From A Point To A Manifold



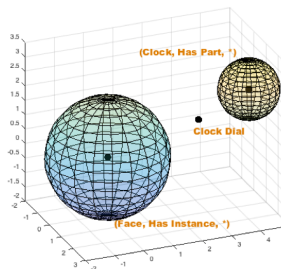
- **Methodology.** To apply the manifold-based principle:

$$\mathcal{M}(\mathbf{h}, \mathbf{r}, \mathbf{t}) = D_r^2$$

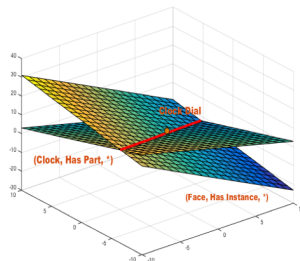
When a head entity and a relation are given, the tail entities lay in a high-dimensional manifold.

$$f_r(h, t) = \|\mathcal{M}(h, r, t) - D_r^2\|^2$$

# ManifoldE: From A Point To A Manifold



(a)



(b)

- Sphere.

$$\mathcal{M}(h, r, t) = \|\mathbf{h} + \mathbf{r} - \mathbf{t}\|_2^2$$

- Hyperplane.

$$\mathcal{M}(h, r, t) = (\mathbf{h} + \mathbf{r}_{\text{head}})^\top (\mathbf{t} + \mathbf{r}_{\text{tail}})$$

# ManifoldE: From A Point To A Manifold

## ► Geometric Perspective.

- Manifold-Based principle extends one point to a whole manifold, to strengthen the stability.
- This way would benefit complex relations.

## ► Algebraic Perspective.

- There are one equation for one triple.
- Thus, if  $d \geq \frac{T}{E+R}$ , the system is far away from ill-posed.

## ► Training.

$$\mathcal{L} = \sum_{(h,r,t) \in \Delta} \sum_{(h',r',t') \in \Delta'} [f_{r'}(h', t') - f_r(h, t) + \gamma]_+$$



# ManifoldE: From A Point To A Manifold

- **Experiments:** Link Prediction.

Datasets	WN18			
Metric	HITS@10(%)		HITS@1(%)	Time(s)
	Raw	Filter	Filter	One Epos
TransE	75.4	89.2	29.5	<b>0.4</b>
TransH	73.0	82.3	31.3	1.4
TransR	79.8	92.0	33.5	9.8
PTransE	-	-	-	-
KG2E	80.2	92.8	54.1	10.7
ManifoldE S.	80.7	92.8	55.8	<b>0.4</b>
ManifoldE H.	<b>84.2</b>	<b>94.9</b>	<b>93.2</b>	0.5

# ManifoldE: From A Point To A Manifold

► **Experiments:** Link Prediction.

Datasets	FB15K			
Metric	HITS@10(%)		HITS@1(%)	Time(s)
	Raw	Filter	Filter	One Epos
TransE	34.9	47.1	29.4	<b>0.7</b>
TransH	48.2	64.4	24.8	4.8
TransR	48.4	68.7	20.0	29.1
PTransE	51.4	84.6	63.3	266.0
KG2E	48.9	74.0	40.4	44.2
ManifoldE S.	<b>55.7</b>	86.2	64.1	<b>0.7</b>
ManifoldE H.	55.2	<b>88.1</b>	<b>70.5</b>	0.8

# ManifoldE: From A Point To A Manifold

- **Experiments:** Triple Classification.

Methods	WN11	FB13	AVG.
SE	53.0	75.2	64.1
NTN	70.4	87.1	78.8
TransE	75.9	81.5	78.7
TransH	78.8	83.3	81.1
TransR	85.9	82.5	84.2
KG2E	85.4	85.3	85.4
ManifoldE Sphere	<b>87.5</b>	87.2	<b>87.4</b>
ManifoldE Hyperplane	86.9	<b>87.3</b>	87.1

# ManifoldE: From A Point To A Manifold

- ▶ In this paper, we study the precise link prediction problem and attribute two reasons to the problem: ill-posed algebraic system and over-restricted geometric form.
- ▶ To alleviate these issues, we propose a novel manifold-based principle and a few models ManifoldE (Sphere/Hyperplane) inspired by the principle. From algebraic perspective, ManifoldE is a nearly well-posed equation system and from a geometric perspective, it expands one point in translation-based principle to a manifold.
- ▶ Extensive experiments show our method achieves substantial improvements against the state-of-the-art baselines.

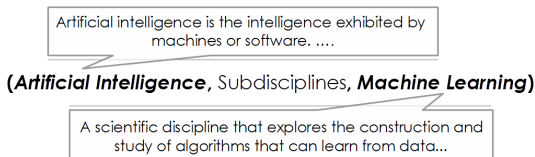
**Thanks.**

# Summaries

1. From the geometric perspective of **DATA**, we propose *TransG* to model multiple relation semantics.
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# SSP: Semantic Space Projection

- ▶ **Problem Definition** To incorporate the textual descriptions with the fact triples.

