Foundation for NeSy: Translational Distance KGE Models

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CS7820: Neurosymbolic AI
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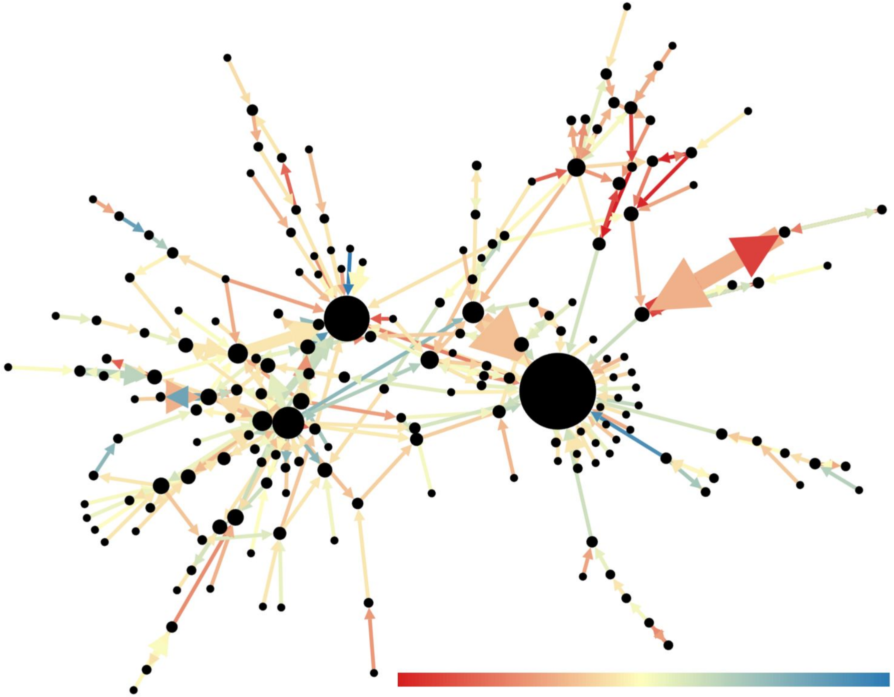
What We Know

CS7810: Graphical Representation of Data

CS7830: Machine Learning Models and Techniques



As presented by NeSy 2023:

1. **Knowledge representation** and **reasoning** using **deep neural networks**;
2. Symbolic **knowledge extraction** from neural and statistical learning systems;
3. **Explainable AI** methods, systems and techniques integrating connectionist and symbolic AI;
4. **Enhancing deep learning** systems **through structured** background knowledge.
5. Neurosymbolic cognitive agents;
6. Biologically-inspired **neurosymbolic integration**;
7. **Integration of logics** and **probabilities** in **neural networks**;
8. **Neurosymbolic** methods for **structure learning, transfer learning, meta, multi-task and continual learning, relational learning**;
9. Novel connectionist systems able to perform traditionally symbolic AI tasks (e.g. abduction, deduction, out-of-distribution learning);
10. Novel symbolic systems able to perform traditionally connectionist tasks (e.g. learning from unstructured data, distributed learning);
11. **Embedding methods** for **structured information**, such as knowledge graphs, mathematical expressions, grammars, knowledge bases, logical theories, etc.
12. **Applications of neurosymbolic** and hybrid systems, including in simulation, finance, healthcare, robotics, semantic web, software engineering, systems engineering, bioinformatics and visual intelligence.

Reading from WSU Researcher, Amit Sheth: https://arxiv.org/abs/2305.00813

Timeline

Introduction to KGE

Translational Distance KGE Models

- TransE, TransR, TransH, RotatE

For each model:

