Stanford CS224W: Reasoning over Knowledge Graphs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu
Announcements

- **Project Proposal** due today
  - Gradescope submissions close at midnight
- **Colab 2** due Thursday
Given an enormous KG, can we complete the KG?

- For a given (head, relation), we predict missing tails.
  - (Note this is slightly different from link prediction task)

Example task: Predict the tail “Science Fiction” for (“J.K. Rowling”, “genre”)
Goal:
- How to perform multi-hop reasoning over KGs?

Reasoning over Knowledge Graphs
- Answering multi-hop queries
  - Path Queries
  - Conjunctive Queries
- Query2Box
Example KG: Biomedicine

Arimidex

Breast Cancer

Headache

Brain Bleeding

Kidney Infection

Fulvestrant

BRCA1

ESR2

ESR1

BIRC2

Short of Breath

CASP8

PIM1
Can we do multi-hop reasoning, i.e., answer complex queries on an incomplete, massive KG?

<table>
<thead>
<tr>
<th>Query Types</th>
<th>Examples: Natural Language Question, Query</th>
</tr>
</thead>
<tbody>
<tr>
<td>One-hop Queries</td>
<td>What adverse event is caused by Fulvestrant? (e:Fulvestrant, (r:Causes))</td>
</tr>
<tr>
<td>Path Queries</td>
<td>What protein is associated with the adverse event caused by Fulvestrant? (e:Fulvestrant, (r:Causes, r:Assoc))</td>
</tr>
<tr>
<td>Conjunctive Queries</td>
<td>What is the drug that treats breast cancer and caused headache? ((e:BreastCancer, (r:TreatedBy)), (e:Migraine, (r:CausedBy))</td>
</tr>
</tbody>
</table>

In this lecture, we only focus on answering queries on a KG! The notation will be detailed next.

One-hop Queries

Path Queries

Conjunctive Queries
Predictive One-hop Queries

- We can formulate knowledge graph completion problems as answering one-hop queries.

  - **KG completion**: Is link \((h, r, t)\) in the KG?

  - **One-hop query**: Is \(t\) an answer to query \((h, r)\)?
    - **For example**: What side effects are caused by drug Fulvestrant?
Generalize one-hop queries to path queries by adding more relations on the path.

An \( n \)-hop path query \( q \) can be represented by

\[
q = (v_a, (r_1, \ldots, r_n))
\]

- \( v_a \) is an “anchor” entity,
- Let answers to \( q \) in graph \( G \) be denoted by \([q]_G\).

Query Plan of \( q \):

Query plan of path queries is a chain.
Question: “What proteins are associated with adverse events caused by Fulvestrant?”

- \( v_a \) is e:Fulvestrant
- \((r_1, r_2)\) is (r:Causes, r:Assoc)
- Query: \((e:Fulvestrant, (r:Causes, r:Assoc))\)
Question: “What proteins are associated with adverse events caused by Fulvestrant?”

- Query: (e:Fulvestrant, (r:Causes, r:Assoc))

Given a KG, how to answer a path query?
We answer path queries by traversing the KG: “What proteins are associated with adverse events caused by Fulvestrant?”

Query: \((e: \text{Fulvestrant}, (r: \text{Causes}, r: \text{Assoc}))\)
We answer path queries by traversing the KG: “What proteins are associated with adverse events caused by Fulvestrant?”

Query: (e:Fulvestrant, (r:Causes, r:Assoc))

Start from the anchor node “Fulvestrant” and traverse the KG by the relation “Causes”, we reach entities {“Brain Bleeding”, “Short of Breath”, “Kidney Infection”, “Headache”}. 
We answer path queries by traversing the KG: “What proteins are associated with adverse events caused by Fulvestrant?”

Query: (e:Fulvestrant, (r:Causes, r:Assoc))

Start from the nodes {“Brain Bleeding”, “Short of Breath”, “Kidney Infection”, “Headache”} and traverse the KG by the relation “Assoc”, we reach entities {“CASP8”, “BIRC2”, “PIM1”}. These are the answers.
However, KGs are incomplete

- Answering queries seems easy: Just traverse the graph.

- But KGs are incomplete and unknown:
  - Many relations between entities are missing or are incomplete
    - For example, we lack all the biomedical knowledge
    - Enumerating all the facts takes non-trivial time and cost, we cannot hope that KGs will ever be fully complete

- Due to KG incompleteness, one is not able to identify all the answer entities
Example: Incomplete KG

- We answer path queries by traversing the KG: “What proteins are associated with adverse events caused by Fulvestrant?”
- Query: (e:Fulvestrant, (r:Causes, r:Assoc))

![Diagram showing relationships between Fulvestrant, adverse events, and proteins like CASP8, BIRC2, PIM1.]

