Knowledge Graph Representation

From Recent Models towards a Theoretical Understanding

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January 27, 2021

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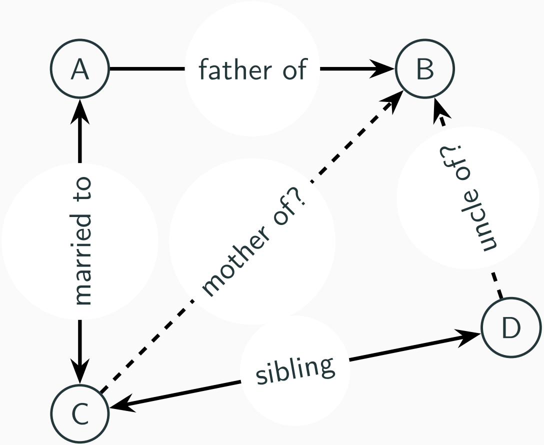
What are Knowledge Graphs?



Entities	$\mathcal{E} = \{A, B, C, D\}$
Relations	$\mathcal{R} = \{\textit{married to}, \textit{father of}, \textit{uncle of}, ...\}$
Knowledge Graph	$\mathcal{G} = \{(A, \textit{father of}, B), (A, \textit{married to}, C), ...\}$

Representing Entities and Relations

Subject and object entities e_s, e_o are represented by **vectors** $\mathbf{e}_s, \mathbf{e}_o \in \mathbb{R}^d$ (embeddings).

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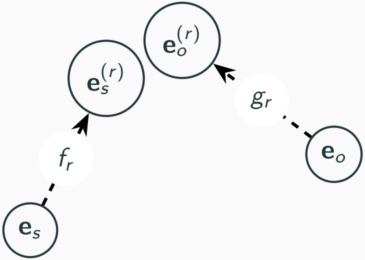

(Edinburgh, capital_of, Scotland)

Score Function

A **score function** $\phi : \mathcal{E} \times \mathcal{R} \times \mathcal{E} \to \mathbb{R}$ brings together entity, relation representations and proximity measure to assign a score $\phi(e_s, r, e_o)$ to each triple, used to predict whether the triple is true or false.

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Rel. Repr. Type	**Example $\phi(e_s, r, e_o)$**	**Model**
Multiplicative	$\mathbf{e}_s^\top \mathbf{W}_r \mathbf{e}_o = \langle \mathbf{e}_s^{(r)}, \mathbf{e}_o \rangle$	DistMult (Yang et al., 2015) TuckER (Balažević et al., 2019b)
Additive	$-\|\mathbf{e}_s + \mathbf{r} - \mathbf{e}_o\|^2$	TransE (Bordes et al., 2013)
Both	$-\|\mathbf{e}_s^\top \mathbf{W}_r^s + \mathbf{r} - \mathbf{e}_o^\top \mathbf{W}_r^o\|^2 + b_s + b_o$	MuRE (Balažević et al., 2019a)

TuckER: Tensor Factorization for Knowledge Graph Completion

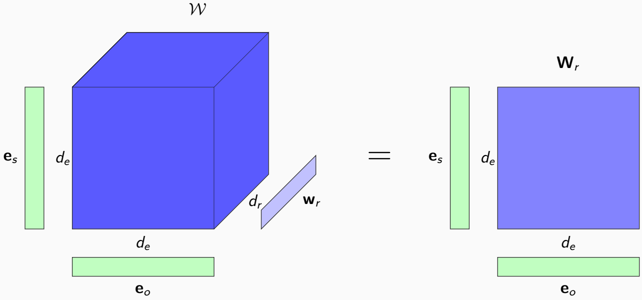

Figure 1: Visualization of the TuckER architecture.

$$\phi_{\text{TuckER}}(e_s, r, e_o) = ((\mathcal{W} \times_1 \mathbf{w}_r) \times_2 \mathbf{e}_s) \times_3 \mathbf{e}_o = \mathbf{e}_s^\top \mathbf{W}_r \mathbf{e}_o$$

