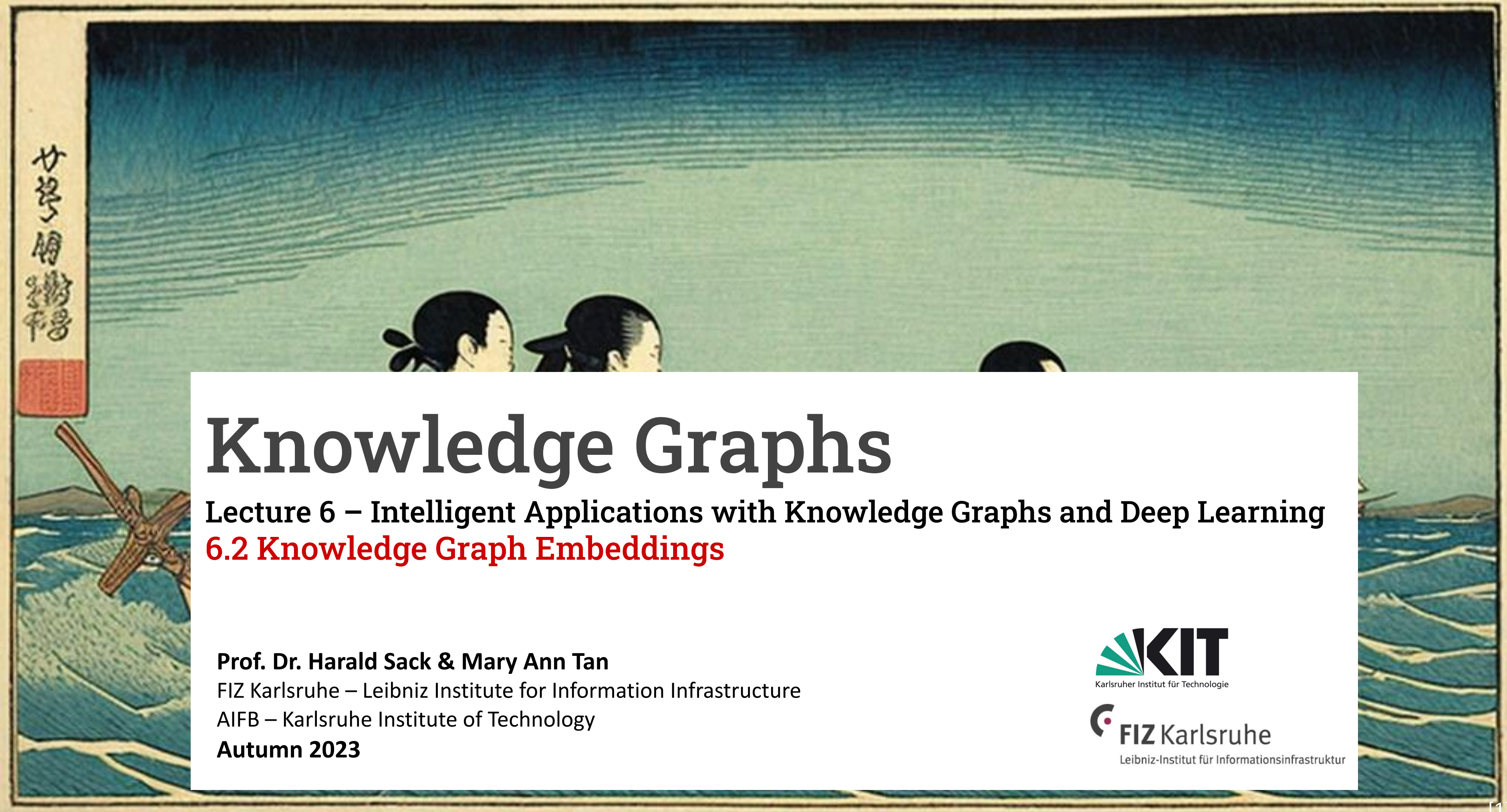

Knowledge Graphs

Lecture 6 – Intelligent Applications with Knowledge Graphs and Deep Learning

6.2 Knowledge Graph Embeddings

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FIZ Karlsruhe – Leibniz Institute for Information Infrastructure
AIFB – Karlsruhe Institute of Technology
Autumn 2023

Karlsruher Institut für Technologie

FIZ Karlsruhe
Leibniz-Institut für Informationsinfrastruktur

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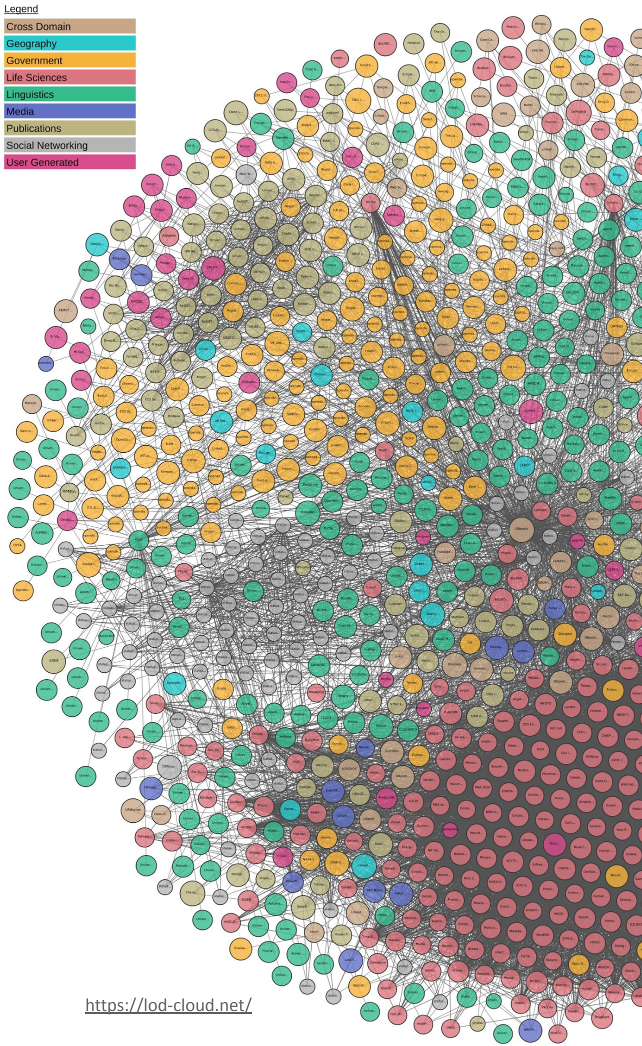
Semantic Similarity