Missing Answer! Answers!
Can KG Completion Help?

Can we first do KG completion and then traverse the completed (probabilistic) KG?

- **No!** The “completed” KG is a **dense graph**!
  - Most \((h, r, t)\) triples (edge on KG) will have some non-zero probability.

- **Time complexity of traversing a dense KG** is exponential as a function of the path length \(L\): \(O(d_{max}^L)\)
Task: Predictive Queries

- We need a way to answer path-based queries over an incomplete knowledge graph.
- We want our approach to implicitly impute and account for the incomplete KG.

**Task: Predictive queries**

- Want to be able to answer arbitrary queries while implicitly imputing for the missing information
- Generalization of the link prediction task
1) Given entity embeddings, how do we answer an arbitrary query?

- Path queries: Using a generalization of TransE
- Conjunctive queries: Using Query2Box
- And-Or Queries: Using Query2Box and query rewriting

(We will assume entity embeddings and relation embeddings are given)

2) How do we train the embeddings?

- The process of determining entity and relation embeddings which allow us to embed a query.
Map queries into embedding space. **Learn to reason in that space**

- Embed query into a single **point** in the Euclidean space: answer nodes are close to the query.
- **Query2Box:** Embed query into a hyper-rectangle (**box**) in the Euclidean space: answer nodes are enclosed in the box.

[Embedding Logical Queries on Knowledge Graphs.](Hamilton, et al., NeurIPS 2018)
[Query2box: Reasoning over Knowledge Graphs in Vector Space Using Box Embeddings.](Ren, et al., ICLR 2020)
**Idea: Traversing KG in Vector Space**

- **Key idea: Embed queries!**
  - Generalize **TransE** to multi-hop reasoning.
  - **Recap: TransE:** Translate $h$ to $t$ using $r$ with score function $f_r(h, t) = -||h + r - t||$.
  - Another way to interpret this is that:
    - **Query embedding:** $q = h + r$
    - **Goal:** query embedding $q$ is close to the **answer embedding** $t$
      $f_q(t) = -||q - t||$

Distance $(q, t)$ is small
Key idea: Embed queries!

- Generalize TransE to multi-hop reasoning.

Given a path query \( q = (v_a, (r_1, \ldots, r_n)) \),

\[
q = v_a + r_1 + \cdots + r_n
\]

- The embedding process only involves vector addition, independent of \# entities in the KG!
Embed path queries in vector space.

- **Question:** “What proteins are associated with adverse events caused by Fulvestrant?”
- **Query:** (e:Fulvestrant, (r:Causes, r:Assoc))

Follow the query plan:

Query Plan

Embedding Process

Fulvestrant
Embed path queries in vector space.

- **Question:** “What proteins are associated with adverse events caused by Fulvestrant?”
- **Query:** $(e: Fulvestrant, (r: Causes, r: Assoc))$

Follow the query plan:

**Query Plan**

**Embedding Process**

- Fulvestrant
- Causes
- Brain Bleeding
- Headache
- Short of Breath
- Kidney Infection
Traversing KG in Vector Space (3)

Embed path queries in vector space.

- **Question:** “What proteins are associated with adverse events caused by Fulvestrant?”
- **Query:** (e:Fulvestrant, (r:Causes, r:Assoc))

Follow the query plan:

**Query Plan**

**Embedding Process**

**Answers!**
Insights:

- We can train **TransE** to optimize knowledge graph completion objective (Lecture 11)

- Since **TransE** can naturally handle *compositional relations*, it can handle path queries by translating in the latent space for multiple hops using addition of relation embeddings.

- For **TransR / DistMult / ComplEx**, since they cannot handle compositional relations, they cannot be easily extended to handle path queries.
Can we answer **more complex queries with logic conjunction operation**?

