Knowledge Graph Embeddings 101

(AKA Neural Link Predictors)

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Main References

Very good introductions to the field:

Very simple models can work surprisingly well:
1. Ruffinelli et al., You CAN Teach an Old Dog New Tricks! On Training Knowledge Graph Embeddings. https://openreview.net/forum?id=BkxSmIBFvr👨💻
Knowledge Graphs

Knowledge Graph — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of relationships between entities.
Knowledge Graphs

Knowledge Graph — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of relationships between entities.

Nodes denote entities.
Edges denote relationships between entities.

Multiple types of relations.
All relations are binary.
Knowledge Graphs

**Knowledge Graph** — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of *relationships between entities*

\[ G = \{ (s, p, o) \} \subseteq E \times R \times E \]

- **s**: subject of the triple
- **p**: predicate of the triple
- **o**: object of the triple

\( E \): set of all entities
\( R \): set of all relation types

(Tour Eiffel, located in, Paris) ∈ \( G \)
Knowledge Graphs

Knowledge Graph — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of relationships between entities

\[ G = \{(s, p, o)\} \subseteq E \times R \times E \]

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<table>
<thead>
<tr>
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<tbody>
<tr>
<td>s</td>
<td>p</td>
<td>o</td>
</tr>
<tr>
<td>Tour Eiffel</td>
<td>Is located in</td>
<td>Paris</td>
</tr>
<tr>
<td>Paris</td>
<td>Is a</td>
<td>Place</td>
</tr>
<tr>
<td>James</td>
<td>Has lived in</td>
<td>Tour Eiffel</td>
</tr>
<tr>
<td>James</td>
<td>Is born on</td>
<td>Jan 1 1984</td>
</tr>
<tr>
<td>James</td>
<td>Has visited</td>
<td>Louvre</td>
</tr>
<tr>
<td>Louvre</td>
<td>Is a</td>
<td>Museum</td>
</tr>
<tr>
<td>Louvre</td>
<td>Is located in</td>
<td>Paris</td>
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<td>Louvre</td>
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</table>
## Knowledge Graphs

| Knowledge Graph | # Triples ($|G|$) | # Entities |
|-----------------|-----------------|------------|
| YAGO            | 120M            | 10M        |
| Wikidata        | 16.7B           | 107M       |
| DBpedia         | 850M            | 6M         |
| GDELT           | 3.5B            | 364M       |
Open World Assumption

Closed-World Assumption — A statement that is true is also known to be true. Therefore, what is not currently known to be true, is false.
Open World Assumption

**Closed-World Assumption** — A statement that is true is also known to be true. Therefore, what is not currently known to be true, is false.

**Open World Assumption** — The absence of a particular statement means, in principle, that the statement has not been made explicitly yet, irrespective of whether it would be true or not. From the absence of a statement alone, we cannot infer that the statement is false.

KGs adopt this assumption
Machine Learning on KGs

Link Prediction/Triple Classification — Predicting the existence (of likelihood of correctness) of edges in the graph.

- Knowledge Graph Completion
- Recommendation
- Question/Query Answering
- Social Network Analysis
- Drug Repurposing/Retargeting
Link-Based Clustering — Identify groups of entities in relational data based on their similarity.

- Customer Segmentation
- Social Network Analysis
- Fraud Detection
- Collaboration Networks
- Biology and Medicine
Machine Learning on KGs

Link Prediction/Triple Classification — Predicting the existence (of likelihood of correctness) of edges in the graph. **Task:** Assign a score proportional to the likelihood that an unseen triple is true.
Link Prediction/Triple Classification — Predicting the existence (of likelihood of correctness) of edges in the graph. **Task:** Assign a score proportional to the likelihood that an unseen triple is true.

**Link Prediction:**

*Learning to Rank problem*

*Information Retrieval Metrics*

*No ground truth negatives*

\[
\langle \text{Louvre}, \text{is located in, } X \rangle
\]
Machine Learning on KGs

**Link Prediction/Triple Classification** — Predicting the existence (of likelihood of correctness) of edges in the graph. **Task:** Assign a score proportional to the likelihood that an unseen triple is true.