From Words to Entities

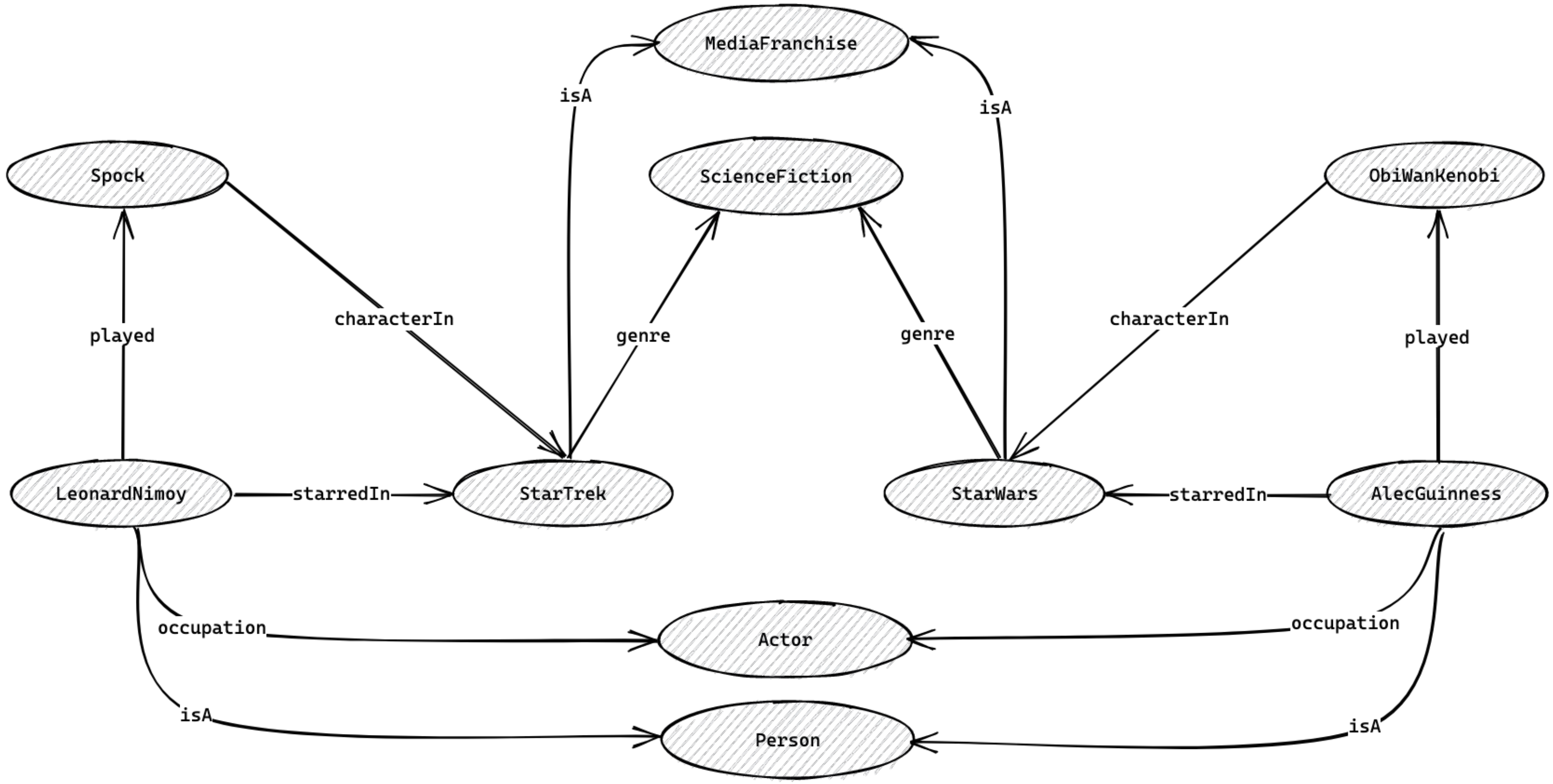
- For **Word Embeddings**, words with similar meanings are mapped to adjacent vectors in a (dense) vector space.
- How can we adapt this concept to (Knowledge) Graphs?
- **When are two nodes (entities) semantically similar?**
  If they can be described by the same/similar facts, e.g.
  - Star wars is a SciFi media franchise and Star Trek is a SciFi media franchise.
  - Alec Guinness is a Person who is an Actor and Leonard Nimoy is a Person who is an Actor.
  - **Is Star wars more similar to Star Trek or to Leonard Nimoy?**



