IT5429E-1-24 (24.1A01)(Fall 2024): Graph Analytics for Big Data

Week 6: Knowledge Graphs - Reasoning

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Many slides are adapted from https://web.stanford.edu/class/cs224w/

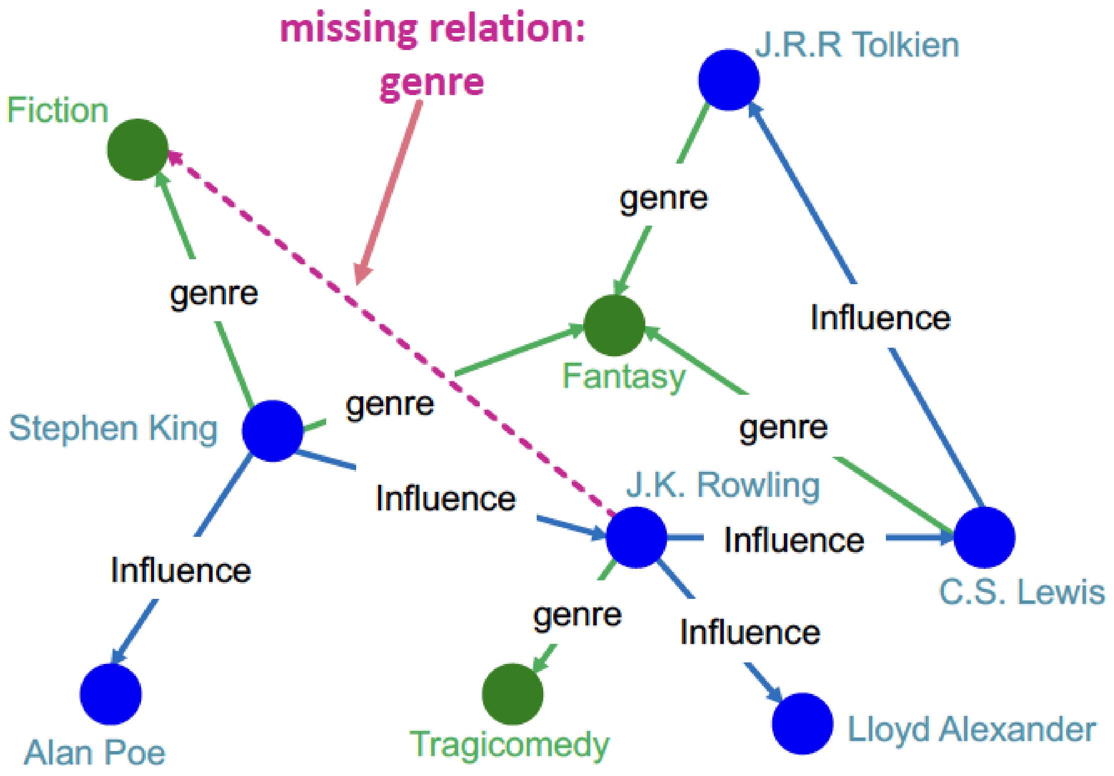
Announcement

- Starting from next week, all lectures will be taught on Zoom
- Zoom link: https://uoregon.zoom.us/j/94399627466?pwd=UaOfNVJWLcDi62sXpyS6iPeTBGIKVQ.1

Recap: KG Completion Task

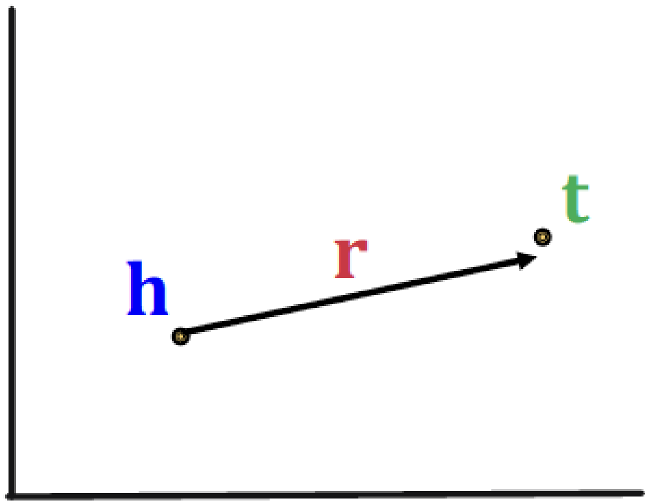
- Given an enormous KG, can we complete the KG?
  - For a given (head, relation), we predict missing tails.
  - Note: this is slightly different from link prediction task.

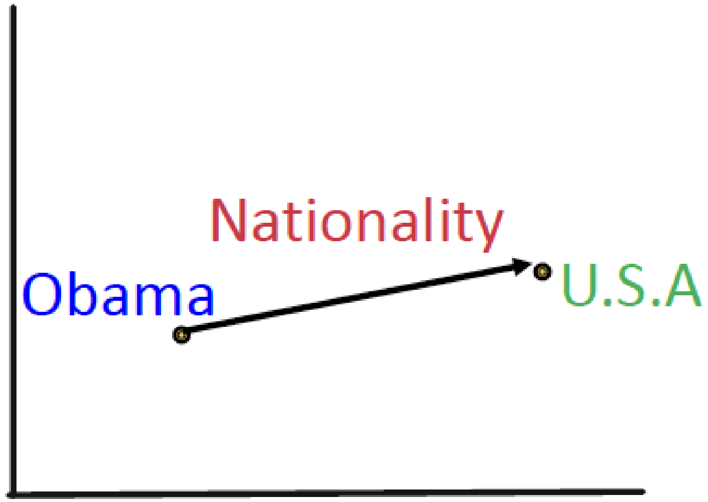
Example task: Predict the tail "Science Fiction" for ("J.K. Rowling", "genre")



TransE

- Intuition: Translation
  - For a triple (h, r, t), let $h, r, t \in \mathbb{R}^d$ be embedding vectors
  - TransE: $h + r \approx t$ if the given link exists; else $h + r \neq t$
- Entity scoring function: $f_r(h, t) = -\,\|h + r - t\|$