**Link Prediction:**
- Learning to Rank problem
- Information Retrieval Metrics
- No ground truth negatives

**Triple Classification:**
- Binary Classification Task/Metrics
- Evaluation requires positive and ground-truth negative examples
Rule-Based Approaches

Logic Programming — Given a set of facts and rules, use deductive reasoning to infer new true facts.

parentOf(Beth, Rick)
parentOf(Morty, Beth)
grandParentOf(X, Y) ← parentOf(X, Z) \land parentOf(Z, Y)

\[ \downarrow \]

grandParentOf(Morty, Rick)
Inductive Logic Programming — Given a set of (positive and negative) facts, identify the *rules* that explain the positive facts without explaining the negative ones.

\[
\text{parentOf(Beth, Rick)} \\
\text{parentOf(Morty, Beth)} \\
\text{pos: grandParentOf(Morty, Rick)} \\
\text{neg: grandParentOf(Beth, Rick)} \\
\ldots \\
\downarrow \\
\text{grandParentOf}(X, Y) \leftarrow \text{parentOf}(X, Z) \land \text{parentOf}(Z, Y)
\]

Rule Mining — (e.g., AMIE+, AnyBURL) extract rules based on the support in the KG.
Introducing (Graph) Representation Learning

Classic Machine Learning Pipeline

Input → Extract Features → Mapping from Features → Output

Learned from data
Introducing (Graph) Representation Learning

Classic Machine Learning Pipeline

Representation Learning Pipeline
Graph Representation Learning

Can we use standard Representation Learning/Deep Learning tools? It’s tricky — CNNs are designed for grids (e.g., images), while RNNs and Transformers are designed for sequences (e.g., text)

Knowledge Graphs, however, have different properties:
No spatial locality, no fixed-node ordering, multi-modal (concepts, textual descriptions, numbers, timestamps..)
We need ad-hoc models that can work with this type of data!
Graph Representation Learning

Idea — Learn representations of nodes and edges in the graph.
Graph Representation Learning

Idea — Learn representations of nodes and edges in the graph
Graph Representation Learning

Idea — Learn representations of nodes and edges in the graph

- Mona Lisa
  - Person, has visited
  - is a friend of
  - is a
  - Painted
  - is about

- Louvre Museum
  - Place
  - is located in

- Paris
  - is a
  - Paris
  \[ \in \mathbb{R}^d \]

- Tour Eiffel
  - tourist attraction
  - Tour Eiffel

- James
  - Person
  - has visited
  - has lived in
  - is on
  - is born on: Jan 1 1984

- Louvre Museum

- Downstream task
Knowledge Graph Embeddings

Knowledge Graph Embedding methods learn *embeddings*, i.e. continuous $d$-dimensional representations, of entities and relations in a KG.
Knowledge Graph Embeddings

KGEs map nodes and edge types ..
Knowledge Graph Embeddings

.. to semantically meaningful dense vector representations ($\in \mathbb{R}^d$)
Knowledge Graph Embeddings

Some KGE models in the recent published literature

Must be able to capture graph properties — relation properties (e.g., (a)symmetry), hierarchies, type constraints, transitivity, homophily, long range dependencies, etc.
## Knowledge Graph Embeddings

<table>
<thead>
<tr>
<th>Model</th>
<th>Symmetry</th>
<th>Antisymmetry</th>
<th>Inversion</th>
<th>Composition</th>
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<tr>
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<td>✗</td>
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<tr>
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<td>✓</td>
<td>✓</td>
<td>✗</td>
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<tr>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

From Sun et al. - RotatE: Knowledge Graph Embeddings by Relational Rotation in Complex Space
Knowledge Graph Embeddings — Components

Encoder:
Given an entity, produces a dense vector representation for (same for relation types):

Scoring Function:
Given the representations, of the subject, predicate, and object of a triple, calculates the likelihood that the fact holds true:

Loss function/Optimiser:
Given a KG, the loss function measures the discrepancy between the scores generated using the encoder and , and the graph. The optimiser finds such that:

$$e \in \mathbb{E}^{\text{enc}}_{\theta}$$

$$e \in \mathbb{R}^{d_e}$$

$$p \in \mathbb{R}^{d_p} \rightarrow p \in \mathbb{R}^{d_p'}$$

$$e \in \mathbb{E}$$

$$f: \mathbb{R}^{d_e} \times \mathbb{R}^{d_p} \times \mathbb{R}^{d_o} \rightarrow \mathbb{R}$$

$$G = \{ \langle s, p, o \rangle \} \subseteq \mathbb{E} \times \mathbb{R} \times \mathbb{E}$$

$$L(G)$$

$$\text{enc}_{\theta}(\cdot)$$

$$\text{f}(\cdot)$$

$$G_{\theta^*} = \operatorname{arg\,min}_{\theta} L(G_{\theta^*})$$
Knowledge Graph Embeddings — Components

**Encoder:** Given an entity $e \in E$, $\text{enc}_\theta(\cdot)$ produces a dense vector representation $e \in \mathbb{R}^d$ for $e$ (same for relation types $p \in R \rightarrow p \in \mathbb{R}^{d'}$):

$$\text{enc}_\theta : E \rightarrow \mathbb{R}^d$$
Knowledge Graph Embeddings — Components