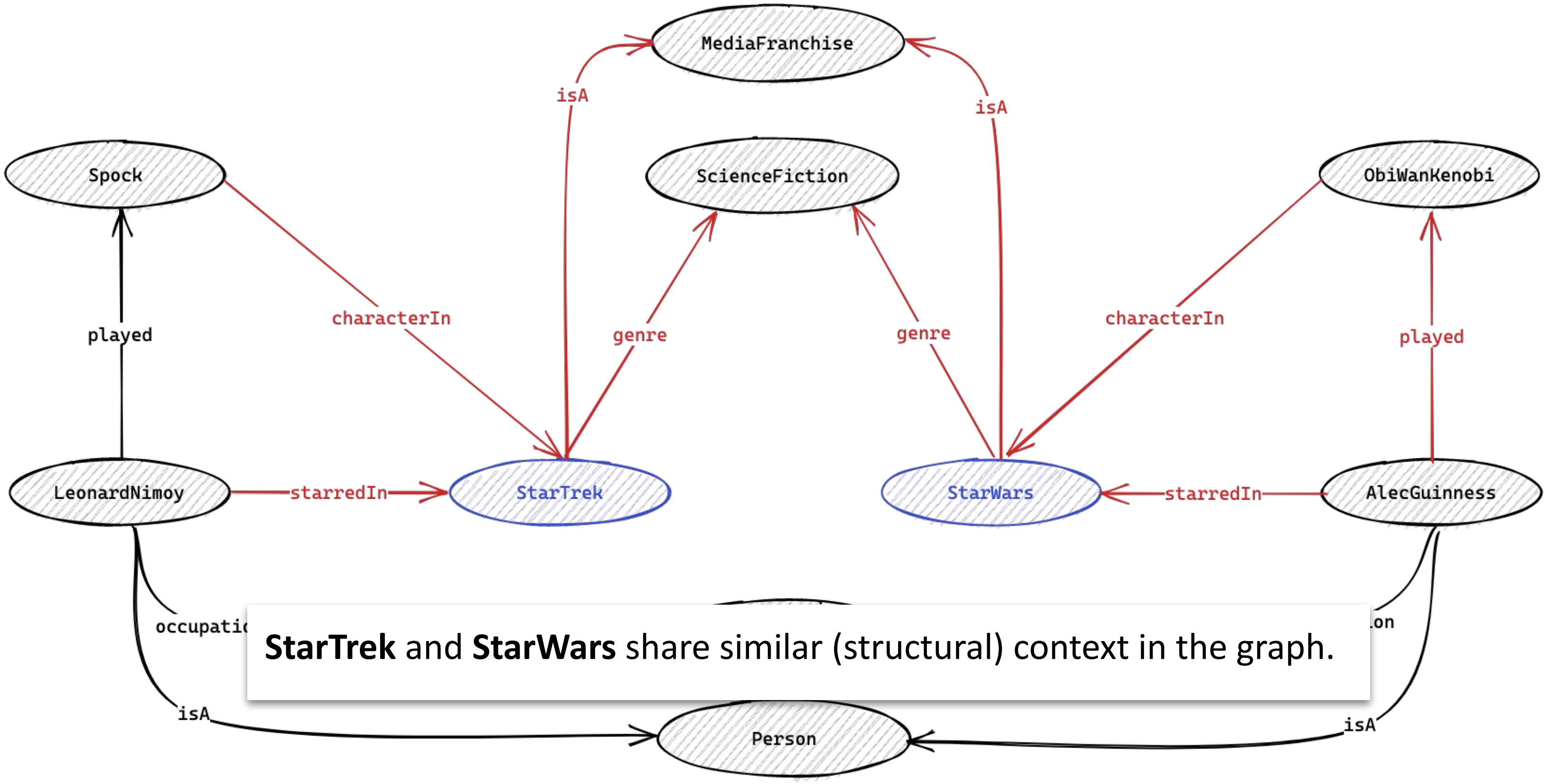
https://lod-cloud.net/

The Linked Open Data Cloud from lod-cloud.net

Semantic Similarity



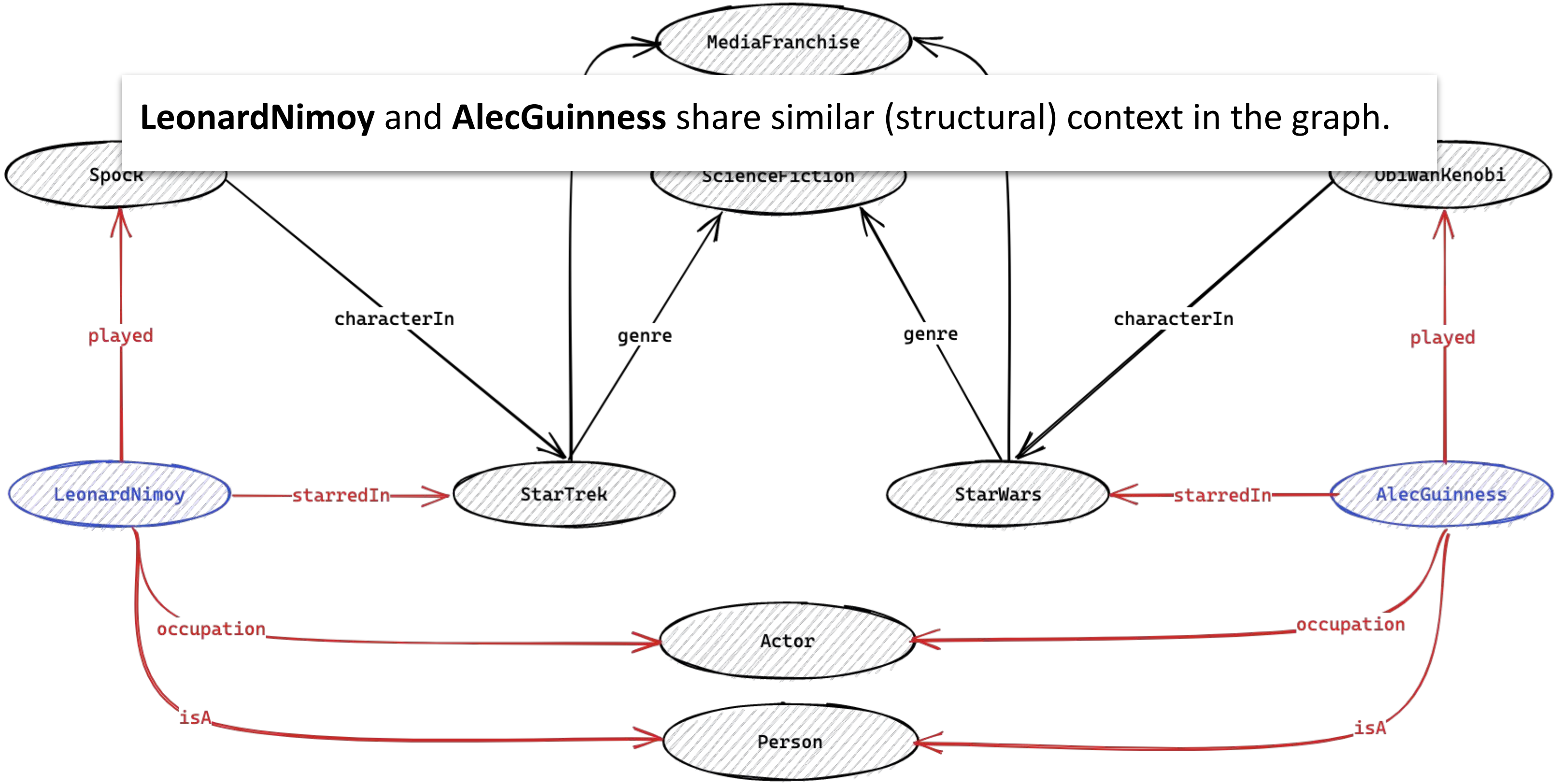
Semantic Similarity



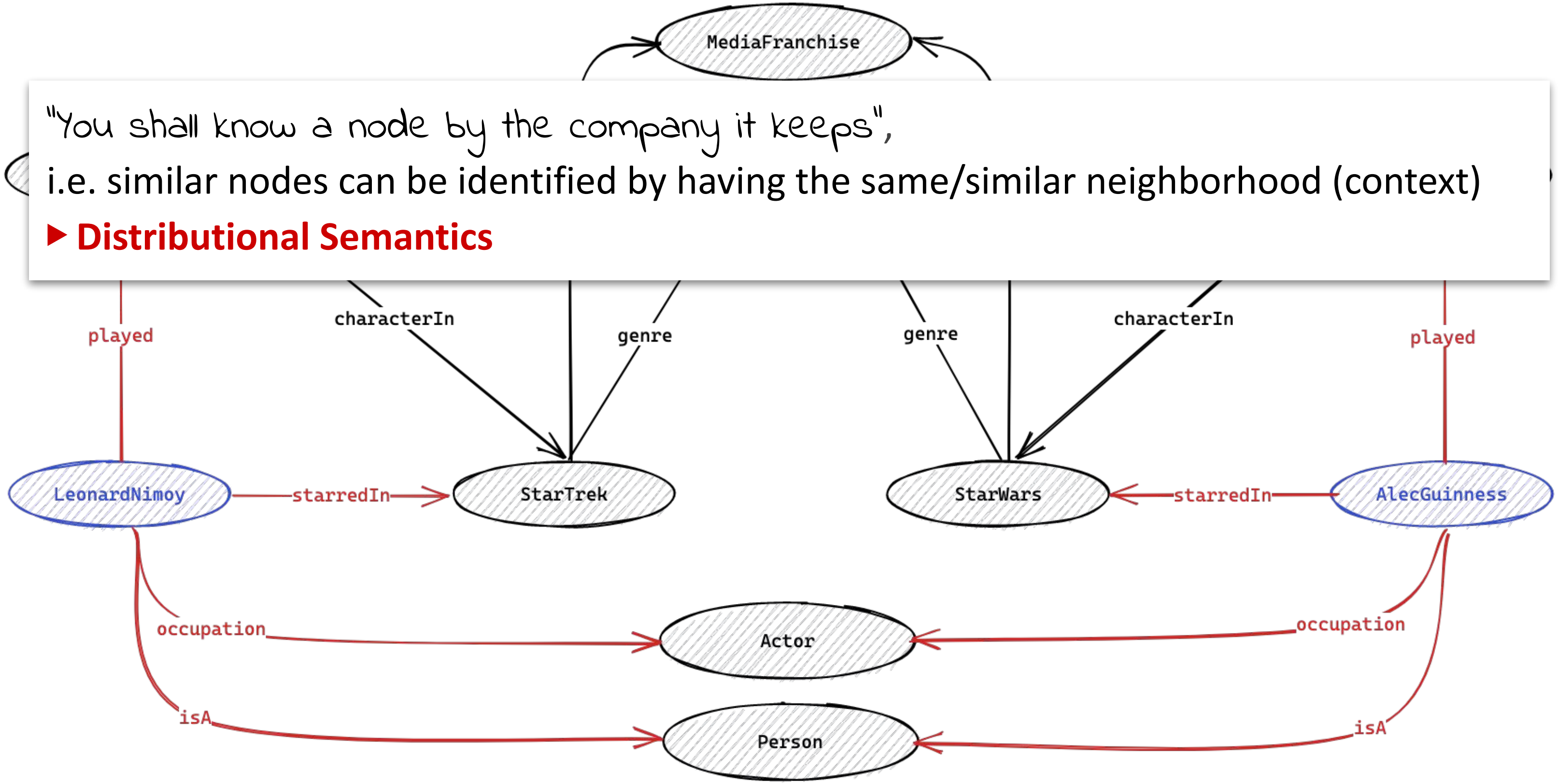
StarTrek and **StarWars** share similar (structural) context in the graph.

