KGC: Knowledge Graph Embedding

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Keywords: KRL, multi-relation learning and statistical relational learning;

Task

定义：将知识图谱中实体/关系的语义嵌入到低维向量空间;

关联：通过学习的向量表达使得图谱补全中链接预测的判别过程可计算;

任务分解: Representation Space + Scoring Function + Encoding Models + Auxiliary Information;

目的：在三元组构成的图谱$(h \in \boldsymbol{E}, t \in \boldsymbol{R}, r \in \boldsymbol{E})$中构建一个打分，使得真实存在的三元组分数比认为构造假的高

Simple Linear Model

TransE

$$-\|h + r - t\|$$

TransX (TranH, TranR, TransD)

$$-\|g_{r,1}(h) + r - g_{r,2}(t)\|$$

DistMult

$$< h, r, t >$$

ComplEx

$$Re(< h, r, \bar{t} >)$$

Relation

- **Symmetry / Antisymetry** (对称)

$$(h, r, t) \in G, (t, r, h) \in G$$

e.g. (A, get_married_with, B), (B, get_married_with, A)

- **Inversion** (可逆)

$$(h, r, t) \in G, (t, r^{-1}, h) \in G$$

e.g. (A, is_son_of, B), (B, is_father_of, A)

- **Composition** (组合)

$$(h, r_1, t_1), (h_n, r_n, t) \rightarrow (h, r, t)$$

e.g. (A, is_the_mother_of, B), (B, is_son_of, C) $\rightarrow$ (A, is_the_wife_of, B)

RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space. ICLR. 2019

With Score Fuction

- Symmetry / Antisymetry (对称)

$$f_r(h,t) = f_r(t,h)$$

$$f_r(h,t) \neq f_r(t,h)$$

- Inversion (可逆)

$$f_r(h,t) = f_{r^{-1}}(t,h)$$

- Composition (组合)

$$f_{r_1}(h,z) \cap f_{r_2}(z,t) => f_r(h,t)$$

Analysis-TransE

$$f_r(h,t) = -\|h + r - t\|$$

$$= -(\|h\|_2^2 + \|r\|_2^2 + \|t\|_2^2 - 2(h^T t + r^T(t-h)))$$

$$=> h^T t + r^T(t-h)$$

- 推得：$-r = r$。当且仅当r=0时，满足对称关系约束，因此TransE并不能有区分地建模任一对称关系；其他关系都能够建模。
- 推得：$-r_1 = r_2$。能够满足可逆关系
- 推得：$h + (r_1 + r_2) = t$。能够满足组合关系

Analysis-DistMult

$$f_r(h,t) = h^T M_r t$$

- 明显的，总存在$h^T M_r t = t^T M_r h$。因此表示对称关系，无法描述非对称关系和可逆关系。
- 往往会将h, t限制为标准向量，则有$h^T M_r t \approx 1 => h^T M_r \approx t^T$, 因此有$h^T M_{r_1} \approx z^T, z^T M_{r_2} \approx t^T => h^T M_{r_1} M_{r_2} \approx t^T$, 能够描述组合关系。

Analysis

Method	Score Function	Symmetry	Anti-	Inversion	Composition
TransE	$-\|h+r-t\|$	X	O	O	O
TransX	$-\|g_{r,1}(h)+r-g_{r,2}(t)\|$	O	O	X	X
DistMult	$< h,r,t >$	O	X	X	O
ComplEx	$Re(< h,r,\bar{t} >)$	O	O	O	X