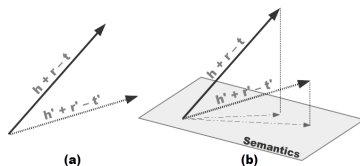


- ▶ **Motivations**
  - ▶ Discovering semantic relevance between entities.
  - ▶ Offering precise semantic expression.
- ▶ **Related Work** could not characterize the correlations.
  - ▶ Jointly:  $\mathbf{w} = \mathbf{e}$ .
  - ▶ DKRL:  $[\mathbf{e}_h, \mathbf{w}_h] \xrightarrow{r} [\mathbf{e}_t, \mathbf{w}_t]$ .

# SSP: Semantic Space Projection

- **Methodology:** Projecting the embedding procedure onto a semantic hyperplane.

$$f_r(h, t) = -\lambda ||\mathbf{e} - \mathbf{s}^\top \mathbf{e}\mathbf{s}||_2^2 + ||\mathbf{e}||_2^2$$



- **Semantic Vector Generation:** Topic Model.
- **Objectives.**

$$\begin{aligned}\mathcal{L} &= \mathcal{L}_{embed} + \mu \mathcal{L}_{topic} \\ \mathcal{L}_{embed} &= \sum_{\substack{(h, r, t) \in \Delta \\ (h', r', t') \in \Delta'}} [f_{r'}(h', t') - f_r(h, t) + \gamma]_+ \\ \mathcal{L}_{topic} &= \sum_{e \in E, w \in D_e} (C_{e,w} - \mathbf{s}_e^\top \mathbf{w})^2\end{aligned}\tag{1}$$

# SSP: Semantic Space Projection

- ▶ **Methodology:** Projecting the embedding procedure onto a semantic hyperplane.

$$f_r(h, t) = -\lambda ||\mathbf{e} - \mathbf{s}^\top \mathbf{e}\mathbf{s}||_2^2 + ||\mathbf{e}||_2^2$$

- ▶ **Correlation Perspective:** There exists the important restriction, that the entities co-occur in a triple should be embedded in the semantic space composed by the associated textual semantics.
- ▶ **Semantic Perspective:** Our model characterizes the strong correlations with a semantic hyperplane, which is capable of taking the advantages of both two semantic effects.
  - ▶ Semantic Relevance.
  - ▶ Precise Semantic Expression.



# SSP: Semantic Space Projection

- **Experiments:** Knowledge Graph Completion.

FB15K	Mean Rank		HITS@10	
TransE	210	119	48.5	66.1
TransH	212	87	45.7	64.4
Jointly	167 <sup>1</sup>	39 <sup>1</sup>	51.7 <sup>1</sup>	77.3 <sup>1</sup>
DKRL(BOW)	200	113	44.3	57.6
DKRL(ALL)	181	91	49.6	67.4
<b>SSP (Std.)</b>	<b>154</b>	<b>77</b>	57.1	78.6
<b>SSP (Joint)</b>	163	82	<b>57.2</b>	<b>79.0</b>

WN18	Mean Rank		HITS@10	
TransE	263	251	75.4	89.2
TransH	401	338	73.0	82.3
<b>SSP (Std.)</b>	204	193	81.3	91.4
<b>SSP (Joint)</b>	<b>168</b>	<b>156</b>	<b>81.2</b>	<b>93.2</b>

# SSP: Semantic Space Projection

- **Experiments:** Entity Classification.

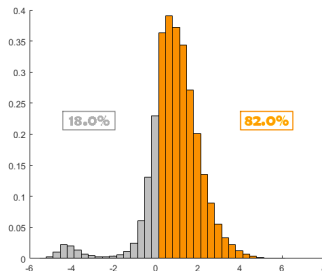
Metrics	FB15K	FB20K
TransE	87.8	-
BOW	86.3	57.5
DKRL(BOW)	89.3	52.0
DKRL(ALL)	90.1	61.9
NMF	86.1	59.6
<b>SSP (Std.)</b>	93.2	-
<b>SSP (Joint)</b>	<b>94.4</b>	<b>67.4</b>

# SSP: Semantic Space Projection

## ► Semantic Relevance Analysis

	<b>SSP(S.)<sub>#≤100</sub></b>	<b>SSP(J.)<sub>#≤100</sub></b>
<b>E<sub>#≥500</sub></b>	601	672
<b>E<sub>#≥1000</sub></b>	275	298
<b>E<sub>#≥2000</sub></b>	80	89
<b>E<sub>#≥3000</sub></b>	32	39
<b>E<sub>#≥5000</sub></b>	3	3

## ► Precise Semantic Expression Analysis



# SSP: Semantic Space Projection

## ► Conclusion.

- In this paper, we propose the knowledge graph embedding model SSP, which jointly learns from the symbolic triples and textual descriptions.
- SSP could interact the triples and texts by characterizing the strong correlations, by which means, the textual descriptions could make more effects to discover semantic relevance and offer precise semantic expression.
- Extensive experiments show our method achieves the substantial improvements against the state-of-the-art baselines.

**Thanks.**

# Summaries

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