Semantic Similarity

LeonardNimoy and **AlecGuinness** share similar (structural) context in the graph.



Semantic Similarity

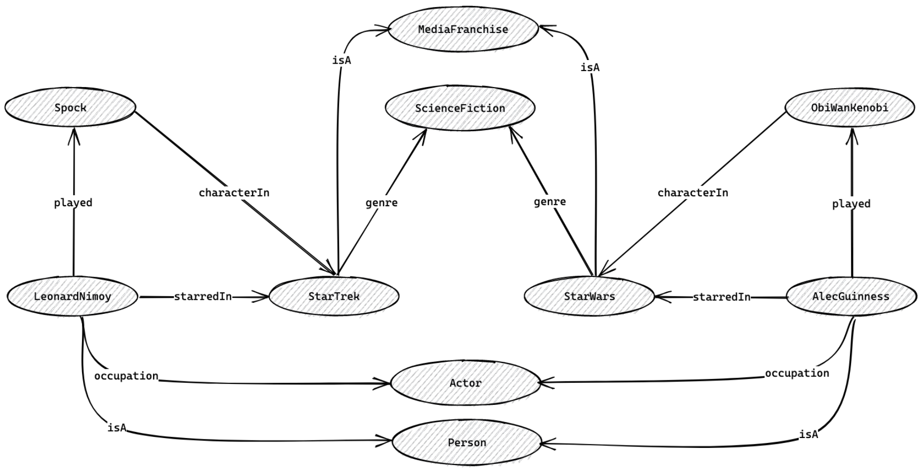


"You shall know a node by the company it keeps",
i.e. similar nodes can be identified by having the same/similar neighborhood (context)