DistMult原文与RotatE表格有冲突

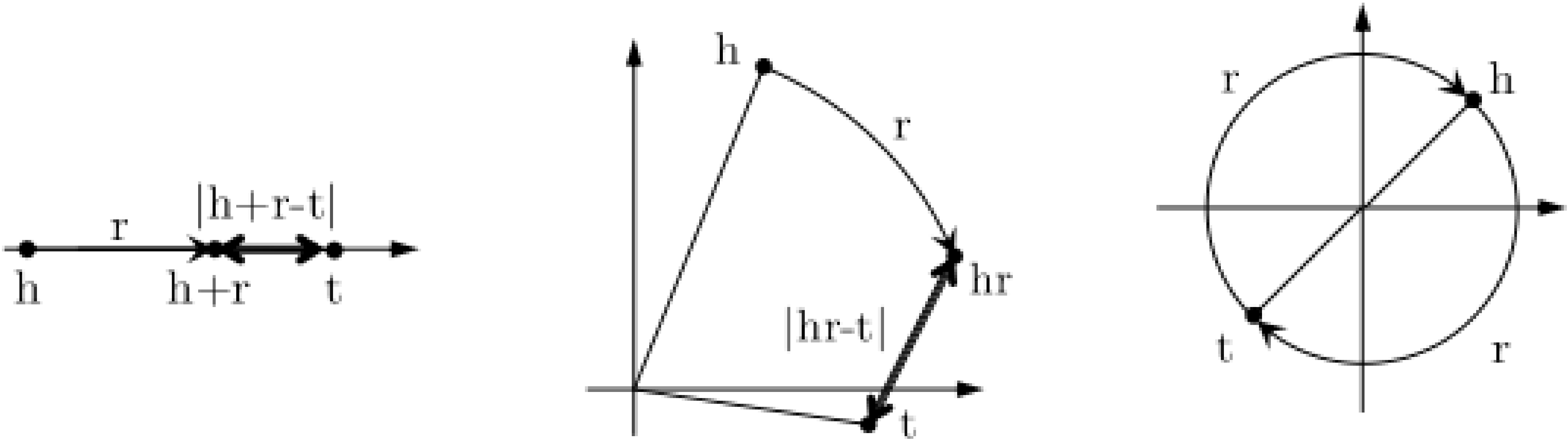
RotatE

$$t = h \circ r, where\ |ri| = 1,$$

- r 是对称关系时，当且仅当r的每一个分量 r_i 满足：$r_i = e^{0/i\pi} = \pm 1$；
- 两个关系r1和r2是逆关系时，当且仅当他们的嵌入是共轭向量：$r_2 = \bar{r}_1$；
- 某个关系 $r_3 = e^{i\theta_3}$ 是其他两个关系 $r_1 = e^{i\theta_1}$ 和 $r_2 = e^{i\theta_2}$ 的组合时，当且仅当 $r_3 = r_1 \circ r_2$ (即，$\theta_3 = \theta_1 + \theta_2$).

RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space. ICLR. 2019

Visualization



(a) TransE models $\mathbf{r}$ as translation in real line.

(b) RotatE models $\mathbf{r}$ as rotation in complex plane.

(c) RotatE: an example of modeling symmetric relations $\mathbf{r}$ with $r_i = -1$

Figure 1: Illustrations of TransE and RotatE with only 1 dimension of embedding.

RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space. ICLR. 2019

TuckER

$$W \times_1 h \times_2 r \times_3 h$$

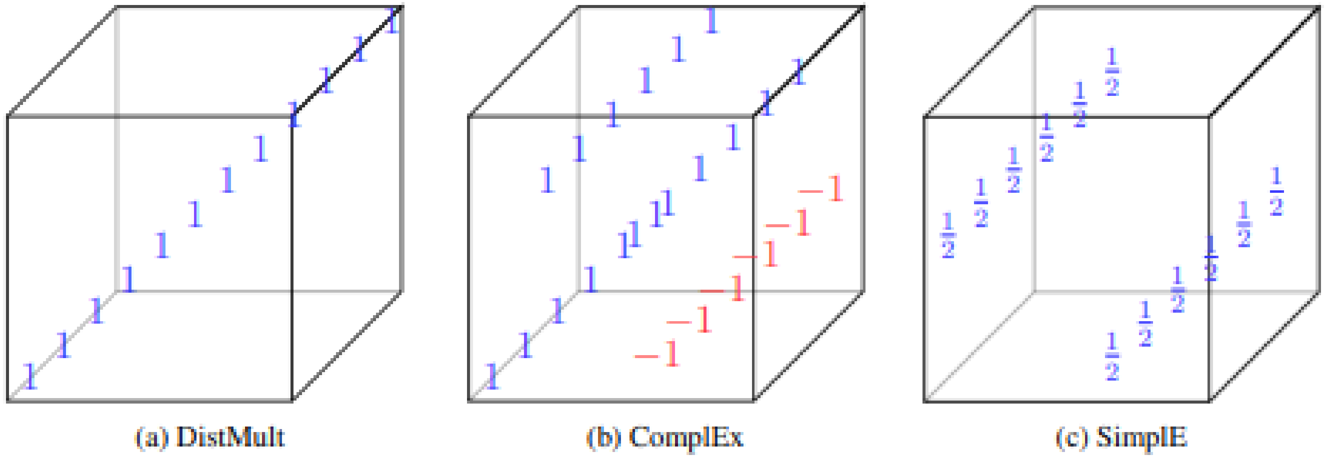


Figure 2: Constraints imposed on the values of core tensor $\mathcal{Z} \in \mathbb{R}^{d_e \times d_e \times d_e}$ for DistMult and $\mathcal{Z} \in \mathbb{R}^{2d_e \times 2d_e \times 2d_e}$ for ComplEx and SimplE. Elements that are set to 0 are represented in white.

NN-Based Method

ConvE

$$f(vec(f([h;r]*w))W)t$$

ConvKB

$$cat(f([h;r;t]*w))W$$

SACN

$$f(vec(M(h,t))W)t$$

HypER

$$f(vec(h*vec^{-1}(rH))W)t$$

其中，$*$为卷积操作，$vec(.)$为reshape为向量,[; ;]为向量拼接

Inference

	WN18RR					FB15k-237				
	MR	MRR	H@10	H@3	H@1	MR	MRR	H@10	H@3	H@1
TransE	3384	.226	.501			357	.294	.465		
DistMult	5110	.430	.490	.440	.390	254	.241	.419	.263	.155
ComplEx	5261	.440	.510	.460	.410	339	.247	.428	.275	.158
RotatE	–	–	–	–	–	**185**	.297	.480	.328	.205
TuckER		.470	.526	.482	.443		.358	.544	.394	.266
ConvE	**4187**	.430	.520	.440	.400	244	.325	.501	.356	.237
HypER	5798	**.465**	**.522**	**.477**	**.436**	250	**.341**	**.520**	**.376**	**.252**

Others

A. '1v1' versus '1vN'

- Faster Inferene
- FROM Ranking-based loss TO Multi-Label Classification

B. Unified Strategy