Encoder: Given an entity $e \in E$, $\text{enc}_\theta(\cdot)$ produces a dense vector representation $e \in \mathbb{R}^d$ for $e$ (same for relation types $p \in R \rightarrow p \in \mathbb{R}^{d'}$):

$$\text{enc}_\theta : E \rightarrow \mathbb{R}^d$$

Scoring Function: Given the representations $s \in \mathbb{R}^d$, $p \in \mathbb{R}^{d'}$, $o \in \mathbb{R}^d$ of the subject $s$, predicate $p$, and object $o$ of a triple $\langle s, p, o \rangle \in E \times R \times E$, calculates the likelihood that the fact holds true:

$$f : \mathbb{R}^d \times \mathbb{R}^{d'} \times \mathbb{R}^d \rightarrow \mathbb{R}$$
Knowledge Graph Embeddings — Components

Encoder: Given an entity \( e \in E \), \( \text{enc}_\theta(\cdot) \) produces a dense vector representation \( e \in \mathbb{R}^d \) for \( e \) (same for relation types \( p \in R \rightarrow p \in \mathbb{R}^{d'} \)):

\[
\text{enc}_\theta : E \rightarrow \mathbb{R}^d
\]

Scoring Function: Given the representations \( s \in \mathbb{R}^d \), \( p \in \mathbb{R}^{d'} \), \( o \in \mathbb{R}^d \) of the subject \( s \), predicate \( p \), and object \( o \) of a triple \( \langle s, p, o \rangle \in E \times R \times E \), calculates the likelihood that the fact holds true:

\[
f : \mathbb{R}^d \times \mathbb{R}^{d'} \times \mathbb{R}^d \rightarrow \mathbb{R}
\]

Loss function/Optimiser: Given a KG \( G = \{\langle s, p, o \rangle\} \subseteq E \times R \times E \), the loss function \( L(G) \) measures the discrepancy between the scores generated using the encoder \( \text{enc}_\theta(\cdot) \) and \( f(\cdot) \), and the graph \( G \). The optimiser finds \( \theta^* \) such that:

\[
\theta^* = \arg \min_{\theta} L(G)
\]
Encoder

**Encoder**: Given an entity $e \in E$, $\text{enc}_\theta(\cdot)$ produces a dense vector representation $e \in \mathbb{R}^d$ for $e$ (same for relation types $p \in R \rightarrow p \in \mathbb{R}^{d'}$):

$$\text{enc}_\theta : E \rightarrow \mathbb{R}^d$$

Simplest possible encoder: **embedding layer** — it stores all entity representations in a $E \in \mathbb{R}^{|E| \times d}$ matrix, where each row is associated with a different entity $e \in E$:

<table>
<thead>
<tr>
<th>Entity</th>
<th>Index</th>
<th>Lookup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paris</td>
<td>$\text{index}(\text{Paris}) \rightarrow 6$</td>
<td>$\mathbf{e}<em>{\text{Paris}} = \mathbf{E}</em>{6,:} \in \mathbb{R}^d$</td>
</tr>
</tbody>
</table>
Scoring Function: Given the representations $s \in \mathbb{R}^d$, $p \in \mathbb{R}^{d'}$, $o \in \mathbb{R}^d$ of the subject $s$, predicate $p$, and object $o$ of a triple $(s, p, o) \in E \times R \times E$, calculates the likelihood that the fact holds true:

$$f : \mathbb{R}^d \times \mathbb{R}^{d'} \times \mathbb{R}^d \rightarrow \mathbb{R}$$

Many possible choices from the literature — a simple one is the TransE scoring function:

$$f(s, p, o) = -\| (s + p) - o \|_2$$

Translation of $s$ with $p$

Distance between $s + p$ and $o$

Bordes et al. Translating Embeddings for Modeling Multi-Relational Data. NIPS 2013
**Scoring Functions**

**RESCAL:** subject and object embeddings $s, o \in \mathbb{R}^d$, predicate embedding $W_p \in \mathbb{R}^{d \times d}$

$$f(s, W_p, o) = s^\top W_p o$$

**DistMult:** subject, predicate, and object embeddings $s, p, o \in \mathbb{R}^d$

$$f(s, p, o) = \langle s, p, o \rangle = (s \odot p)^\top o = \sum_{i=1}^{d} s_i p_i o_i$$

*Problem —* $\langle \text{Louvre}, \text{locatedIn}, \text{Paris} \rangle$ and $\langle \text{Paris}, \text{locatedIn}, \text{Louvre} \rangle$ have the same score!