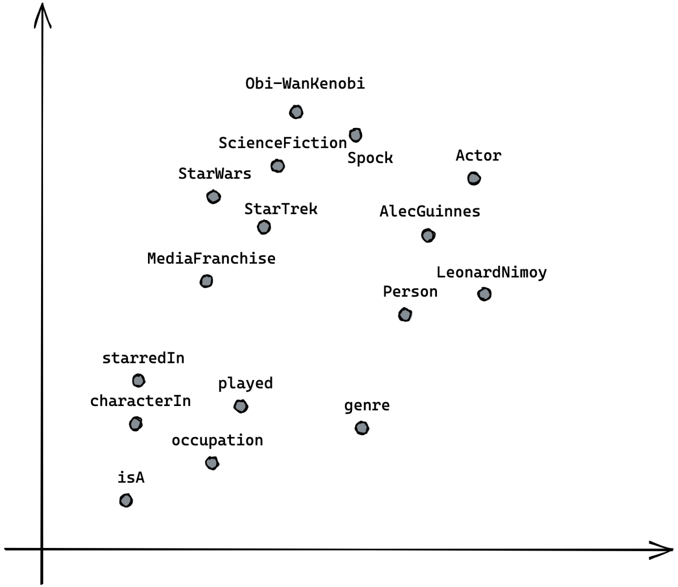
▶ **Distributional Semantics**

Knowledge Graph Embeddings (KGE)

(Knowledge) Graph Representation



Vector Space Representation



Idea: Learn embedding of **entities** and **relations** in a low-dimensional vector space such that **“similar” entities and relations in the graph** have **vector representations that are close together**.

KGE Design Rationale

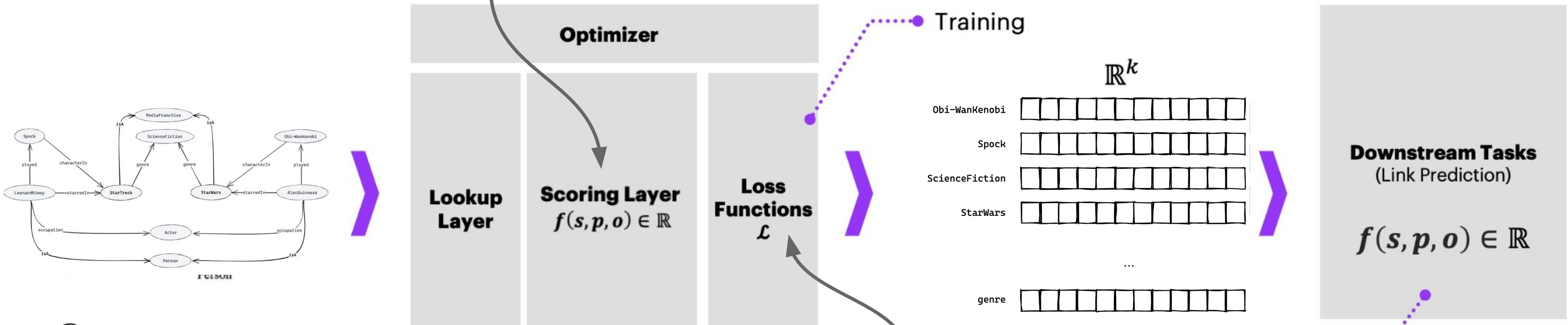
Capture Knowledge Graph Patterns:

- **Symmetry** <LukeSkywalker siblingOf PrincessLeia>
- **Asymmetry** <LukeSkywalker childOf DarthVader>
- **Inversion** <LukeSkywalker childOf DarthVader>
  <DarthVader fatherOf LukeSkywalker>
- **Composition** <LeonardNimoy played Spock>
  <Spock characterIn StarTrek>
  <LeonardNimoy starredIn StarTrek>
- also capture
  - Hierarchies, Type constraints, Transitivity, Reflexivity and Irreflexivity, etc.
  - Literals including Multimodality and Data Type semantics.

KGE Construction Kit

High score = high chances for the fact (s,p,o) to be true

② Scoring Layer $f(s,p,o) \in \mathbb{R}$



① Knowledge Graph G

③ Loss Functions $\mathcal{L}$

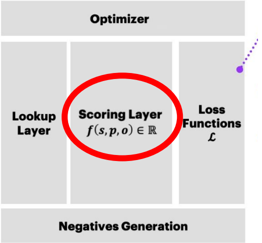
④ Negatives Generation

Pays a penalty if score of positive triple less than score of synthetic negative

Create "corrupted" versions of existing triples as negative triples

Costabello, L. et al, *ECAI-20 Tutorial: Knowledge Graph Embeddings: From Theory to Practice*, 2020

KGE Construction Kit – Scoring Function

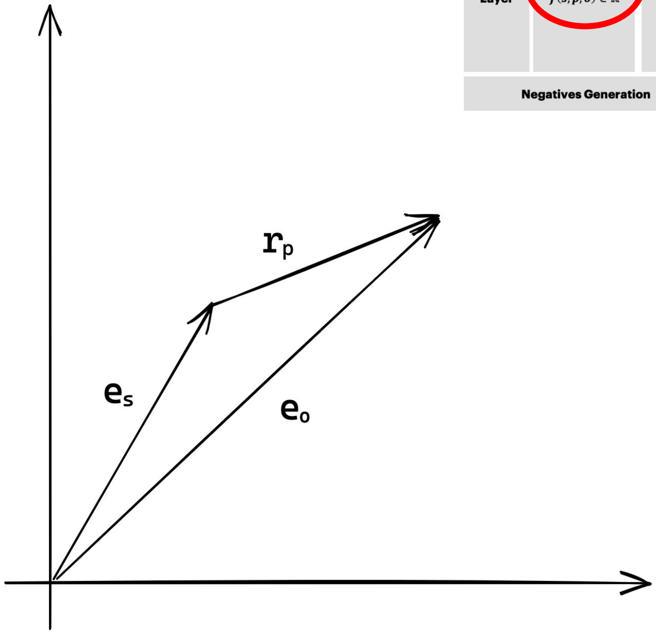


- Scoring function f assigns a score to a triple (s,p,o)
  High Score = high probability that the triple (s,p,o) is a true fact.

- **Translation-based Scoring Functions**
  - **TransE**: Translation Embeddings

$$f_{TransE} = -\|(e_s + r_p) - e_o\|_n$$

  - Exploits a distance based scoring function
  - Measures plausibility of a fact as distance between two entities
  - also TransH, TransR, TransD, TransSparse, TransM, TransEdge, …

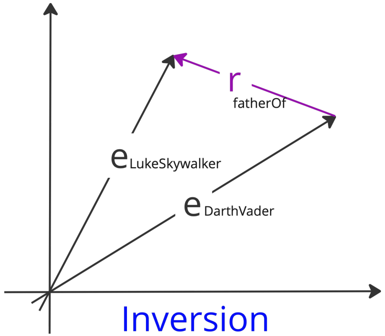


Bordes et al, *Translating Embeddings for Modeling Multi-relational Data*, 2013.

