Lecture 1: Relational Data & Embedding Models

Relational Learning
Course Organisation
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Advanced Topics in Machine Learning: Research-oriented and somewhat less conventional course.
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For both themes, there will be a live-streamed guest lecture towards the end of the term. Please follow the announcements on the course website.
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**Practicals:** There are 6 practicals planned. These practicals will provide you the necessary technical skills for the projects. Two of these practicals are specifically dedicated for discussing the assessment papers and helping you to form groups, depending on your interests.
Course Structure: Relational Learning
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These topics are covered for the first time in the scope of this course, and so the material is new. Please email me if you spot any problems in the slides and I will revise them accordingly.
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- Relational data
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• Relational data
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- Summary
Relational Data
Relational Data

Protein Networks
Relational Data

Molecule Networks
Relational Data

Recommender Systems
Relational Data

Social Networks
Knowledge Graphs, as graph-structured data models, storing relations (e.g., isFriendOf) between entities (e.g., Alice, Bob) and thereby capture structured knowledge.
Knowledge Graphs
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Nairobi capitalOf Kenya
Knowledge Graphs

- Kenya
  - capitalOf
  - cityIn
- Nairobi
Knowledge Graphs

- capitalOf: Nairobi, Kenya
- cityIn: Kenya
- locatedIn: Africa
Knowledge Graphs

- Kenya: capitalOf
- Nairobi: cityIn
- locatedIn: Africa

Diagram showing relationships between Kenya, Nairobi, and Africa.
Knowledge Graphs

- Nairobi, Kenya
- Somalia, Ethiopia, Africa
- capitalOf: Nairobi
- locatedIn: Somalia, Ethiopia, Africa
- neighbourOf: Somalia, Ethiopia
- cityIn: Nairobi

Diagram:
- Nairobi (Kenya) connected to Somalia (Ethiopia) by neighbourOf
- Somalia (Ethiopia) and Ethiopia connected to Africa by locatedIn
- Nairobi connected to Kenya by capitalOf
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- Diagram showing relations between countries and their capital cities.
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- We sometimes write $U$ to denote the set of all possible facts over $E$ and $R$. 
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  • Can KGs be mediators for developing more reliable and interpretable models for ML?
  • How to make learning and reasoning compatible?
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Somewhat surprisingly, many of these patterns can be represented as linear translations.

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For example, the result of a vector calculation \( \text{vec}(\text{“Madrid”}) - \text{vec}(\text{“Spain”}) + \text{vec}(\text{“France”}) \) is closer to \( \text{vec}(\text{“Paris”}) \) than to any other word vector.”

(Mikolov et. al, 2013)

Figure 2 (Mikolov et. al, 2013): 2-dimensional PCA projection of the 1000-dimensional Skip-gram vectors of countries and their capital cities. The figure illustrates ability of the model to automatically organize concepts and learn implicitly the relationships between them, as during the training no supervised information about what a capital city means is given.
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- **Knowledge Graph Example:**
  - **Nodes:** Somalia, Ethiopia, Kenya, Africa, Nairobi
  - **Edges:**
    - capitalOf: Somalia -> Kenya
    - locatedIn: Kenya -> Somalia, Nairobi
    - neighbourOf: Ethiopia -> Somalia
    - cityIn: Nairobi -> Somalia, Kenya
    - locatedIn: Somalia -> Africa, Kenya

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**Intuition:** Real-world data lies in **low dimensional** manifolds, so if existing facts in a KG exhibit common patterns then one can embed them into low-dimensional vector-spaces and use them to predict new facts.
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**Idea**: Represent entities and relations as **embeddings**, while capturing latent properties of the knowledge graph, i.e., similar entities and relationships will be represented with similar embeddings. Use such similarities to rank new predictions.
Knowledge Graph Embedding Models
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Most of the existing approaches can be described in term of the following criteria:

(i) **Model representation**: How are the entities and relations represented?

(ii) **Scoring function**: How is the likelihood of a fact to be true defined?