- **Conjunctive Queries**: “What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

  \[
  ((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy)))
  \]

**Query plan:**

- ESR2
- Assoc
- TreatedBy
- Intersection
- Short of Breath
- CausedBy
- Intersection
“What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

((e:ESR2, r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))
“What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy)))

Traverse KG from anchor nodes: ESR2 and Short of Breath:

Traverse from the first anchor “ESR2” by relation “Assoc”, we reach a set of entities {“Lung Cancer”, “Breast Cancer”}
“What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

Traverse KG from anchor nodes: ESR2 and Short of Breath:

Traverse from the set of entities {“Lung Cancer”, “Breast Cancer”} by relation TreatedBy, we reach a set of entities {“Paclitaxel”, “Arimidex”, “Fulvestrant”}
“What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy)))

Traverse KG from anchor nodes: ESR2 and Short of Breath:

Traverse from the second anchor “Short of Breath” by relation “CausedBy”, we reach a set of entities {“Fulvestrant”, “Ketamin”, “Paclitaxel”}
“What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy)))

Traverse KG from anchor nodes: ESR2 and Short of Breath:

We take intersection between the two sets and get the answers {“Fulvestrant”, “Paclitaxel”}
“What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CauseBy)))

Traverse KG from anchor nodes: ESR2 and Short of Breath:

If this link is missing, then we cannot find Fulvestrant to be an answer.
How can we use embeddings to implicitly impute the missing (ESR2, Assoc, Breast Cancer)?

**Intuition:** ESR2 interacts with both BRCA1 and ESR1. Both proteins are associated with breast cancer.
“What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

\[
((e:\text{ESR2}, (r:\text{Assoc}, r:\text{TreatedBy})), (e:\text{Short of Breath}, (r:\text{CausedBy})))
\]

**Query plan:**

Each intermediate node represents a set of entities, how do we represent it? How do we define the intersection operation in the latent space?
Stanford CS224W: Query2Box: Reasoning over KGs Using Box Embeddings
How can we answer more complex queries with logical conjunction operation?

Query plan:

1. Each intermediate node represents a set of entities; how do we represent it?
2. How do we define the intersection operation in the latent space?
Box Embeddings

- Embed queries with hyper-rectangles (boxes)
  \[ q = (\text{Center}(q), \text{Offset}(q)) \]

For example, we can embed the adverse events of Fulvestrant with a box that enclose all the answer entities.
Key Insight: Intersection

- Intersection of boxes is well-defined!
- When we traverse the KG to find the answers, each step produces a set of reachable entities.
- How can we better model these sets?
  - Boxes are a **powerful abstraction**, as we can project the center and control the offset to model the set of entities enclosed in the box.

```
<table>
<thead>
<tr>
<th>Short of Breath</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kidney Infection</td>
</tr>
<tr>
<td>Headache</td>
</tr>
</tbody>
</table>
```
Things to figure out:

- **Entity embeddings (# params: \(d|V|\))**:
  - Entities are seen as zero-volume boxes

- **Relation embeddings (# params \(2d|R|\))**:
  - Each relation takes a box and produces a new box

- **Intersection operator \(f\)**:
  - New operator, inputs are boxes and output is a box
  - Intuitively models intersection of boxes

---

**Notation**

- \(d\): out degree
- \(|V|\): # entities
- \(|R|\): # relations
Embed queries in vector space: “What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

\(((e:\text{ESR2}, (r:\text{Assoc, } r:\text{TreatedBy})), (e:\text{Short of Breath}, (r:\text{CausedBy}))))

Traverse KG from anchor nodes: ESR2 and Short of Breath:
**Projection Operator**

- **Intuition:**
  - Take the current box as input and use the relation embedding to **project and expand** the box!
- $P : \text{Box} \times \text{Relation} \rightarrow \text{Box}$

  \[
  \text{Cen}(q') = \text{Cen}(q) + \text{Cen}(r) \\
  \text{Off}(q') = \text{Off}(q) + \text{Off}(r)
  \]

"×" (cross) means the projection operator is a **relation** from any box and **relation** to a new box.
embed queries in vector space: “What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?”

- Traverse KG from anchor nodes: ESR2 and Short of Breath:
- Use projection operator again following the query plan.

Query Plan

Embedding Space
“What is the drug that causes Short of Breath and treats disease associated with protein ESR2?”

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy)))

- Use projection operator again following the query plan.
“What is the drug that causes Short of Breath and treats disease associated with protein ESR2?”

\[
((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy)))
\]

- Use projection operator again following the query plan.

### Query Plan

- ESR2
- Assoc
- TreatedBy
- Short of Breath
- CausedBy

### Embedding Space

- Breast Cancer
- Lung Cancer
- Arimidex
- Paclitaxel
- Fulvestrant
- Ketamin
- ESR2
- Short of Breath
- CausedBy
- TreatedBy
“What is the drug that causes Short of Breath and treats disease associated with protein ESR2?”