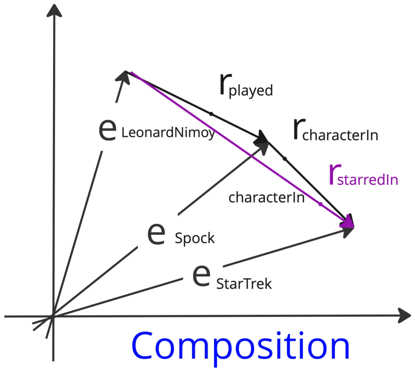
KGE Design Rationale

Capture Knowledge Graph Patterns:

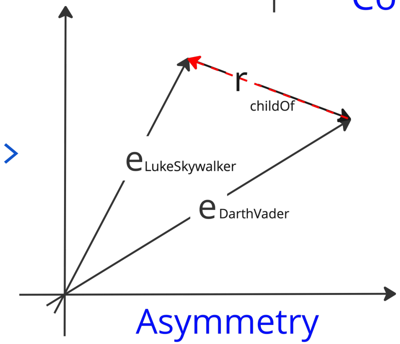
- **Inversion**
  <LukeSkywalker childOf DarthVader>
  <DarthVader fatherOf LukeSkywalker>
- **Composition** <LeonardNimoy played Spock>
  <Spock characterIn StarTrek>
  <LeonardNimoy starredIn StarTrek>
- **Asymmetry** <LukeSkywalker childOf DarthVader>
- **Symmetry** <LukeSkywalker siblingOf PrincessLeia>



Inversion



Composition



Asymmetry

- Other approaches can capture:
  - Hierarchies, Type constraints, Transitivity, Reflexivity and Irreflexivity, etc.
  - Literals including Multimodality and Data Type semantics.

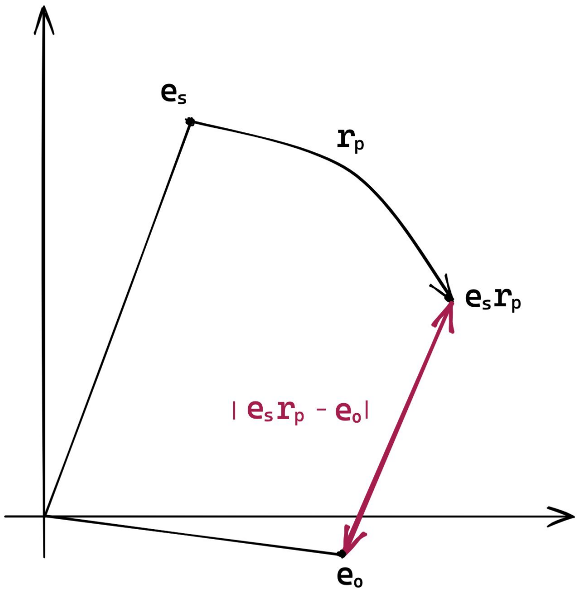
KGE Construction Kit – Scoring Function

Translation-based Scoring Functions

- **RotatE**: relations modelled as rotations in complex space $\mathbb{C}$: element-wise product between complex embeddings

$$f_{RotatE} = -\|(e_s \cdot r_p) - e_o\|_n$$

- Defines relations as rotation from head to tail
- Score function measures the angular distance between head and tail elements



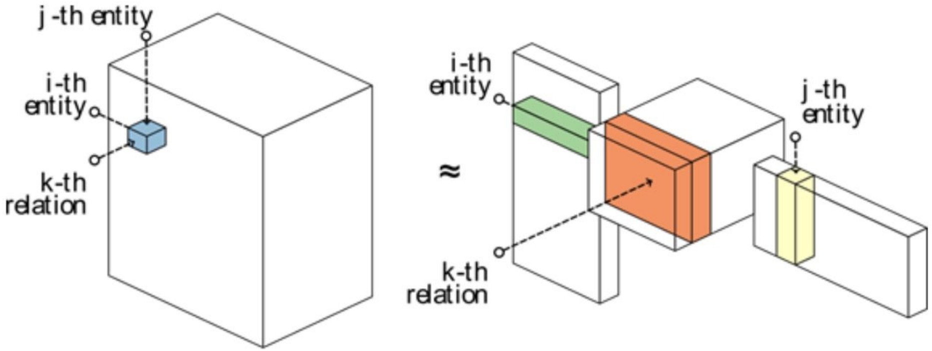
Sun et al, 2019

KGE Construction Kit – Scoring Function

Factorization-based Scoring Functions

- **RESCAL**: low-rank factorization with tensor product.

$$f_{RESCAL} = e_s^T W_r e_o$$



- Three-way factorization of an adjacency tensor that represents the knowledge graph.

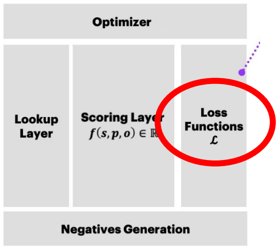
- Captures latent semantics of a knowledge graph through associate entities with vectors and represents each relation as a matrix that models pairwise interaction between entities.

Nickel et al, *A Three-Way Model for Collective Learning on Multi-Relational Data*, 2011.

KGE Construction Kit – Scoring Function

- **Factorization-based Scoring Functions**
  - **DistMult** (bilinear diagonal model, dot product)
  - **ComplEx** (complex embeddings, Hermitian dot product, extension of DistMult)
- **Further Scoring Functions**
  - **ConvE** (reshaping and convolution)
  - **ConvKB** (convolutions and dot product)
  - PTransE, DeepWalk, RDF2Vec, R-GCN, HolE, SimplE, QuatE, MurP, etc.

KGE Construction Kit – Loss Function



- **Pairwise Margin-based Hinge Loss:**
  Pays a penalty if the score of a positive triple is smaller than the score of a negative (synthetic) triple by margin γ.

$$\mathcal{L}(\Theta) = \sum_{t^+ \in \mathcal{G}} \sum_{t^- \in \mathcal{C}} \max(0, [\gamma + \underbrace{f(t^-;\Theta)}_{\text{Score assigned to a \textbf{synthetic negative triple}}} - \underbrace{f(t^+;\Theta)}_{\text{Score assigned to a \textbf{true triple}}}])$$

- Many more:
  - Negative Log-Likelihood / Cross Entropy
  - Binary Cross-Entropy
  - Self-Adversarial
  - etc.