**ComplEx:** subject, predicate, and object embeddings $s, p, o \in \mathbb{C}^d$

$$f(s, p, o) = \Re \left( \langle s, p, \overline{o} \rangle \right)$$

where $\Re(x)$ denotes the real part of $x \in \mathbb{C}^d$ and $\overline{x} \in \mathbb{C}^d$ denotes its complex conjugate.
**Evaluation**

**Binary Classification Metrics** — we have a set of test triples representing true and false facts (positive and negative examples); we try to classify each test triple in its correct class, and then calculate the accuracy of our classifier:

\[ + \langle \text{Louvre}, \text{locatedIn}, \text{Paris} \rangle \]
\[ - \langle \text{Louvre}, \text{locatedIn}, \text{Edinburgh} \rangle \]
\[ + \langle \text{Tour Eiffel}, \text{locatedIn}, \text{Paris} \rangle \]
\[ - \langle \text{Tour Eiffel}, \text{locatedIn}, \text{London} \rangle \]

\[ \Rightarrow \quad \text{Accuracy} = \frac{\# \text{ Correct Classifications}}{\# \text{ Test Triples}} \]

Requires translating the scores produced by \( f(\cdot) \) in a binary decision — a way to do this is to find a threshold score that maximises the accuracy on some held-out validation set.
Information Retrieval Metrics — we have a set of test triples $T$ representing true facts (positive examples). For each test triple we hide the object, and measure how well we can recover it using the model; then repeat the operation for the subject.

<table>
<thead>
<tr>
<th>Subject</th>
<th>Predicate</th>
<th>Object</th>
<th>Score</th>
<th>Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>Louvre</td>
<td>locatedIn</td>
<td>London</td>
<td>0.4</td>
<td>2</td>
</tr>
<tr>
<td>Louvre</td>
<td>locatedIn</td>
<td>Edinburgh</td>
<td>0.2</td>
<td>3</td>
</tr>
<tr>
<td>Louvre</td>
<td>locatedIn</td>
<td>Paris</td>
<td>1.4</td>
<td>1</td>
</tr>
<tr>
<td>Louvre</td>
<td>locatedIn</td>
<td>Mars</td>
<td>-0.5</td>
<td>4</td>
</tr>
</tbody>
</table>

Mean Reciprocal Rank: $\text{MRR} = \frac{1}{|T|} \sum_{t \in T} \frac{1}{\text{Rank}_t}$

Hits@$k$: $\text{Hits}@k = \frac{|\{t \in T \mid \text{Rank}_t \leq k\}|}{|T|}$
Loss Functions

**Loss function:** Given a KG $G = \{\langle s, p, o \rangle \} \subseteq E \times R \times E$, the loss function $L(G)$ measures the discrepancy between the scores generated using the encoder $\text{enc}_\theta(\cdot)$ and the scoring function $f(\cdot)$, and the graph $G$.

In a nutshell — they measure to which extent triples in the graph receive lower scores than triples *not* in the graph. A first example is the *margin-based ranking loss*:

$$L(G) = \sum_{t \in G} \sum_{t' \in N(t)} \left[ \gamma - f(t) + f(t') \right]_+$$

where $t \in G$ is a triple from the graph $G$, $t'$ is a corruption of $t$ obtained by changing either the subject or the object of $t$, and $\mathbf{t}$ denotes the embedding of $t$.

Bordes et al. Translating Embeddings for Modeling Multi-Relational Data. NIPS 2013
Minimising a Loss Function

**Optimiser:** Given a KG $G = \{\langle s, p, o \rangle \} \subseteq E \times R \times E$ and a loss function $L(G)$ for an encoder $\text{enc}_\theta(\cdot)$ and scoring function $f(\cdot)$, the optimiser finds $\theta^*$ such that:

$$\theta^* = \arg \min_{\theta} L(G)$$

Most common solution (by far) is based on **Gradient Descent** — in a nutshell:

1. Initialise $\theta^{(0)}$ (the embeddings) randomly
   - E.g., based on a validation MRR
2. Until convergence, for $i = 1, \ldots, n$:
   - $\theta^{(i)} = \theta^{(i-1)} - \eta \nabla_\theta [L(G) + \lambda \Omega(\theta)]$
   - **Learning rate — hyperparameter**
   - $\Omega(\theta)$ controls the magnitude of $\theta$
   - **Updated parameters**
   - **Gradient of $L(G) + \lambda \Omega(\theta)$ wrt. $\theta$**

Follow best practices from Representation/Deep Learning.