- A Use-Case
- Scoring Function

Understanding Evaluation Metrics

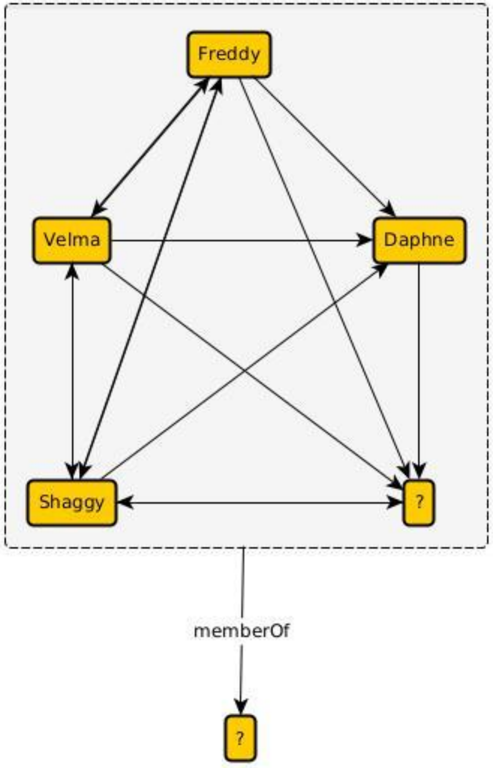
Overall Research Continuation

- Semantic Matching Models

Knowledge Graph Embedding

Integrating a KG (the set of triples) into a vector plane

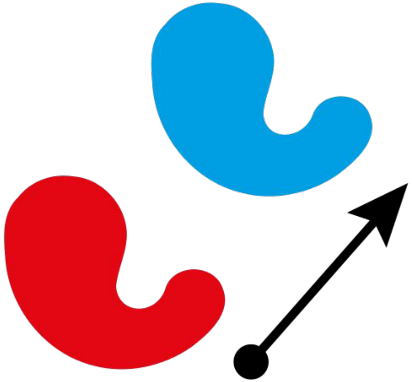
- Inferring “facts” from the KG
- Discovering new triples
- Completing missing links
- Analyzing clusterability



Translational Distance

- These models rely on geometric translations for KGE
- As stated in the TransH paper:

  "[K]nowledge graph embedding represents an entity as a k-dimensional vector h (or t) and defines a scoring function $f_r(h, t)$ to measure the plausibility of the triplet (h, r, t) in the embedding space. The score function implies a transformation r on the pair of entities which characterizes the relation r."



- Entity E1 exists at position (x,y)
- Relationship R1 modifies position by (x+a, y+b)
- What Entity E2 also exists at (x+a, y+b)?

Common Connectivity Patterns

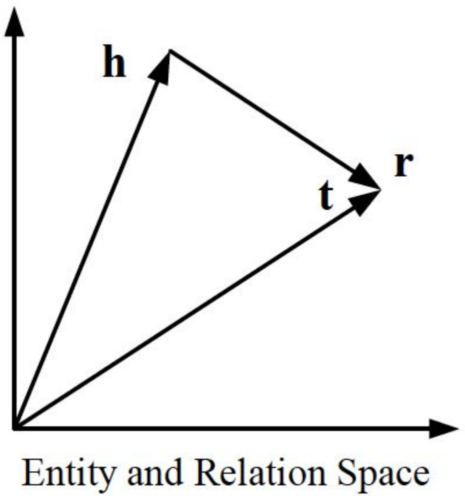
- Symmetric
- Anti-Symmetry
- Inversion
- Composition
- Cardinality Relationships (1-to-1, m-to-n)

TransE (2013)

Use-Case

- Handles 1-to-1 entity matching problems wrt. Head, Relationship, and Tail
- The scoring function can be used to answer what head entity and tail entity is with respect to a relationship that applies translation
- Represents Entities and Relationships on a *single* Embedding Space

Scoring Function (h,r,t) = (h+r-t)

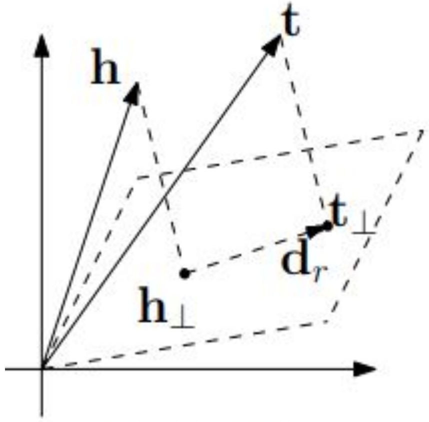


TransH (2014)

Scoring Function:
$\| (h - w_r^T h w_r) + d_r - (t - w_r^T t w_r) \|$
where d_r is a translation vector, and w_r is a norm vector

Use-Case

- distributed representation of entities across different relations
- implements a hyperplane of existence that allows for the relationship-specific translation on entities
    - relationship-specific allows for coverage of more broad representation



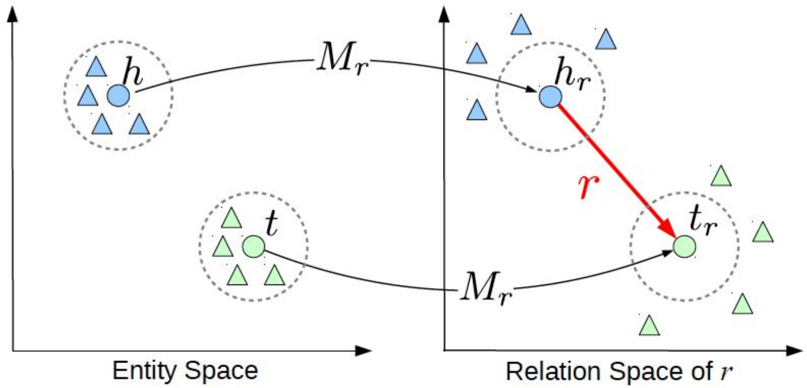
(b) TransH

TransR (2015)

Use-Case

- Handles m-to-n
- Maps entity-space and relationship-space to their own respective vector spaces.
- Provides capabilities to now represent various relationship r's affect between entity and tail