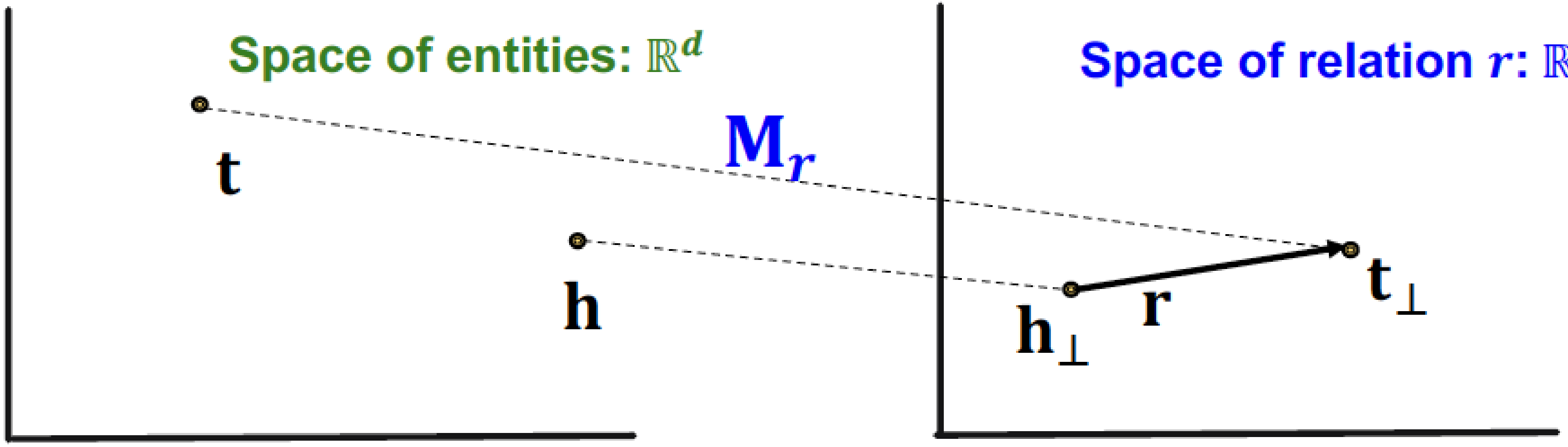




TransR

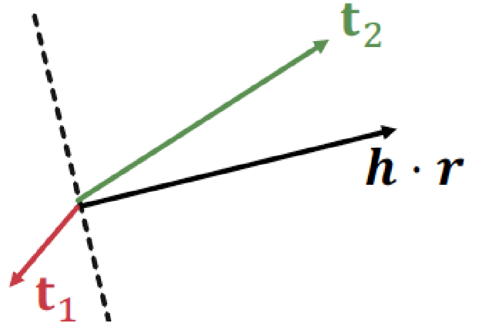
- TransR: model entities as vectors in the entity space $\mathbb{R}^{d}$ and model each relation as vector in relation space $r \in \mathbb{R}^{k}$ with $M_r \in \mathbb{R}^{k \times d}$ as the projection matrix.
- $h_\perp = M_r h, t_\perp = M_r t$
- Score function: $f_r(h,t) = -\|h_\perp + r - t_\perp\|$

Use M_r to project from entity space $\mathbb{R}^d$ to relation space $\mathbb{R}^k$!!



DistMult

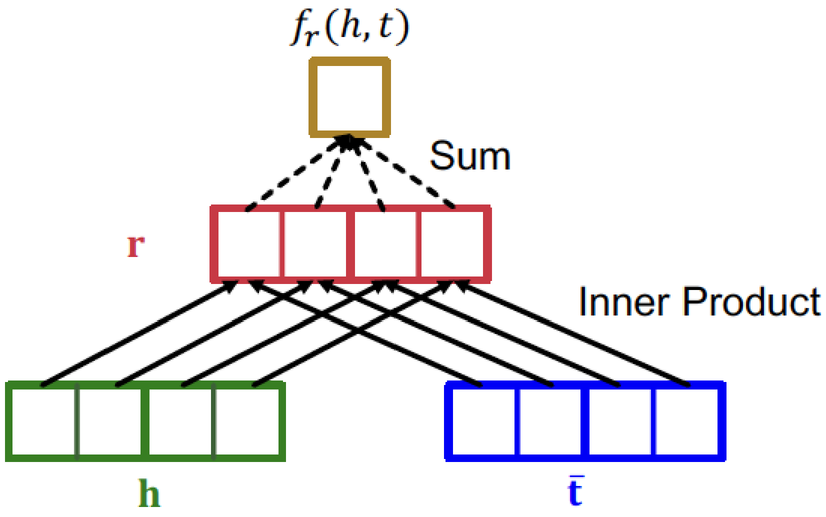
- DistMult: Entities and relations using vectors in $\mathbb{R}^k$
- Score function: $f_r(h,t) = \langle h, r, t \rangle = \sum_i h_i \cdot r_i \cdot t_i$
- $h, r, t \in \mathbb{R}^k$
- Intuition of the score function: Can be viewed as a cosine similarity between $h \odot r$ and t where $\odot$ is the Hadamard product (elementwise product)
- Example: $f_r(h, t_1) < 0, \quad f_r(h, t_2) > 0$



ComplEx

- Based on Distmult, ComplEx embeds entities and relations in Complex vector space
- ComplEx: model entities and relations using vectors in $\mathbb{C}^k$
- Score function: $f_r(h,t) = \mathrm{Re}(\sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{t}}_i)$

$$
\begin{aligned}
&= \langle \mathrm{Re}(\mathbf{h}_i), \mathrm{Re}(\mathbf{r}_i), \mathrm{Re}(\mathbf{t}_i) \rangle \\
&+ \langle \mathrm{Re}(\mathbf{h}_i), \mathrm{Im}(\mathbf{r}_i), \mathrm{Im}(\mathbf{t}_i) \rangle \\
&+ \langle \mathrm{Im}(\mathbf{h}_i), \mathrm{Re}(\mathbf{r}_i), \mathrm{Im}(\mathbf{t}_i) \rangle \\
&- \langle \mathrm{Im}(\mathbf{h}_i), \mathrm{Im}(\mathbf{r}_i), \mathrm{Re}(\mathbf{t}_i) \rangle
\end{aligned}
$$



Model Relation Properties

- Different models are…
  - …based on different geometric intuitions
  - …capture different types of relations (have different expressivity)

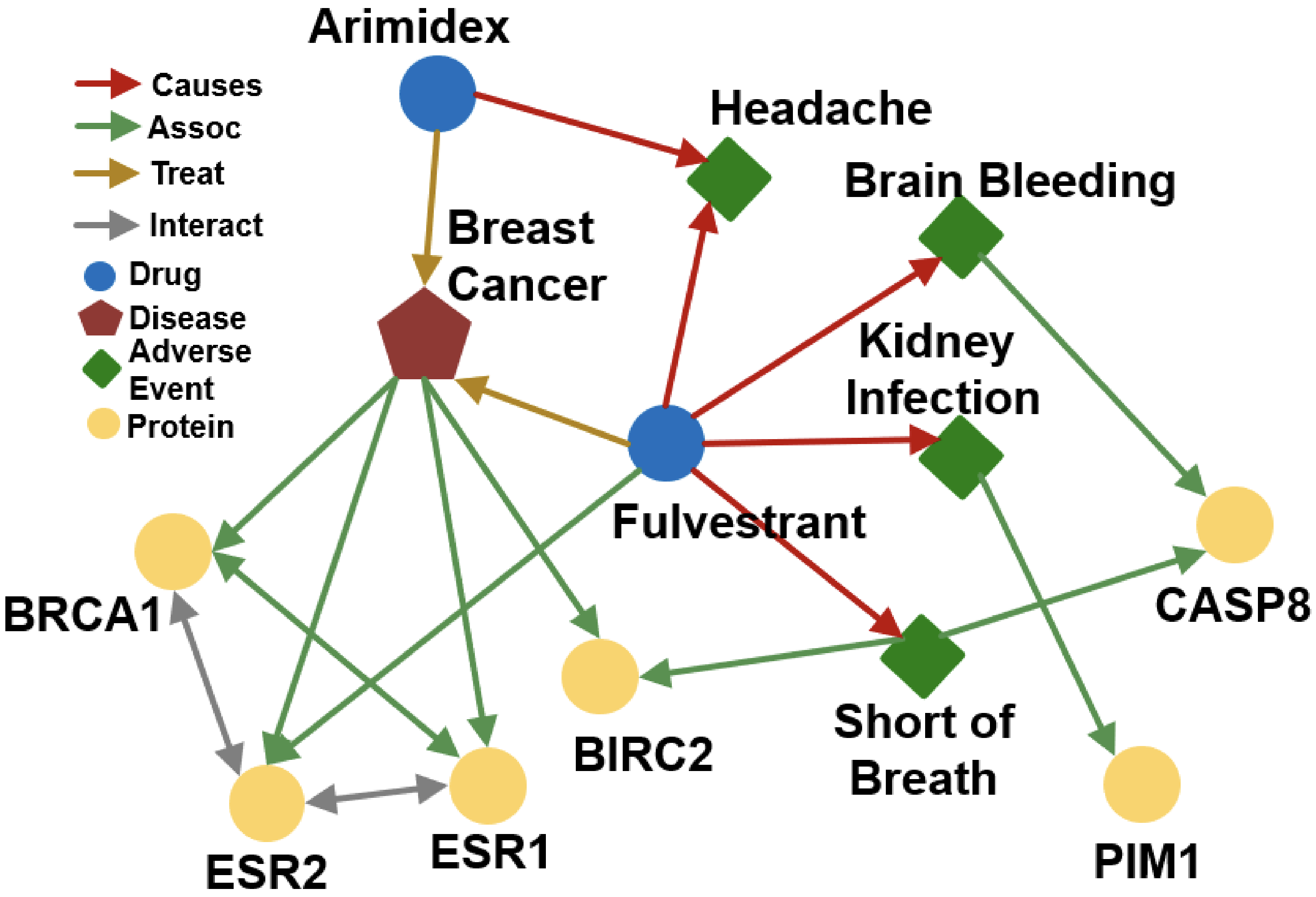
Model	Score	Embedding	Sym.	Antisym.	Inv.	Compos.	1-to-N
TransE	$-\|\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|\|$	$\mathbf{h},\mathbf{t},\mathbf{r} \in \mathbb{R}^k$	✗	✓	✓	✓	✗
TransR	$-\|\|\boldsymbol{M}_r\mathbf{h}+\mathbf{r} - \boldsymbol{M}_r\mathbf{t}\|\|$	$\mathbf{h},\mathbf{t} \in \mathbb{R}^k$, $\mathbf{r} \in \mathbb{R}^d$, $\boldsymbol{M}_r \in \mathbb{R}^{d \times k}$	✓	✓	✓	✓	✓
DistMult	$<\mathbf{h},\mathbf{r},\mathbf{t}>$	$\mathbf{h},\mathbf{t},\mathbf{r} \in \mathbb{R}^k$	✓	✗	✗	✗	✓
ComplEx	$\mathrm{Re}(<\mathbf{h},\mathbf{r},\bar{\mathbf{t}}>)$	$\mathbf{h},\mathbf{t},\mathbf{r} \in \mathbb{C}^k$	✓	✓	✓	✗	✓