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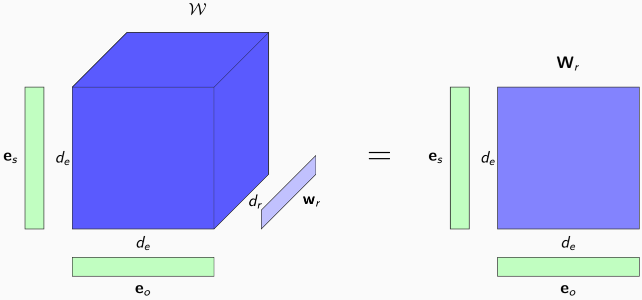

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Multi-task learning: Rather than learning distinct relation matrices $\mathbf{W}_r$, the core tensor $\mathcal{W}$ contains a shared pool of "prototype" relation matrices that are linearly combined using parameters of the relation embedding $\mathbf{w}_r$.

(Balažević et al., 2019a)

MuRE: Multi-relational Euclidean Graph Embeddings

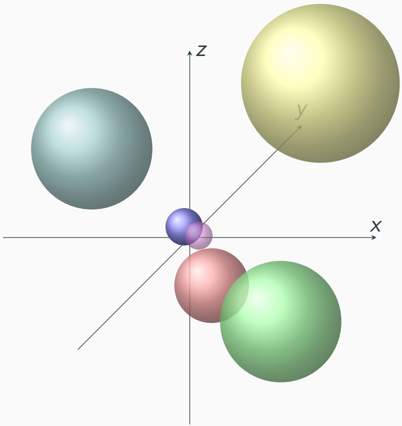

Figure 2: MuRE spheres of influence.

$$\phi_{\text{MuRE}} = -d(\mathbf{R}\mathbf{e}_s, \mathbf{e}_o + \mathbf{r})^2 + b_s + b_o$$

(Balažević et al., 2019b)

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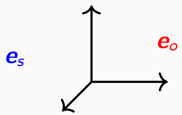

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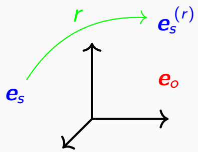

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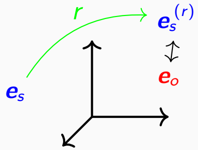

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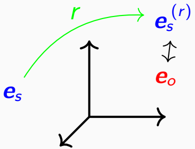

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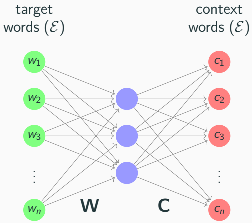

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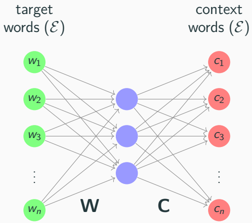

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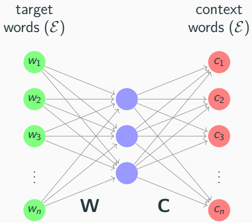

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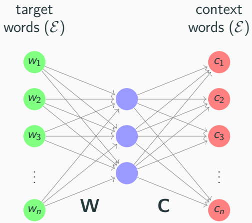

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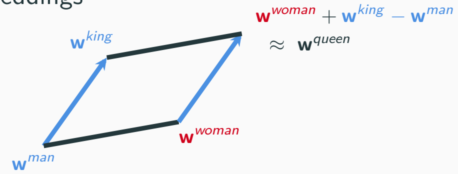
  - **similar** words $\Rightarrow$ close embeddings
  - **analogies** (often) $\Rightarrow$



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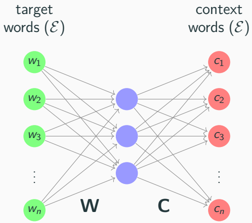

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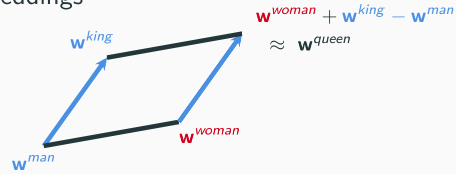

- **Aim**: relate the understanding of this to knowledge graph relations

Understanding word embeddings: the W2V Loss Function

$$-\ell_{W2V} = \sum_{i,j} \#(w_i, c_j) \log \sigma(\mathbf{w}_i^\top \mathbf{c}_j) + \frac{k\#(w_i)\#(c_j)}{D} \log(\sigma(-\mathbf{w}_i^\top \mathbf{c}_j))$$

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$\Rightarrow$ Embedding $\mathbf{w}_i$ is a (non-linear) projection of row i of the PMI matrix*, a **PMI vector** $\mathbf{p}^i$.