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy)))

- How do we take intersection of boxes?
Geometric Intersection Operator $\mathcal{I}$
- Take multiple boxes as input and produce the intersection box
- **Intuition:**
  - The center of the new box should be "close" to the centers of the input boxes
  - The offset (box size) should shrink (since the size of the intersected set is smaller than the size of all the input set)
- $\mathcal{I} : \text{Box} \times \cdots \times \text{Box} \rightarrow \text{Box}
Geometric Intersection Operator $\mathcal{I}$

- $\mathcal{I} : \text{Box} \times \cdots \times \text{Box} \to \text{Box}$

\[
Cen(q_{\text{inter}}) = \sum_{i} w_i \odot Cen(q_i)
\]

\[
w_i = \frac{\exp(f_{cen}(Cen(q_i)))}{\sum_{j} \exp(f_{cen}(Cen(q_j)))}
\]

Intuition: The center should be in the red region!

Implementation: The center is a weighted sum of the input box centers.

$w_i \in \mathbb{R}^d$ is calculated by a neural network $f_{cen}$ (with trainable weights).

$w_i$ represents a “self-attention” score for the center of each input $Cen(q_i)$. 

Hadamard product (element-wise product)
Geometric Intersection Operator $J$

- $J : \text{Box} \times \cdots \times \text{Box} \rightarrow \text{Box}$

$$
\text{Off}(q_{\text{inter}}) \\
= \min(\text{Off}(q_1), ..., \text{Off}(q_n)) \\
\circ \sigma(f_{\text{off}}(\text{Off}(q_1), ..., \text{Off}(q_n)))
$$

**Intuition:** The offset should be smaller than the offset of the input box

**Implementation:** We first take minimum of the offset of the input box, and then we make the model more expressive by introducing a new function $f_{\text{off}}$ to extract the representation of the input boxes with a sigmoid function to guarantee shrinking.

- $f_{\text{off}}$ is a neural network (with trainable parameters) that extracts the representation of the input boxes to increase expressiveness

Sigmoid function: squashes output in (0,1)
“What is the drug that causes Short of Breath and treats disease associated with protein ESR2?”

\[(\text{e:ESR2, (r:Assoc, r:TreatedBy)}, (\text{e:Short of Breath, (r:CausedBy)}))\]

- Use box intersection operator

![Diagram showing the query plan and embedding space](image)
How do we define the score function $f_q(v)$ (negative distance)?

($f_q(v)$ captures inverse distance of a node $v$ as answer to $q$)

Given a query box $q$ and entity embedding (box) $v$,

$$d_{box}(q, v) = d_{out}(q, v) + \alpha \cdot d_{in}(q, v)$$

where $0 < \alpha < 1$.

**Intuition**: if the point is enclosed in the box, the distance should be downweighted.

$$f_q(v) = -d_{box}(q, v)$$
Can we embed complex queries with union? E.g.: “What drug can treat breast cancer or lung cancer?”

**Conjunctive queries + disjunction** is called **Existential Positive First-order (EPFO)** queries. We’ll refer to them as **AND-OR** queries.

Can we also design a disjunction operator and embed AND-OR queries in low-dimensional vector space?
Can we embed AND-OR queries in a low-dimensional vector space?

No! Intuition: Allowing union over arbitrary queries requires high-dimensional embeddings!

Example:
- Given 3 queries $q_1, q_2, q_3$, with answer sets:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$
- If we allow union operation, can we embed them in a two-dimensional plane?
Example:

- Given 3 queries $q_1, q_2, q_3$, with answer sets:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$
- If we allow union operation, can we embed them in two-dimensional plane?

We want red dots (answers) to be in the box while the blue dots (negative answers) to be outside the box.
Example:

- Given 3 queries $q_1, q_2, q_3$, with answer sets:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?

We want red dots (answers) to be in the box while the blue dots (negative answers) to be outside the box.
Example:

- Given 3 queries $q_1, q_2, q_3$, with answer sets:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$

- If we allow union operation, can we embed them in two-dimensional plane?

We want red dots (answers) to be in the box while the blue dots (negative answers) to be outside the box.
Example:

- Given 3 queries $q_1, q_2, q_3$, with answer sets:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$
- If we allow union operation, can we embed them in a two-dimensional plane?

We want red dots (answers) to be in the box while the blue dots (negative answers) to be outside the box.
Example:

- Given 3 queries $q_1, q_2, q_3$, with answer sets:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$
- If we allow union operation, can we embed them in two-dimensional plane?