Today: Reasoning over KGs

- 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

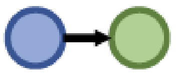


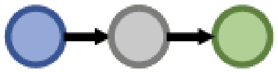
Predictive Queries on KG

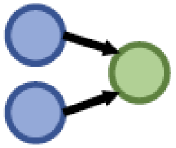
- Can we do multi-hop reasoning, i.e., answer complex queries on an incomplete, massive KG?

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

- In this lecture, we only focus on answering queries on a KG!


One-hop Queries


Path Queries


Conjunctive Queries

Predictive One-hop Queries

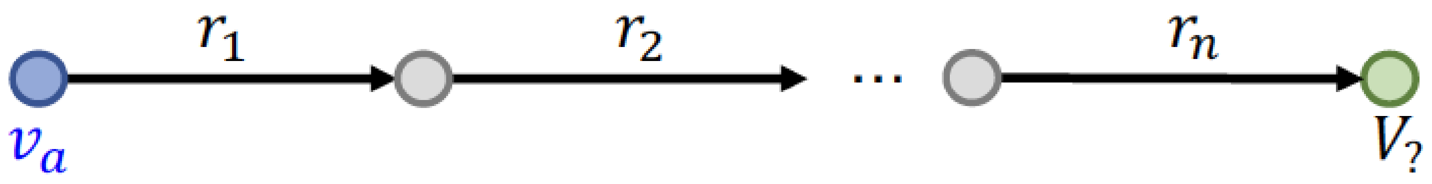
- We can formulate knowledge graph completion problems as answering one-hop queries.

- 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?

Path Queries

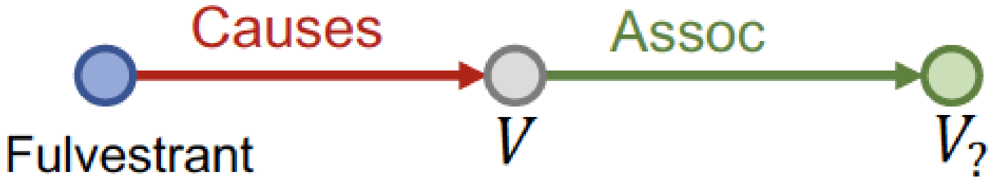
- Generalize one-hop queries to path queries by adding more relations on the path.
- An n-hop path query q can be represented by $q = \left(v_a, (r_1, r_2, \cdots, r_n)\right)$
  - v_a is an "anchor" entity
  - Let answers to q in graph G be denoted by $[\![q]\!]_G$
- Query plan for q



  - Query plan of path queries is a chain.

Path Queries

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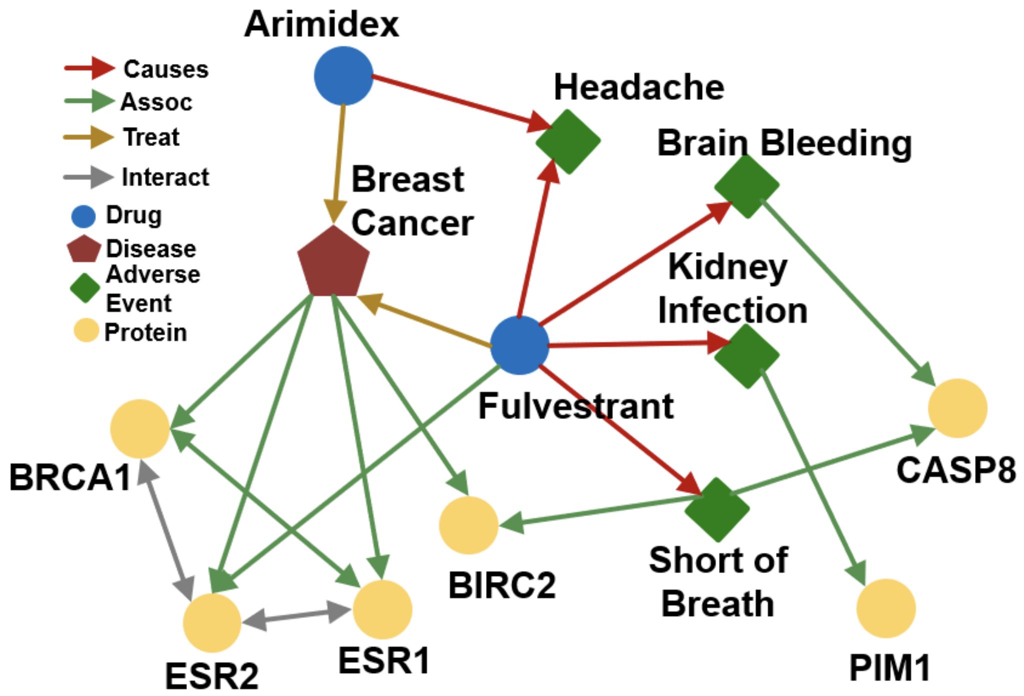
- Query: (e:Fulvestrant, (r:Causes, r:Assoc))

Path Queries

- 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?