(* drop k term as artefact of the W2V algorithm.)

PMI Vectors

$$\mathbf{p}^i \;=\; \left\{\log \frac{p(c_j|w_i)}{p(c_j)}\right\}_{c_j \in \mathcal{E}} \;=\; \log \frac{p(\mathcal{E}|w_i)}{p(\mathcal{E})} \qquad (\mathcal{E} = \text{dictionary of all words})$$

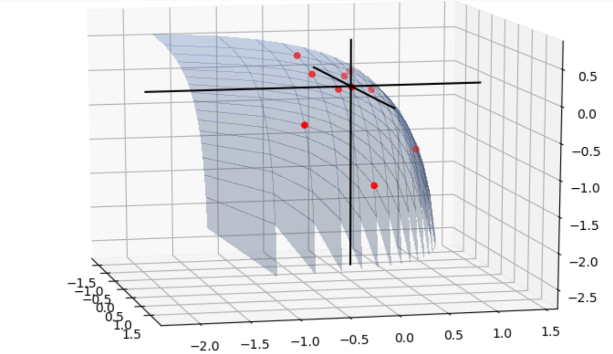

Figure 3: The PMI surface $\mathcal{S}$ with example PMI vectors of words (red dots)

PMI Vector Interactions = Semantics (Similarity)

Similarity: similar words, e.g. synonyms, induce similar distributions, $p(\mathcal{E}|w)$, over context words.

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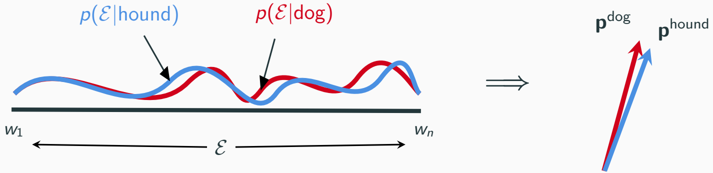

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&= \mathbf{p}^k + \underbrace{\underbrace{\log \frac{p(\mathcal{E}|w_i,w_j)}{p(\mathcal{E}|w_k)}}_{\rho^{\{i,j\},k}}}_{\text{paraphrase error}} - \underbrace{\underbrace{\log \frac{p(w_i,w_j|\mathcal{E})}{p(w_i|\mathcal{E})p(w_j|\mathcal{E})}}_{\boldsymbol{\sigma}^{i,j}} + \underbrace{\log \frac{p(w_i,w_j)}{p(w_i)p(w_j)}}_{\tau^{i,j}}}_{\text{independence error}}
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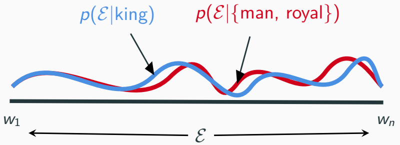

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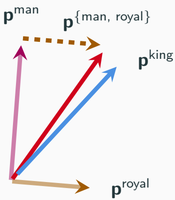

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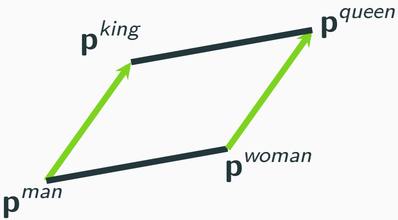
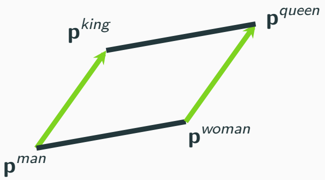


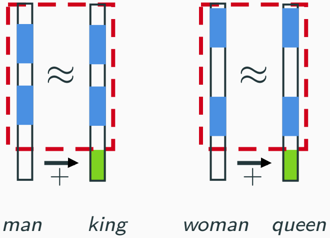
(Allen and Hospedales, 2019; Allen et al., 2019)

From Analogies to Relations



Analogy

⇔



Relation

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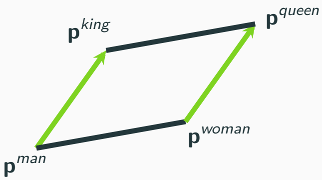