We want red dots (answers) to be in the box while the blue dots (negative answers) to be outside the box.
Example:

- Given 3 queries $q_1, q_2, q_3$, with answer sets:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?

We want red dots (answers) to be in the box while the blue dots (negative answers) to be outside the box.
Example:

- Given 3 queries $q_1, q_2, q_3$, with answer sets:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$
- If we allow union operation, can we embed them in two-dimensional plane?

For 3 points, 2-dimension is okay!

How about 4 points?
Example 2:

- Given 4 queries $q_1, q_2, q_3, q_4$ with answers:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$, $[q_4] = \{v_4\}$,
  - If we allow union operation, can we embed them in two-dimensional plane?
Example 2:

- Given 4 queries $q_1, q_2, q_3, q_4$ with answers:
  - $[q_1] = \{v_1\}$, $[q_2] = \{v_2\}$, $[q_3] = \{v_3\}$, $[q_4] = \{v_4\}$,
- If we allow union operation, can we embed them in two-dimensional plane?

We cannot design a box embedding for $q_2 \lor q_4$, that only $v_2$ and $v_4$ are in the box but $v_1$ and $v_3$ are outside the box.
Can we embed AND-OR queries in low-dimensional vector space?

- **Conclusion**: Given any $M$ conjunctive queries $q_1, \ldots, q_M$ with non-overlapping answers, we need dimensionality of $\Theta(M)$ to handle all OR queries.
  - For real-world KG, such as FB15k, we find $M \geq 13,365$, where $|V| = 14,951$.
  - Remember, this is for arbitrary OR queries.
Since we cannot embed AND-OR queries in low-dimensional space, can we still handle them?  
- **Key idea**: take all unions out and only do union at the last step!
Any AND-OR query can be transformed into equivalent DNF, i.e., disjunction of conjunctive queries.

Given any AND-OR query $q$,

$$q = q_1 \lor q_2 \lor \cdots \lor q_m$$

where $q_i$ is a conjunctive query.

Now we can first embed each $q_i$ and then “aggregate” at the last step!
Distance Between $q$ and an Entity

- **Distance** between entity embedding and a DNF $q = q_1 \lor q_2 \lor \cdots \lor q_m$ is defined as:
  $$d_{box}(q, v) = \min(d_{box}(q_1, v), \ldots, d_{box}(q_m, v))$$

- **Intuition:**
  - As long as $v$ is the answer to one conjunctive query $q_i$, then $v$ should be the answer to $q$.
  - As long as $v$ is close to one conjunctive query $q_i$, then $v$ should be close to $q$ in the embedding space.
Distance between entity embedding and a DNF $q = q_1 \lor q_2 \lor \cdots \lor q_m$ is defined as:

$$d_{box}(q, v) = \min(d_{box}(q_1, v), \ldots, d_{box}(q_m, v))$$

The process of embedding any AND-OR query $q$

1. Transform $q$ to equivalent DNF $q_1 \lor \cdots \lor q_m$
2. Embed $q_1$ to $q_m$
3. Calculate the (box) distance $d_{box}(q_i, v)$
4. Take the minimum of all distance
5. The final score $f_q(v) = -d_{box}(q, v)$
Stanford CS224W: How to Train Query2box

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu
Overview and Intuition (similar to KG completion):

- Given a query embedding $q$, maximize the score $f_q(v)$ for answers $v \in q$ and minimize the score $f_q(v')$ for negative answers $v' \notin q$.

Trainable parameters:

- Entity embeddings with $d|V|$ # params
- Relation embeddings with $2d|R|$ # params
- Intersection operator

How to achieve a query, its answers, its negative answers from the KG to train the parameters?

How to split the KG for query answering?
Generate a set of training queries \((q, v, v')\).
Train entity embeddings and operators to minimize the loss (i.e., to answer the training queries correctly).

Each training query provides a “constrain” on the embeddings of entities.

Training loop:
1) Get query \((q, v, v')\)
2) Using current operators, embed \(q\)
3) Compute the loss to update entity embs. and operators
Training: Details

Training:

1. Sample a query $q$ from the training graph $G_{\text{train}}$, answer $v \in [q]_{G_{\text{train}}}$, and non-answer $v' \notin [q]_{G_{\text{train}}}$.