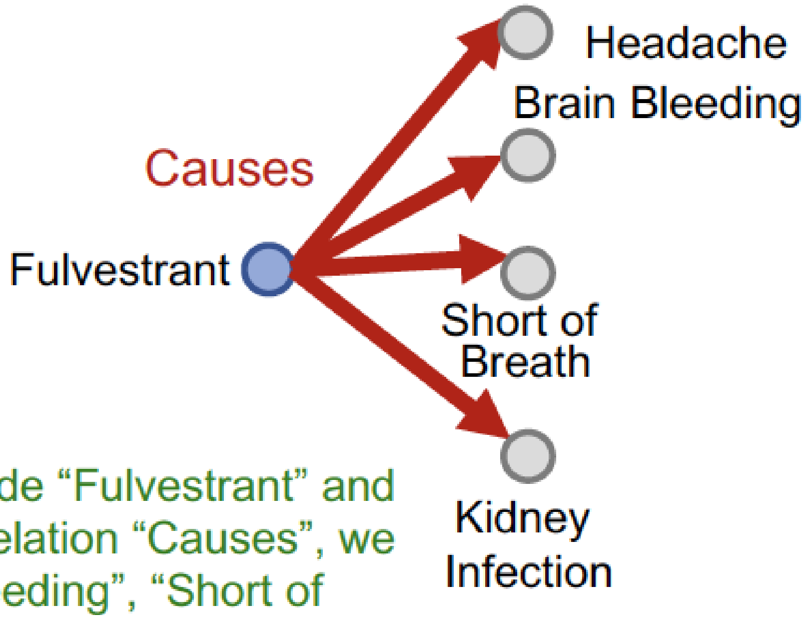
Traversing Knowledge Graphs

- 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).

Traversing Knowledge Graphs

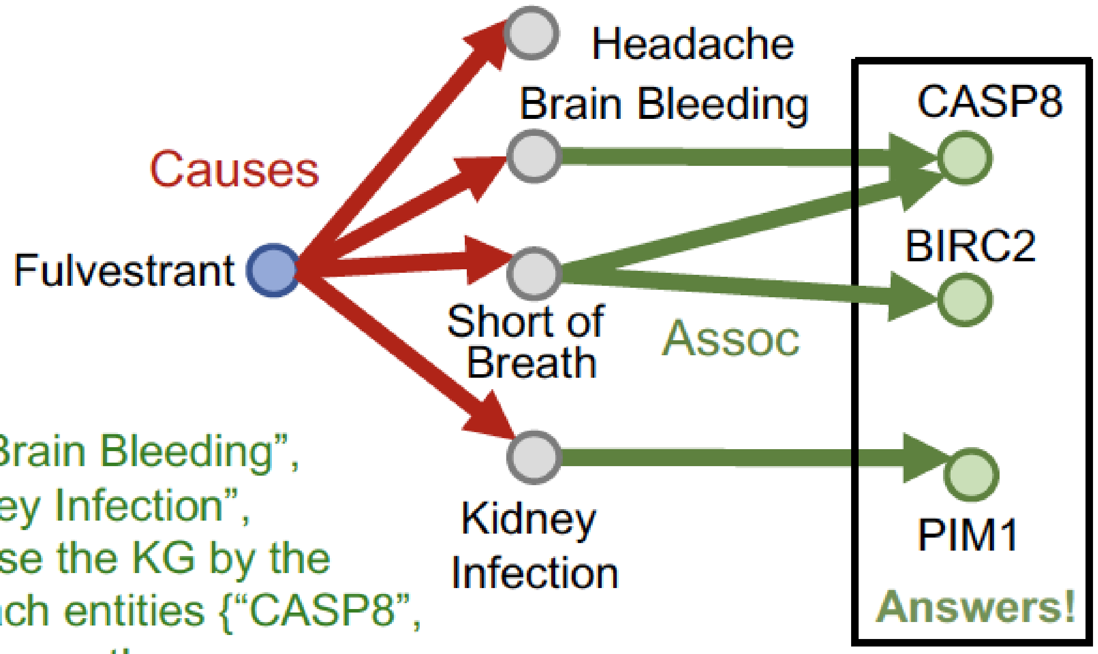
- We answer path queries by traversing the KG: “What proteins are associated with adverse events caused by Fulvestrant?”
- Query: (e:Fulvestrant, (r:Causes, r:Assoc))



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”}.

Traversing Knowledge Graphs

- 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.

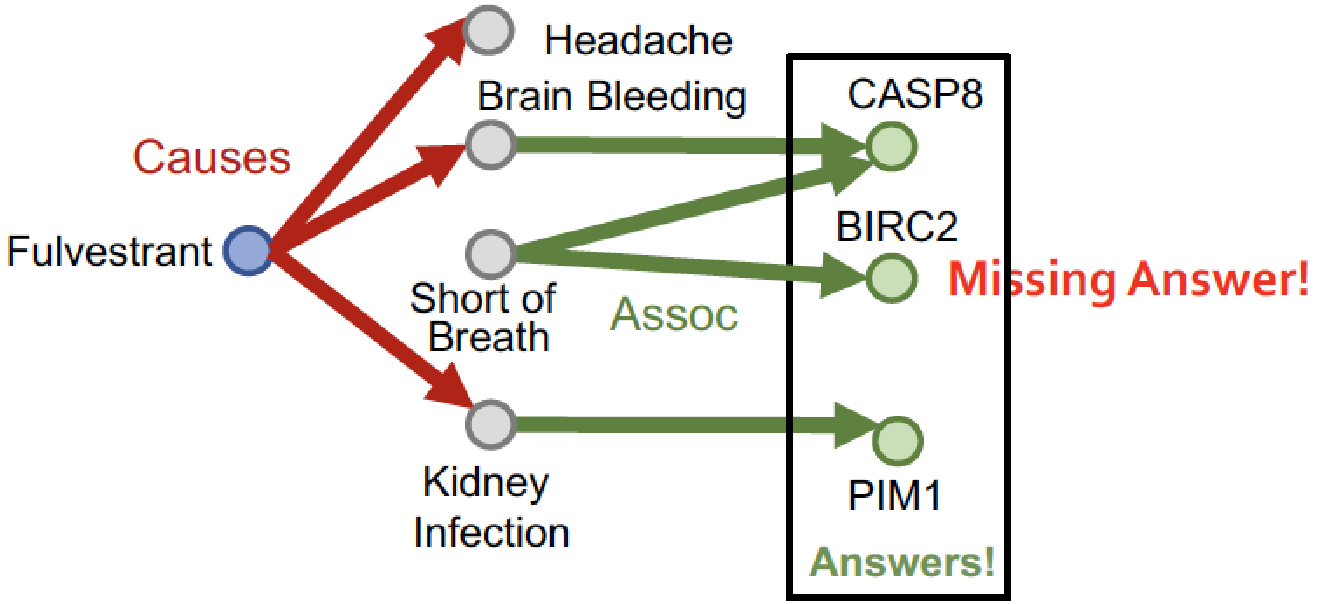
However, KGs are Incomplete

- 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!

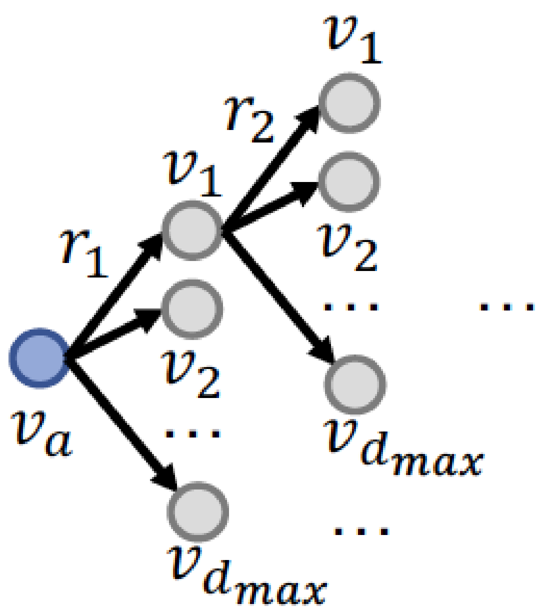
Example: Incomplete KG

- 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))



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.