Analogy

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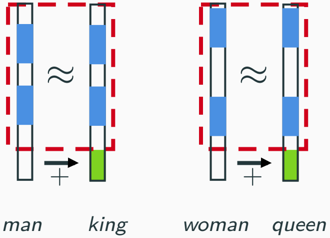
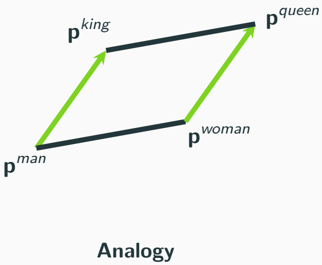


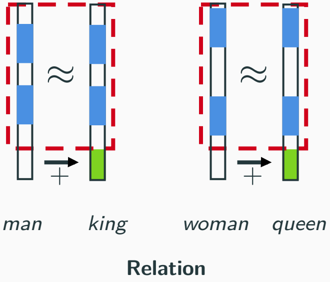
Relation

- Analogies contain common **binary word relations**, similar to KGs.

From Analogies to Relations



$\Leftrightarrow$



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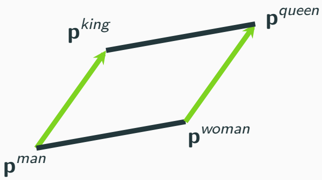

Analogy

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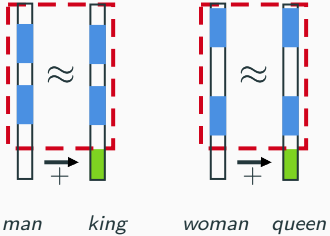
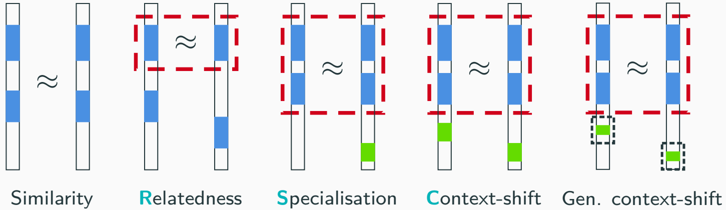


Relation

- Analogies contain common **binary word relations**, similar to KGs.
- For certain analogies ("specialisations"), the associated "vector offset" gives a **transformation that represents the relation**.
- Not all relations fit this semantic pattern, but we have insight to consider geometric aspects (**relation conditions**) of other relation types.

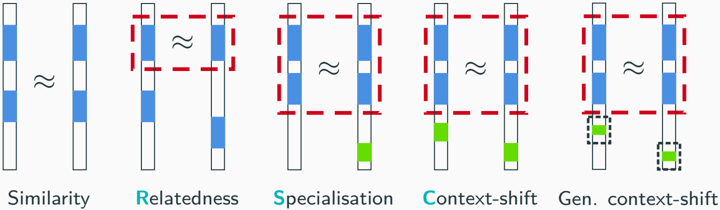
Categorising Relations: semantics → relation requirements



Relationships between PMI vectors for different relation types.

blue/green = strong word association (PMI$>$ 0); red = relatedness; black = context sets

Categorising Relations: semantics → relation requirements



Relationships between PMI vectors for different relation types.
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Categorisation of WN18RR relations.

Type	Relation	Examples *(subject entity, object entity)*
R	verb_group	*(trim_down_VB_1, cut_VB_35)*, *(hatch_VB_1, incubate_VB_2)*
	derivationally_related_form	***(lodge_VB_4, accommodation_NN_4)***, *(question_NN_1, inquire_VB_1)*
	also_see	*(clean_JJ_1, tidy_JJ_1)*, *(ram_VB_2, screw_VB_3)*
S	hypernym	*(land_reform_NN_1, reform_NN_1)*, *(prickle-weed_NN_1, herbaceous_plant_NN_1)*
	instance_hypernym	***(yellowstone_river_NN_1, river_NN_1)***, *(leipzig_NN_1, urban_center_NN_1)*
C	member_of_domain_usage	*(colloquialism_NN_1, figure_VB_5)*, *(plural_form_NN_1, authority_NN_2)*
	member_of_domain_region	***(rome_NN_1, gladiator_NN_1), (usa_NN_1, multiple_voting_NN_1)***
	member_meronym	*(south_NN_2, sunshine_state_NN_1)*, *(genus_carya_NN_1, pecan_tree_NN_1)*
	has_part	*(aircraft_NN_1, cabin_NN_3)*, *(morocco_NN_1, atlas_mountains_NN_1)*
	synset_domain_topic_of	*(quark_NN_1, physics_NN_1)*, *(harmonize_VB_3, music_NN_4)*

Categorical completeness: are all relations covered?