(iii) **Loss function**: What is the objective function to be minimised?
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Well-known families of models classified in terms of model representation:

- **Translational models**: Embed entities as points in vector space, and model relations as translations operating on the embeddings of the entities.

- **Bilinear models**: Embed entities and relations into vector space, and model relations as a **bilinear product** between entity and relation embeddings.

- **Neural models**: Embed the entities and relations using a **neural** network (e.g., convolutional neural network).
KG Embedding Models: Basic Idea
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Train a KG Embedding Model $M$

Score all facts

$M_{\text{score}} :: U \mapsto \mathbb{R}$
KG Embedding Models: Basic Idea

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**Problem:** KGs typically store only positive information, and so encode only the facts that are true. There are no real negative examples to train with!
Negative Sampling
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The idea is to corrupt true facts, and then use some of these corrupted facts as negative examples.
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A corrupted fact is obtained by replacing only the head (resp., only the tail) entity in a true fact in $G$ with an entity in $E$. Formally, for a true fact $r(h, t) \in G$, we define the set of all corrupted facts as:
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$$C^{r(h,t)} = \{r(e, t) \mid e \neq h \in E, r(e, t) \notin G\} \cup \{r(h, e) \mid e \neq t \in E, r(h, e) \notin G\}.$$
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Negative sampling is not ideal, as random sampling can clearly give a potentially correct fact as a negative fact, and require it to be ranked lower, misleadingly.
Model Expressiveness
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Would theoretical inexpressivity surface in practice?

Theoretical inexpressivity of a model may not surface empirically, especially if the benchmark datasets are not very complex. Knowing the expressive limitations of a model, however, it is easy to design datasets to empirically observe its limitations.
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One well-known example inference pattern is symmetry: A relation $r \in R$ is symmetric if, for any choice of entities $e_1, e_2 \in E$, whenever a fact $r(e_1, e_2)$ holds, then so does $r(e_2, e_1)$. 
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How can model inductive capacity be studied?

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One well-known example inference pattern is symmetry: A relation $r \in R$ is symmetric if, for any choice of entities $e_1, e_2 \in E$, whenever a fact $r(e_1, e_2)$ holds, then so does $r(e_2, e_1)$.

As a result, if a model learns a symmetry pattern for a relation $r$, then it can infer facts in the symmetric closure of $r$, thus providing a strong inductive bias.
Inference Patterns
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An inference pattern specifies a logical property over a KG, which means that such patterns can be formalised using logical rules. To formalise this, let us extend our relational vocabulary over $E$ and $R$ with a set $V$ of variables. A first-order atom is an expression of the form $r(x_i, x_j)$, where $r \in R$, and $x_i, x_j \in V$. 
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A Boolean combination of first-order atoms is defined inductively using logical constructors $\neg$, $\land$, $\lor$, e.g., $\phi_1(x_1, x_3) = r_1(x_1, x_2) \land r_2(x_2, x_2)$ and $\phi_2(x_3, x_4) = r_2(x_3, x_4) \lor \neg r_3(x_4, x_3)$ are Boolean combinations of first-order atoms.
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and

$$\phi_2(x_3, x_4) = r_2(x_3, x_4) \lor \neg r_3(x_4, x_3)$$

are Boolean combinations of first-order atoms.

For the purposes of this lecture, we are interested in universally quantified first-order rules of the form:

$$\forall x_1 \ldots x_k \phi(x_1 \ldots x_k) \Rightarrow \psi(x_1 \ldots x_l),$$

with $k \geq l$. The semantics of such universally quantified first-order rules is that of first-order logic, restricted to a finite domain (as the set $E$ of entities is finite).
Inference Patterns
We can express the \textit{symmetry} inference pattern for a relation $r \in R$, in the form of such a logical rule as follows:

$$\forall x, y \ r(x, y) \Rightarrow r(y, x),$$

which holds if and only if the relation $r$ is symmetric, i.e., the rule is invalidated if there exists two entities $e_1, e_2 \in E$, where $r(e_1, e_2)$ is true, but $r(e_2, e_1)$ is not.
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Similarly, we can express that the relations $r_1, r_2 \in R$ are the inverse of each other in terms of two rules:

$$\forall x, y \ r_1(x, y) \Rightarrow r_2(y, x),$$

$$\forall x, y \ r_2(x, y) \Rightarrow r_1(y, x).$$

In this case, we will use the standard abbreviation $\Leftrightarrow$ and write $\forall x, y \ r_1(x, y) \Leftrightarrow r_2(y, x)$. 
## Inference Patterns