Scoring Function (h,r,t) = (h_r+r-t_r)

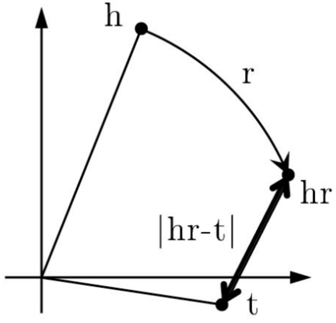


RotatE (2019)

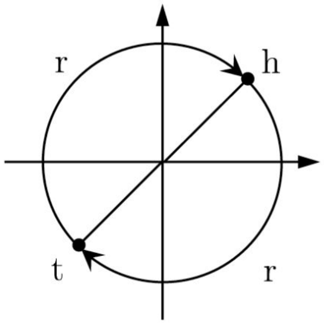
Use-Case

- Each relation represented as a rotation from the head entity to a tail entity
- Rotational Representation also allows for:
    - symmetry/antisymmetry, inversion, and composition

Scoring Function (h,r,t) = $\| h \circ r - t \|$



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



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

Evaluation Metrics

Hits@K: The correct results show up in the first *k*-options

Mean Rank: Average Ordinal Ranking across all elements of the KGE

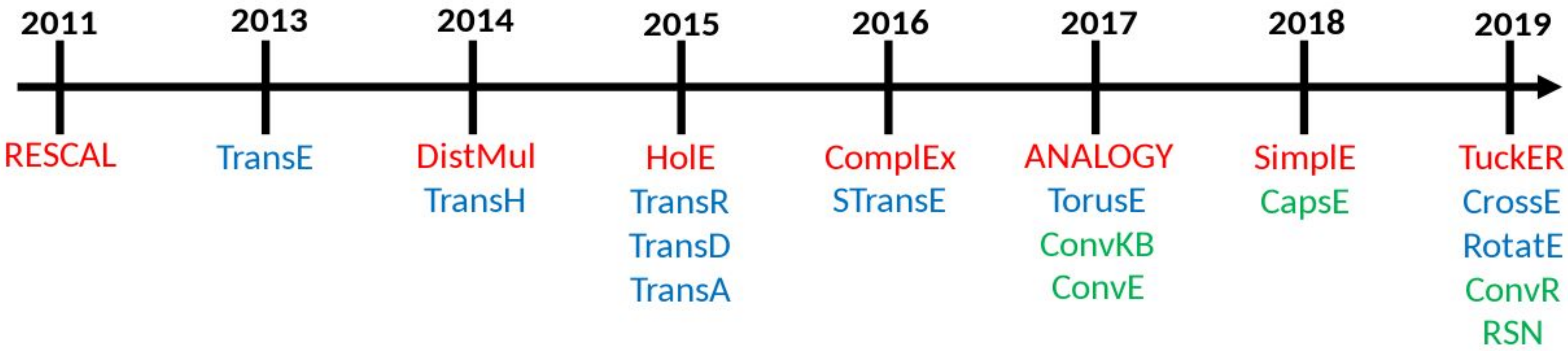
Mean Reciprocal Rank: How likely is it, the correct option appears in the first, second, third, … nth place?

In Summary

Models	score function $f(\mathbf{h}, \mathbf{r}, \mathbf{t})$
TransE [2]	$-\|\|\mathbf{h} + \mathbf{r} - \mathbf{t}\|\|_{1/2}$
TransR [10]	$-\|\|M_r \mathbf{h} + \mathbf{r} - \mathbf{M_r t}\|\|_2^2$
DistMult [20]	$\mathbf{h}^\top \mathrm{diag}(\mathbf{r})\mathbf{t}$
ComplEx [16]	$\mathrm{Real}(\mathbf{h}^\top \mathrm{diag}(\mathbf{r})\bar{\mathbf{t}})$
RESCAL [12]	$\mathbf{h}^\top \mathbf{M_r t}$
RotatE [15]	$-\|\|\mathbf{h} \circ \mathbf{r} - \mathbf{t}\|\|^2$

Method	symm	Anti	Inv	Comp
TransE	–	✓	✓	–
TransR	–	✓	✓	✓
RESCAL	✓	–	✓	✓
DistMulti	✓	–	–	–
ComplEx	✓	✓	✓	–
RotateE	✓	✓	✓	✓

In Summary



2011
RESCAL
2013
TransE
2014
DistMul
TransH
2015
HolE
TransR
TransD
TransA
2016
ComplEx
STransE
2017
ANALOGY
TorusE
ConvKB
ConvE
2018
SimplE
CapsE
2019
TuckER
CrossE
RotatE
ConvR
RSN

Semantic Matching

Questions that continue the research for KGE:

- How can we integrate KGE with AI to understand and represent semantics? (synonyms/antonyms, defining contextual meanings and word associations)
  - What relationship can be inferred if an AI is presented “cat” and “mouse”?

References

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