KGE Construction Kit – Negatives Generation

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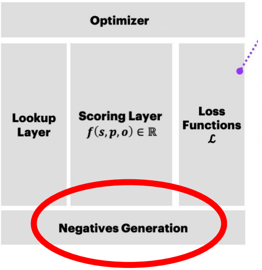


- Knowledge Graphs only contain positive statements (true statements).
- Where do negative examples (i.e., false statements) come from?
- **Synthetic Negative Generation**
  - Local Closed World Assumption: the KG is only locally complete.
  - "Corrupted" versions of a triple as synthetic negatives:

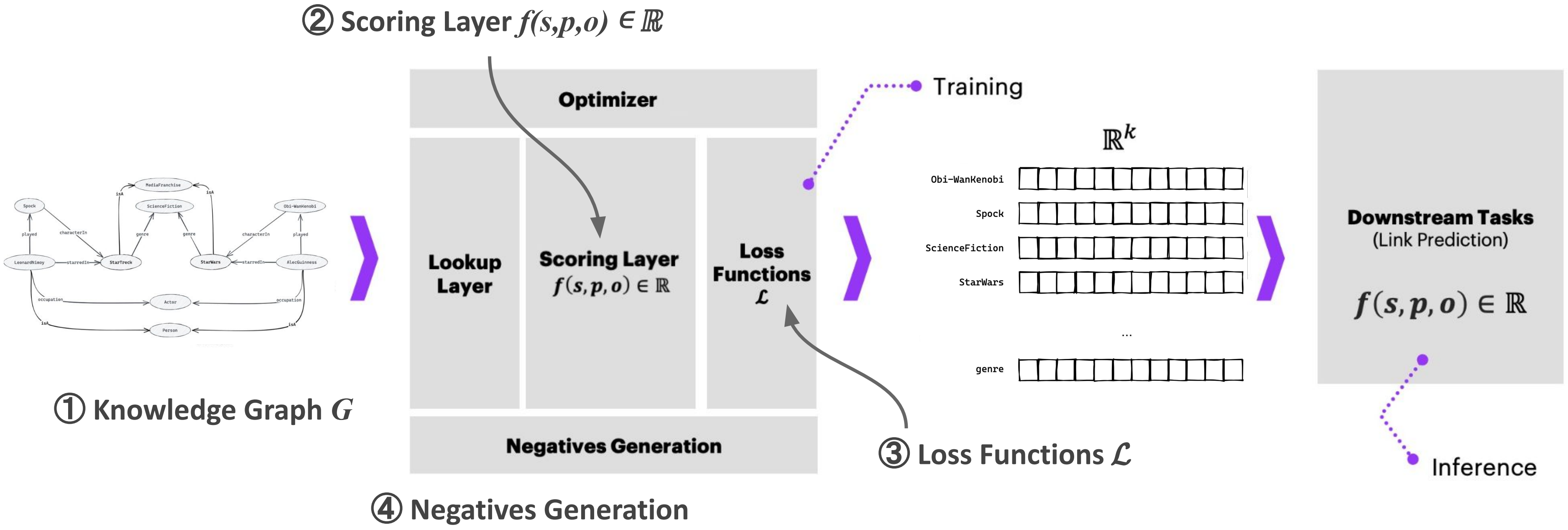
$$\mathcal{C} = \{\underbrace{(\hat{s}, p, o)}_{\text{corrupted } \textbf{subject}} | \hat{s} \in \mathcal{E} \cup \underbrace{(s, p, \hat{o})}_{\text{corrupted } \textbf{object}} | \hat{o} \in \mathcal{E}\}$$

- Example:

$\mathcal{E}$={AlecGuinness, StarWars, Obi-WanKenobi}
$t \in \mathcal{G}$ = (LeonardNimoy played Spock)

$\mathcal{C}_t$={ (AlecGuinness played Spock),
(StarWars played Spock),
(LeonardNimoy played AlecGuinness),
(LeonardNimoy played StarWars), …}