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</tr>
<tr>
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</tr>
<tr>
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List of inference patterns commonly used in the literature and the corresponding logical rules. It is assumed that $r_1 \neq r_2 \neq r_3$. 
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List of inference patterns commonly used in the literature and the corresponding logical rules. It is assumed that $r_1 \neq r_2 \neq r_3$.

These patterns are very prominent in many datasets. While these patterns and the corresponding rules are not very expressive, they already are a challenge for KGE models, as it is already hard for existing systems to capture these patterns.
Empirical Evaluation
Empirical Evaluation: Ranking
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The most common empirical evaluation task for KGE methods is based on entity ranking. The knowledge graph $G$ is partitioned into a set of training ($G_{tr}$), validation ($G_{v}$), and test facts ($G_{test}$).
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$$r(\_ , t) = \{ r(e, t) \mid e \in E, r(e, t) \notin G_{tr} \cup G_v \cup G_{test} \} \cup \{ r(h, t) \} ,$$

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Importantly, all facts that occur in the training, validation, or test data are filtered out from these sets (except the test fact itself). This is to ensure that other facts known to be true do not affect the ranking. This is the so-called filtered evaluation which has become standard practice in experimental evaluation (Bordes et al., 2013).
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The rank of the entity $e$ relative to the facts $r(_, t)$, denoted $\text{rank}(e \mid r(_, t))$, is the rank of the fact $r(e, t)$ in $r(_, t)$; similarly, the rank of the entity $e$ relative to the facts $r(h, _)$, denoted $\text{rank}(e \mid r(h, _))$, is the rank of the fact $r(h, e)$ in $r(h, _)$. 

Empirical Evaluation: Metrics
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Mean rank (MR) is the average rank of true facts against their corrupted counterparts:

\[
\frac{1}{2 |G_{test}|} \sum_{r(h,t)\in G_{test}} \left( \text{rank}(h \mid r(\_, t)) + \text{rank}(t \mid r(h, \_)) \right)
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Hits@k is the proportion of true facts with rank at most k:

\[
\frac{1}{2 | G_{test} |} \sum_{r(h,t) \in G_{test}} \left( \mathbf{1}(\text{rank}(h \mid r(\_, t)) \leq k) + \mathbf{1}(\text{rank}(t \mid r(h, \_)) \leq k) \right),
\]

where \( \mathbf{1}(c) \) is the indicator function that returns 1, if \( c \) is true, and 0, otherwise.
Empirical Evaluation: Datasets
FB15k (Bordes et al., 2013): A subset of Freebase (Bollacker et al., 2008), where a large part of the test facts \( r(x, y) \) can be directly inferred via an inverse relation \( r'(y, x) \), which makes the inversion pattern very prominent (Toutanova & Chen, 2015). Other patterns on FB15k are symmetry/antisymmetry and composition patterns.
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**YAGO3-10**: A subset of the YAGO3 (Mahdisoltani et al., 2015), where all entities appear in at least 10 facts.
## Empirical Evaluation: Datasets

| Dataset    | |E|   | |R|   | Training facts | Validation facts | Test facts |
|------------|---------|--------|--------|----------------|------------------|---------------|
| FB15K-237  | 14,541  | 237    | 272,115| 17,535         | 20,466           |
| WN18RR     | 40,943  | 11     | 86,835 | 3,034          | 3,034            |
| YAGO3-10   | 123,182 | 37     | 1,079,040| 5,000         | 5,000            |
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Datasets with their respective #entities (|E|), #relations (|R|), and #facts.
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• We have not introduced/evaluated any specific model: Next lecture!
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