2. Embed the query $q$.
   - Use current operators, to compute query embedding.

3. Calculate the score $f_q(v)$ and $f_q(v')$.

4. Optimize embeddings and operators to minimize the loss $\ell$ (maximize $f_q(v)$ while minimize $f_q(v')$):

$$\ell = -\log \sigma(f_q(v)) - \log(1 - \sigma(f_q(v')))$$
Generate queries from multiple query templates:
How can we generate a complex query?

- We start with a **query template**
- **Query template** is an abstraction of the query
- We generate a query by instantiating every variable with a concrete entity and relation from the KG
  - E.g., instantiate **Anchor1** with **ESR2** (a node on KG)
  - E.g., instantiate **Rel1** with **Assoc** (an edge on KG)
- **How to instantiate query template given a KG?**

**Query**

\[
(e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))
\]

**Query Template**

\[
((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3)))
\]

---

**Diagram:**

1. ESR2
2. Assoc
3. TreatedBy
4. Intersection
5. Short of Breath
6. CausedBy
7. Intersection
8. Projection
9. Projection
10. Intersection

---

**Image:**

- [Image](image-url)
### How to instantiate a query template given a KG?

**Query Template**

```
((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3)))
```

**Knowledge Graph**

- Lung Cancer
- Paclitaxel
- Breast Cancer
- Arimidex
- TreatedBy
- Fulvestrant
- Short of Breath
- CausedBy
- Ketamin
- ESR2

**Overview:**

Start from instantiating the **answer node** of the query template and then iteratively instantiate the other edges and nodes until we ground **all the anchor nodes**.
How to instantiate a query template given a KG?

Start from instantiating the root node of the query template.

Randomly pick one entity from KG as the root node, e.g., we pick **Fulvestrant**.
How to instantiate a query template given a KG?

Now we look at intersection. What we have is that the intersection of the sets of entities is **Fulvestrant**, then naturally the two sets should also contain **Fulvestrant**.
How to instantiate a query template given a KG?

We instantiate the **Projection edge** in the template by randomly sample one relation associated with the current entity **Fulvestrant**. For example, we may select relation **TreatedBy**, and check what entities are connected to **Fulvestrant** with **TreatedBy**: \{Breast Cancer\}.
How to instantiate a query template given a KG?

We first look at one branch and ground the Projection edge with the relation associated with Breast Cancer, e.g., Assoc. Then we check what entities are connected to Breast Cancer with Assoc: {ESR2}. 
How to instantiate a query template given a KG?

Then we look at the second branch and ground the **Projection edge** with the relation associated with **Fulvestrant**, e.g., **CausedBy**. Then we check what entities are connected to **Fulvestrant** with **CausedBy**: \{Short of Breath\}. 
How to instantiate a query template given a KG?

**Query Template**

```
((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3)))
```

**Knowledge Graph**

- **CausedBy**: ESR2 → Breast Cancer
- **Assoc**: Breast Cancer → Lung Cancer
- **TreatedBy**: Fulvestrant → Arimidex
- **TreatedBy**: Fulvestrant → Paclitaxel
- **CausedBy**: Short of Breath → Ketamin

We select entity from **Short of Breath**, set it as the anchor node.
How to instantiate a query template given a KG?

Now, we instantiated a query $q$!

$q$: $((e:\text{ESR2}, (r:\text{Assoc}, r:\text{TreatedBy})), (e:\text{Short of Breath}, (r:\text{CausedBy})))$

• The query $q$ must have answers on the KG and one of the answers is the instantiated answer node: Fulvestrant.
• We may obtain the full set of answers $\llbracket q \rrbracket_G$ by KG traversal.
• We can sample negative answers $\nu' \notin \llbracket q \rrbracket_G$
What do box embeddings actually learn?

Example: “List male instrumentalists who play string instruments”

We use t-SNE to reduce the embedding space to a 2-dimensional space, in order to visualize the query results.
“List male instrumentalists who play string instruments”
“List male instrumentalists who play string instruments”
“List male instrumentalists who play string instruments”
“List male instrumentalists who play string instruments”

# of instrumentalists: 472

TPR: 98.4%
FPR: 0.01%
“List male instrumentalists who play string instruments”
"List male instrumentalists who play string instruments"
“List male instrumentalists who play string instruments”

- TP
- FN
- FP
- TN

# of answers: 396

TPR: 99.4%
FPR: 0.01%
We introduce answering predictive queries on large knowledge graphs.

The key idea is to embed queries by navigating the embedding space!

- We embed the query by composing learned operators
- Embedding of the query is close to its answers in the embedding space