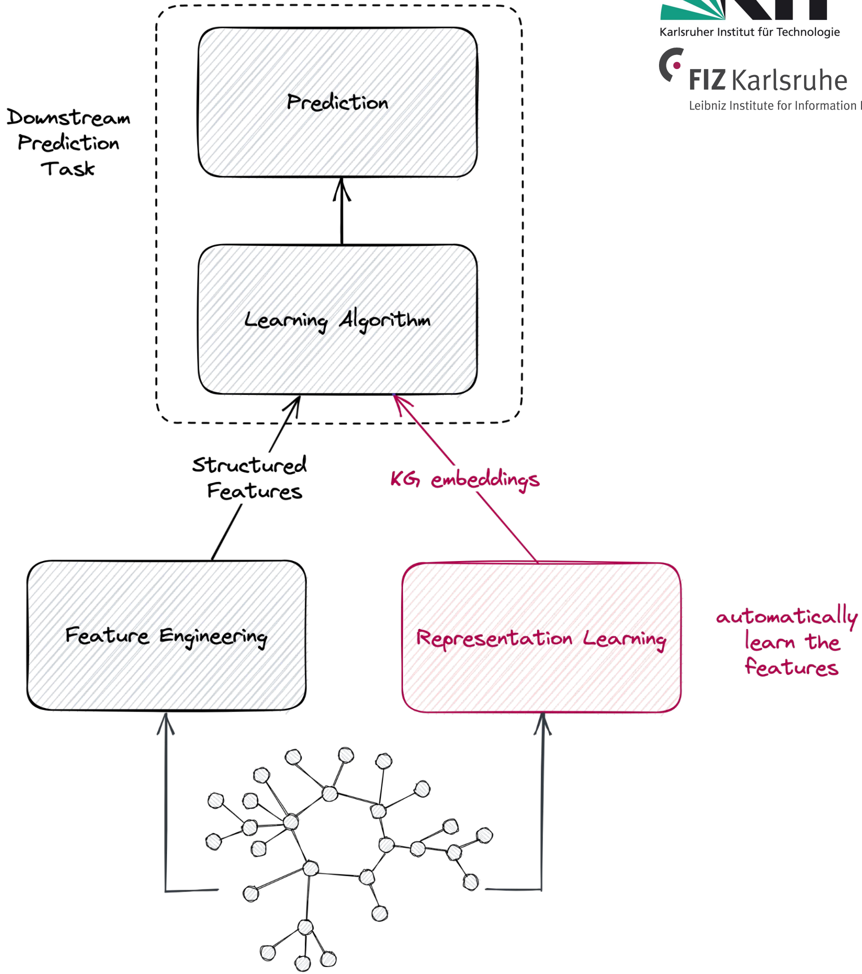
KGE Construction Kit

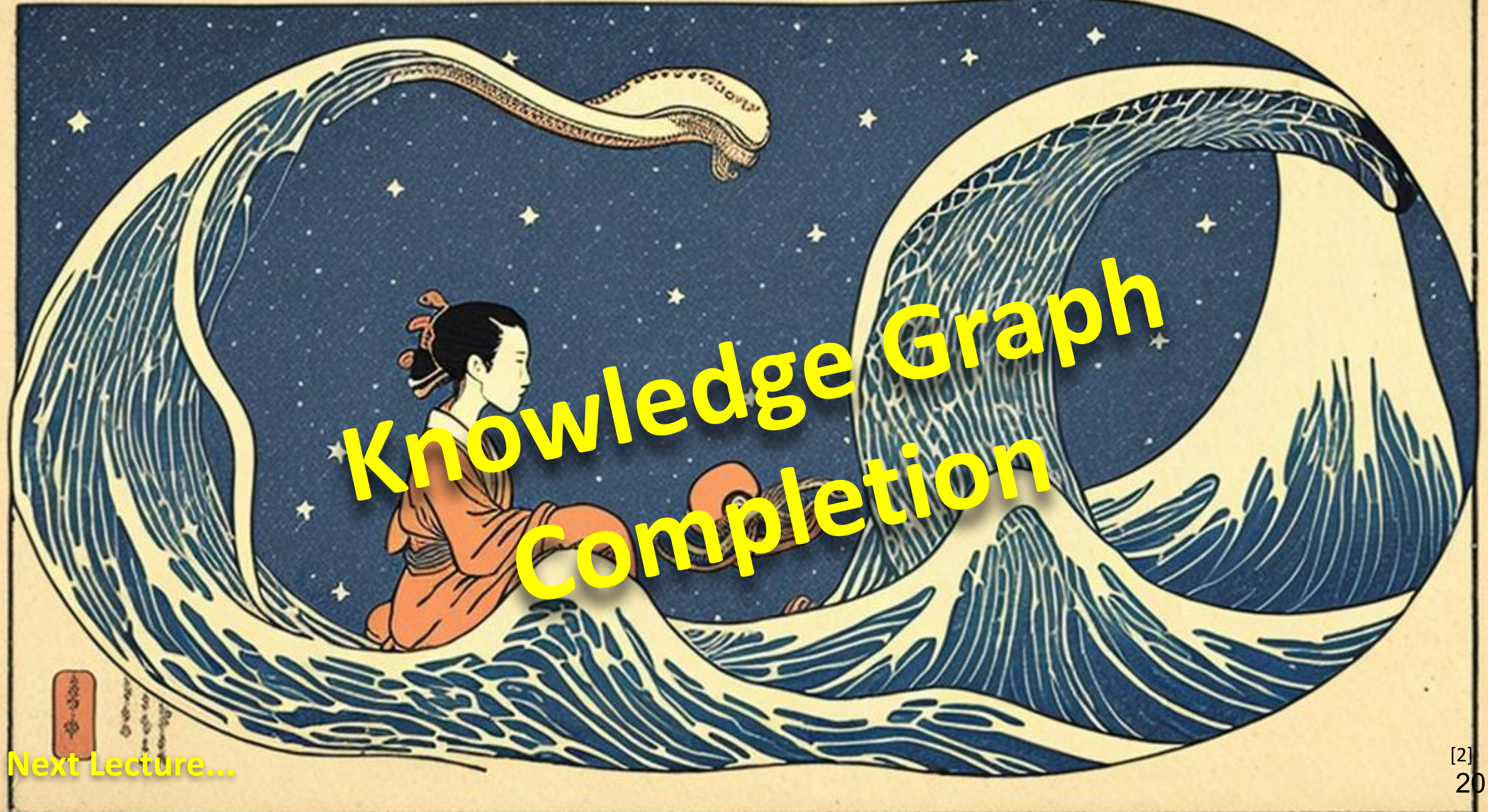


Costabello, L. et al, [ECAI-20 Tutorial: Knowledge Graph Embeddings: From Theory to Practice](), 2020.

Graph Representation Learning

- In **traditional ML for graphs**, we have to
  - extract node, link and graph-level features and
  - learn a model that maps features to labels.
- **Graph Representation Learning** alleviates the need to do feature engineering **every single time**.





Knowledge Graph Completion

Next Lecture...

[2]

Bibliographic References:

- Costabello, L. et al (2020), *ECAI-20 Tutorial: Knowledge Graph Embeddings: From Theory to Practice*.
- Bordes, A., Usunier, N., García-Durán, A., Weston, J., & Yakhnenko, O. (2013). *Translating Embeddings for Modeling Multi-relational Data*. NIPS.
- Zhiqing Sun, Zhi-Hong Deng, Jian-Yun Nie, Jian Tang: *RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space*. ICLR 2019.
- Nickel, M., Tresp, V., & Kriegel, H. (2011). *A Three-Way Model for Collective Learning on Multi-Relational Data*. International Conference on Machine Learning.

Picture References:

[1] “On this colorized woodcut in the style of Hiroshige we see a pensive cupid together with a beautiful female angel, bothe are melancholically watching two sailing ships on the vast ocean of flat Earth driven towards the edge of the world, where the waters are pouring down in the empty universe.”, created via ArtBot, Deliberate, 2023, [CC-BY-4.0], https://tinybots.net/artbot

[2] “On this colorized woodcut in the style of Hokusai we see a pensive woman together together giant octopus who melancholically entangles the knowledge graph that extends into the vast empty space of the universe to the galaxies and stars.”, created via ArtBot, Deliberate, 2023, [CC-BY-4.0], https://tinybots.net/artbot