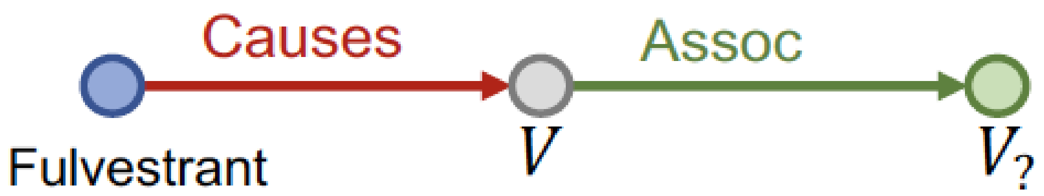
- Time complexity of traversing a dense KG is exponential as a function of the path length L:

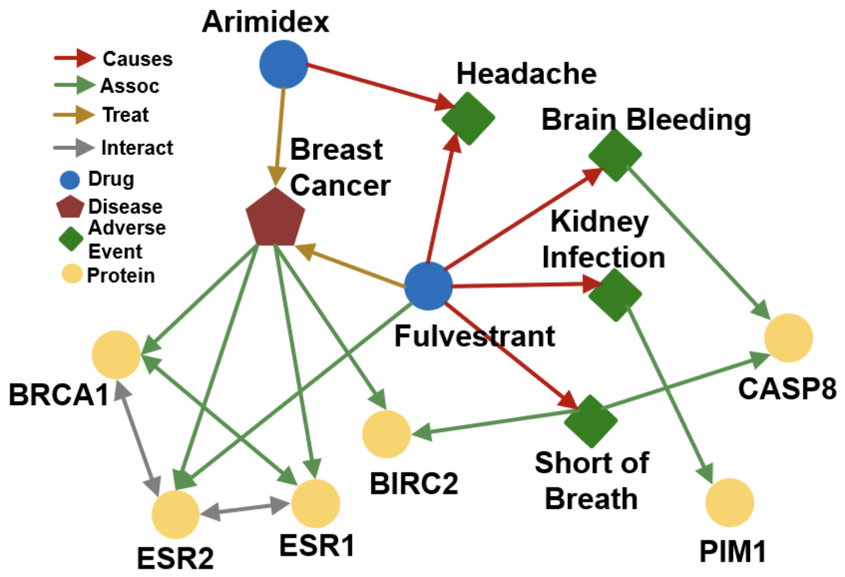
$$O(d_{max}^L)$$

  - d_{max}: max degree

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





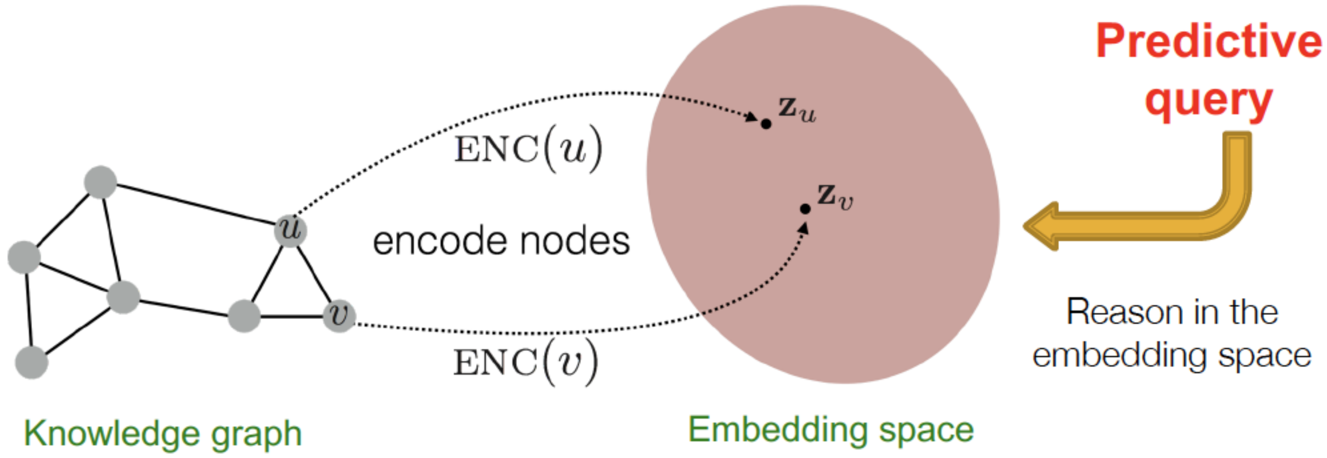
Outline

- 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

- How do we train the embeddings?
  - The process of determining entity and relation embeddings which allow us to embed a query.

Answering Predictive Queries on KGs

General Idea

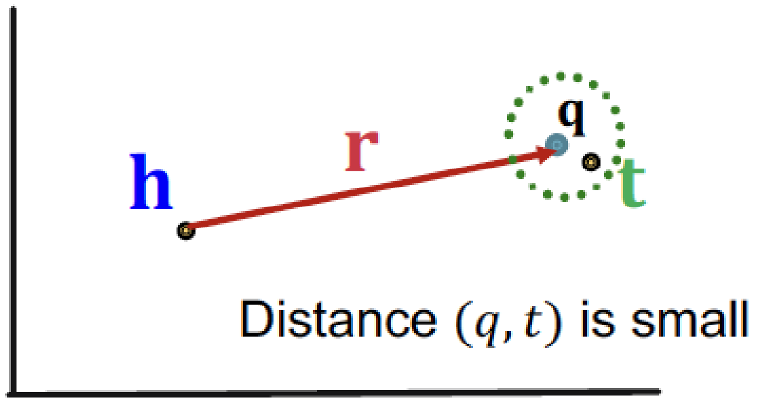


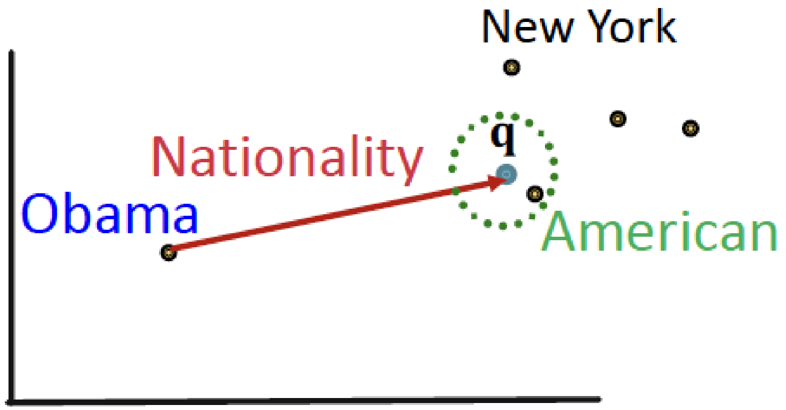
- Map queries into embedding space. Learn to reason in that space
  - Embed query into a single point in the Euclidean space: answer nodes are close to the query.
  - Query2Box: Embed query into a hyper-rectangle (box) in the Euclidean space: answer nodes are enclosed in the box.

1. Embedding Logical Queries on Knowledge Graphs. Hamilton, et al., NeurIPS 2018
2. Query2box: Reasoning over Knowledge Graphs in Vector Space Using Box Embeddings. Ren, et al., ICLR 2020

Idea: Traversing KG in Vector Space

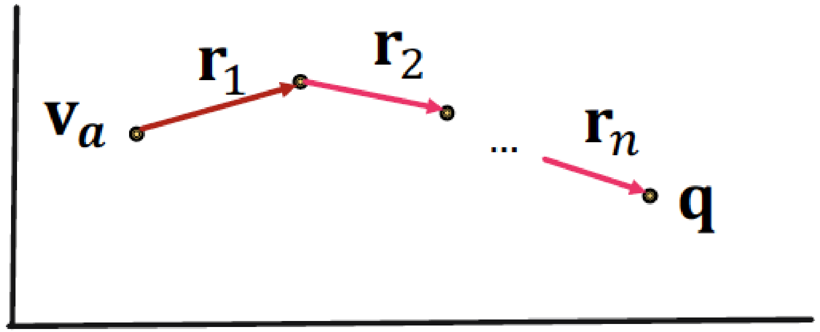
- Key idea: Embed queries!
  - Generalize TransE to multi-hop reasoning.
  - Recap: TransE: Translate **h** to **t** using **r** with score function $f_r(h,t) = -\|h+r-t\|$.
  - Another way to interpret this is that:
    - Query embedding: $\mathbf{q} = \mathbf{h} + \mathbf{r}$
    - Goal: query embedding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





Traversing KG in Vector Space

- Key idea: Embed queries!
  - Generalize TransE to multi-hop reasoning.
- Given a path query $q = (v_a, (r_1, r_2, \cdots, r_n))$



$$\mathbf{q} = \mathbf{v}_a + \mathbf{r}_1 + \cdots + \mathbf{r}_n$$

- The embedding process only involves vector addition, independent of # entities in the KG!