- View PMI vectors as *sets of word features* and **relation types as set operations**:
  - similarity $\Rightarrow$ set equality
  - relatedness $\Rightarrow$ subset equality (relation-specific)
  - context-shift $\Rightarrow$ set difference (relation-specific)

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  - irrelevant.

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- **Conjecture**: the relation types identified partition the set of semantic relations.

Relations as mappings between embeddings

R: $\mathcal{S}$-relatedness requires both entity embeddings $\boldsymbol{e}_s, \boldsymbol{e}_o$ to share a common subspace component $\mathbb{V}_{\mathcal{S}}$

- project onto $\mathbb{V}_{\mathcal{S}}$ (multiply by matrix $\boldsymbol{P}_r \in \mathbb{R}^{d\times d}$) and compare.
- Dot product: $(\boldsymbol{P}_r\boldsymbol{e}_s)^\top(\boldsymbol{P}_r\boldsymbol{e}_o) = \boldsymbol{e}_s^\top\boldsymbol{P}_r^\top\boldsymbol{P}_r\boldsymbol{e}_o = \boldsymbol{e}_s^\top\boldsymbol{M}_r\boldsymbol{e}_o$
- Euclidean distance: $\|\boldsymbol{P}_r\boldsymbol{e}_s - \boldsymbol{P}_r\boldsymbol{e}_o\|^2 = \|\boldsymbol{P}_r\boldsymbol{e}_s\|^2 - 2\boldsymbol{e}_s^\top\boldsymbol{M}_r\boldsymbol{e}_o + \|\boldsymbol{P}_r\boldsymbol{e}_o\|^2$

S/C: requires $\mathcal{S}$-relatedness and relation-specific component(s) ($\boldsymbol{v}_r^s$, $\boldsymbol{v}_r^o$).

- project onto a subspace (by $\boldsymbol{P}_r \in \mathbb{R}^{d\times d}$) corresponding to $\mathcal{S}$, $\boldsymbol{v}_r^s$ and $\boldsymbol{v}_r^o$ (i.e. test $\mathcal{S}$-relatedness while preserving relation-specific components);
- add relation-specific $\boldsymbol{r} = \boldsymbol{v}_r^o - \boldsymbol{v}_r^s \in \mathbb{R}^d$ to transformed embeddings.
- Dot product: $(\boldsymbol{P}_r\boldsymbol{e}_s + \boldsymbol{r})^\top\boldsymbol{P}_r\boldsymbol{e}_o$
- Euclidean distance: $\|\boldsymbol{P}_r\boldsymbol{e}_s + \boldsymbol{r} - \boldsymbol{P}_r\boldsymbol{e}_o\|^2$ (*cf* **MuRE**: $\|\boldsymbol{R}\boldsymbol{e}_s + \boldsymbol{r} - \boldsymbol{e}_o\|^2$)

Summary

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Summary

- **Theoretic**: a derivation of geometric components of relation representations from word co-occurrence statistics.

- **Interpretability**: associates geometric model components with semantic aspects of relations.

- **Empirically supported**: justifies relative link-prediction performance of a range of models on real datasets:

$$\underbrace{\textbf{additive \& multiplicative}}_{\text{MuRE* (Balažević et al., 2019a)}} \quad > \quad \underbrace{\textbf{multiplicative}}_{\substack{\text{TuckER (Balažević et al., 2019b)} \\ \text{DistMult (Yang et al., 2015)}}} \quad \textit{or} \quad \underbrace{\textbf{additive}}_{\text{TransE (Bordes et al., 2013)}}$$

*Note: MuRE was inspired by the vector offset of analogies.

Thanks!

Any questions?

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