Traversing KG in Vector Space (1)

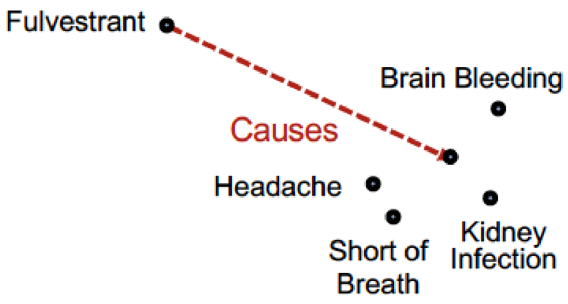
- Embed path queries in vector space.
- Question: "What proteins are associated with adverse events caused by Fulvestrant?"
- Query: (e:Fulvestrant, (r:Causes , r:Assoc))
- Follow the query plan:

Traversing KG in Vector Space (2)

- 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:

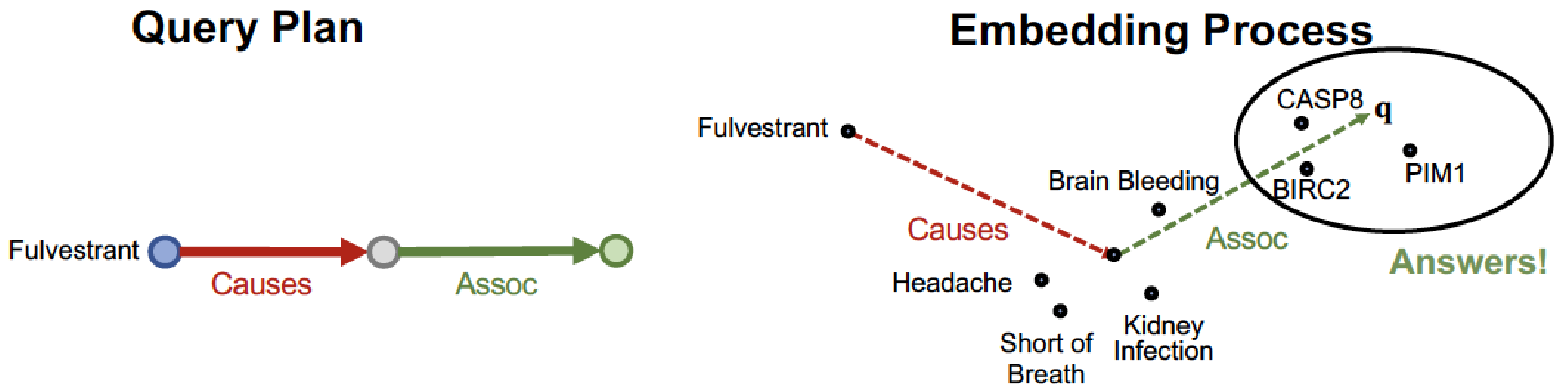
Query Plan

Embedding Process



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:

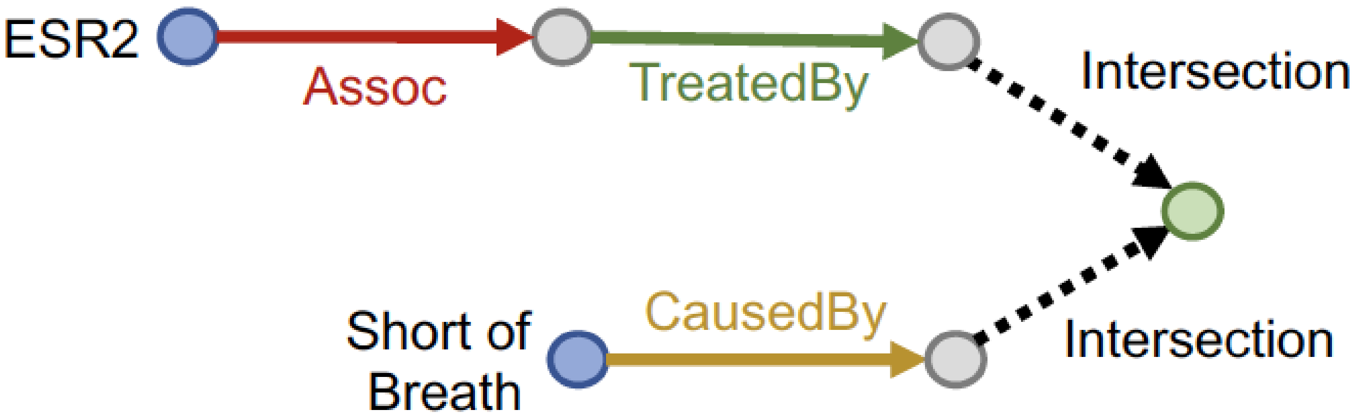


Traversing KG in Vector Space (4)

- Insights:
  - We can train TransE to optimize knowledge graph completion objective
  - 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 DistMult / ComplEx, since they cannot handle compositional relations, they cannot be easily extended to handle path queries.

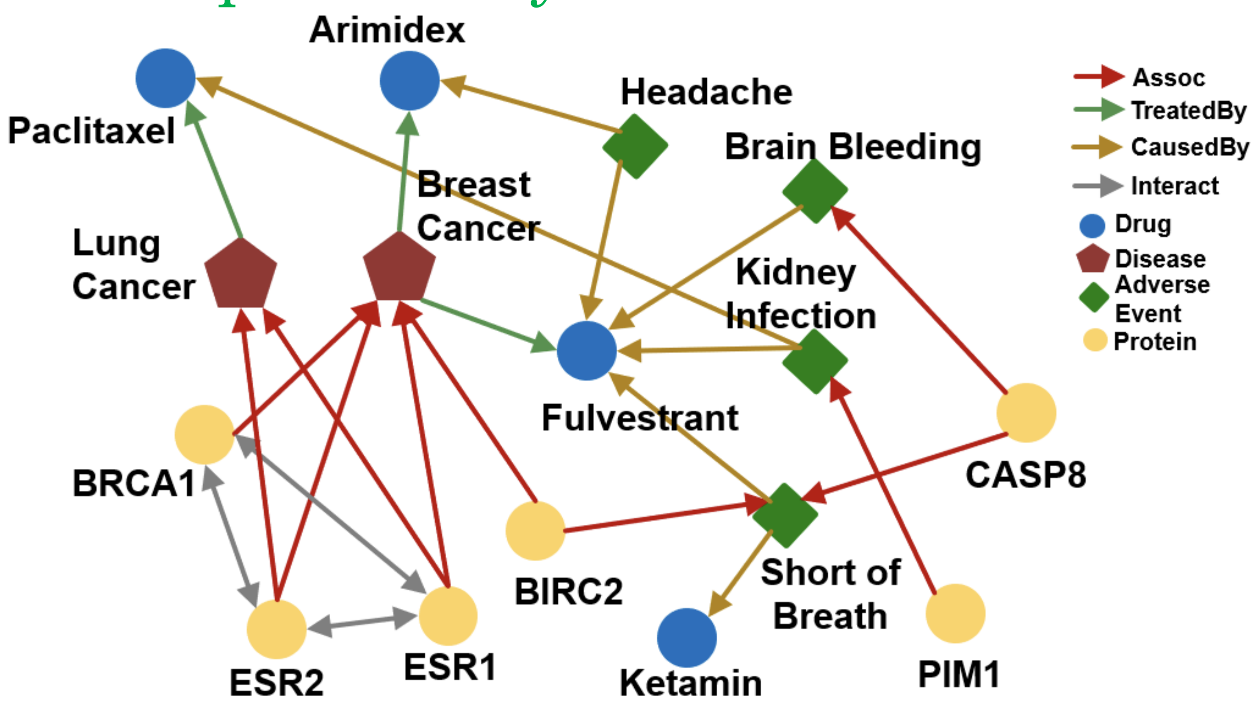
Conjunctive Queries

- 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:



Conjunctive Queries

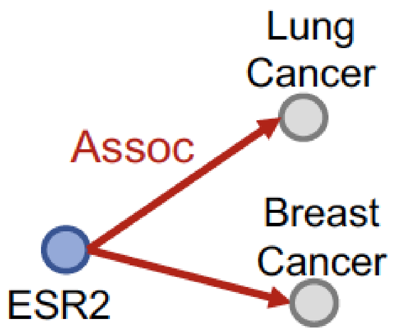
- Conjunctive Queries: "What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"
- ((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))
- How do we answer the question by KG traversal?



Traversing KG for Conjunctive Queries

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

Breath:

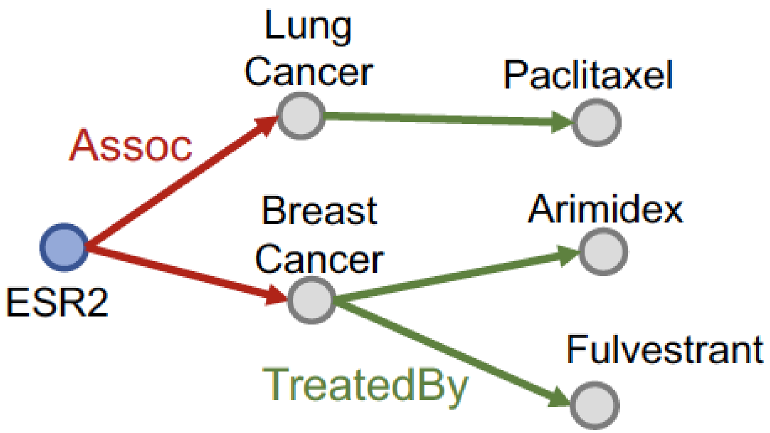


Traverse from the first anchor "ESR2" by relation "Assoc", we reach a set of entities {"Lung Cancer", "Breast Cancer"}

Traversing KG for Conjunctive Queries

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

Breath:

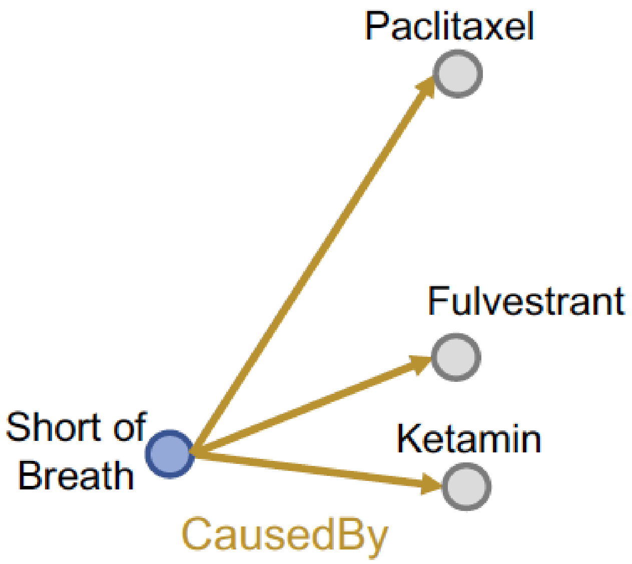


Traverse from the set of entities {"Lung Cancer", "Breast Cancer"} by relation TreatedBy, we reach a set of entities {"Paclitaxel", "Arimidex", "Fulvestrant"}

Traversing KG for Conjunctive Queries

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

Breath:

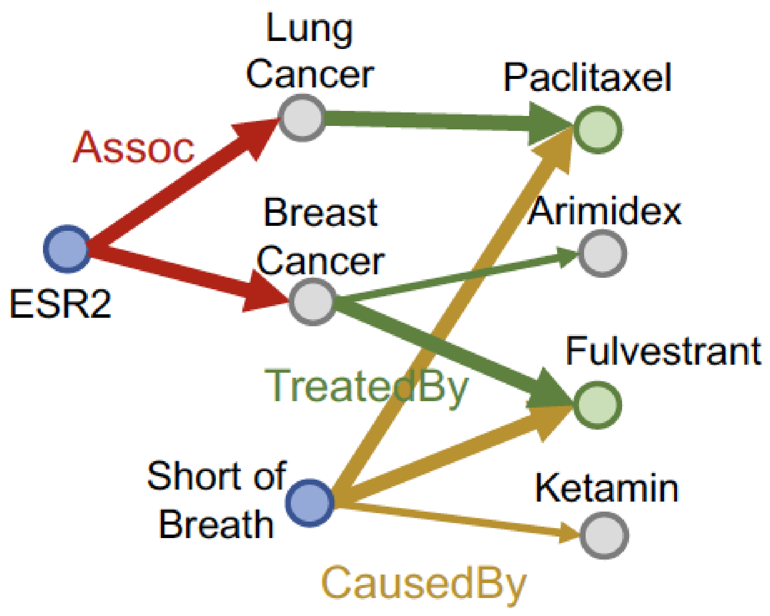


Traverse from the second anchor "Short of Breath" by relation "CausedBy", we reach a set of entities {"Fulvestrant", "Ketamin", "Paclitaxel"}

Traversing KG for Conjunctive Queries

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

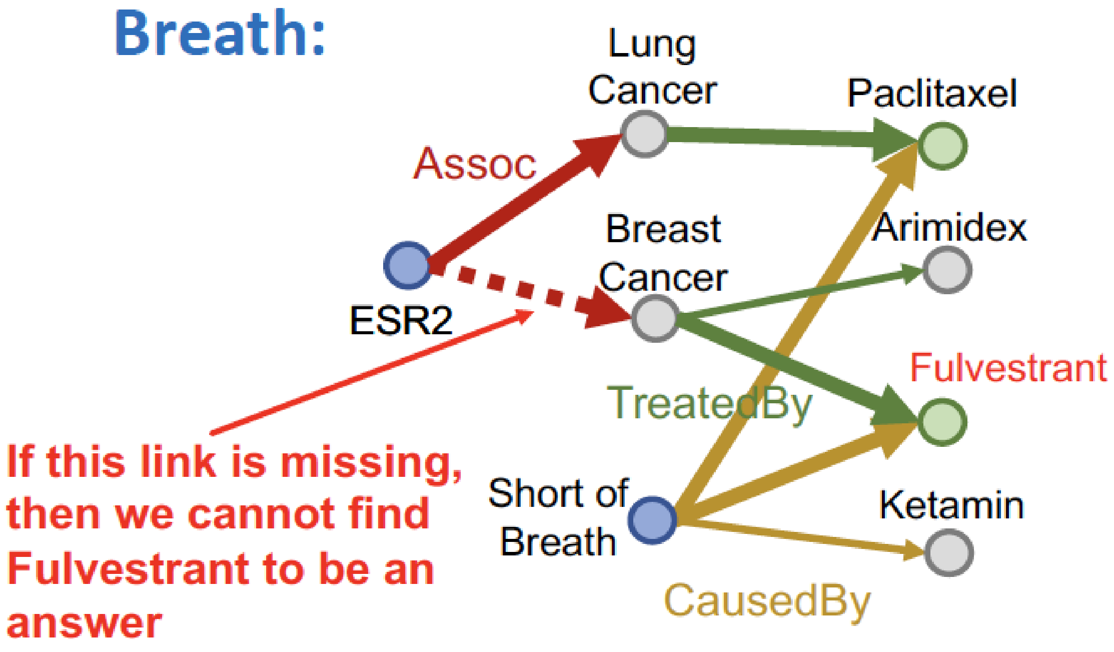
Breath:



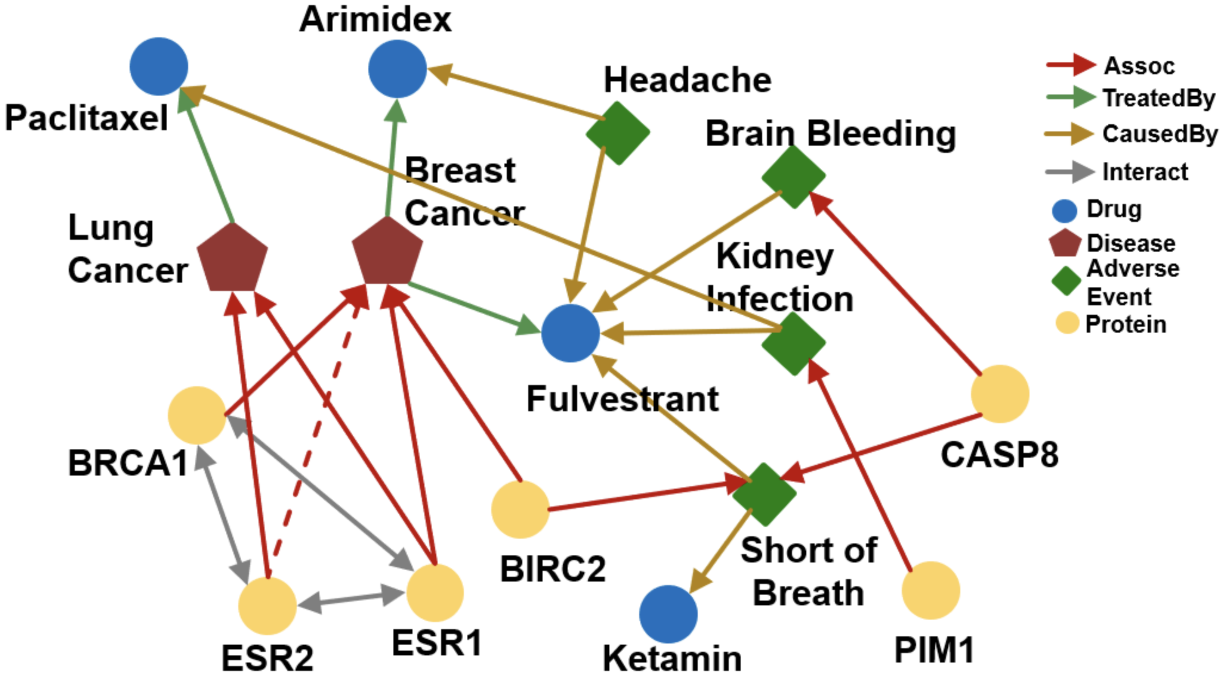
We take intersection between the two sets and get the answers {"Fulvestrant", "Paclitaxel"}

Traversing KG for Conjunctive Queries

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



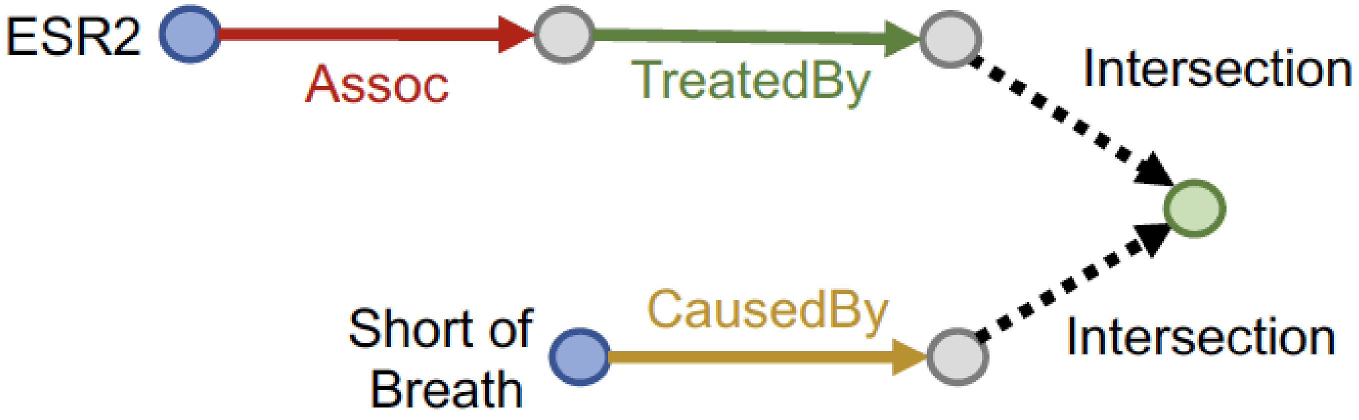
Traversing KG for Conjunctive Queries



- 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.

Traversing KG in Vector Space

- 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:

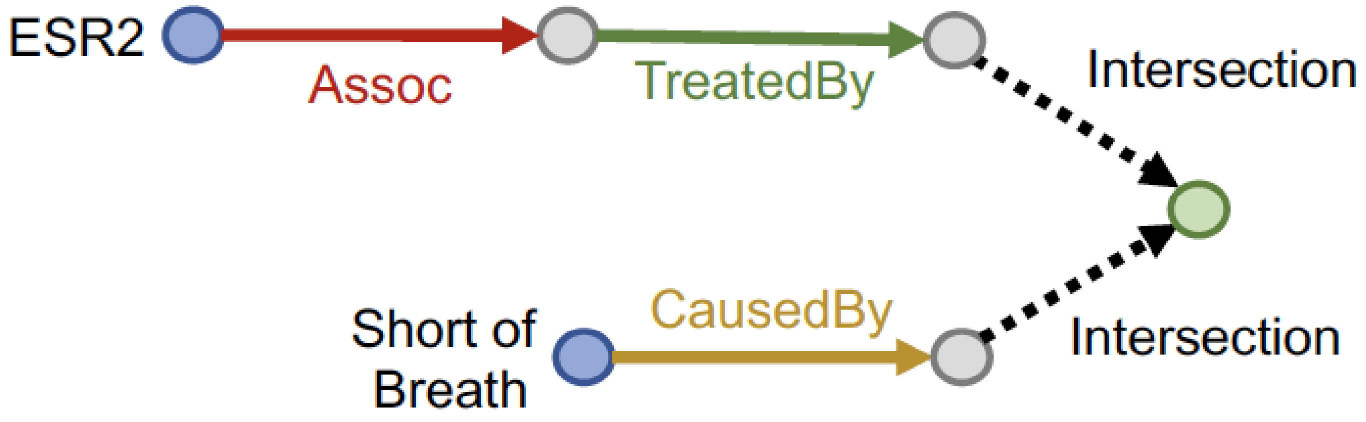


- Each intermediate node represents a set of entities, how do we represent it? How do we define the intersection operation in the latent space?

Query2Box: Reasoning over KGs Using Box Embedding

Conjunctive Queries

- How can we answer more complex queries with logical conjunction operation?
- Query plan:

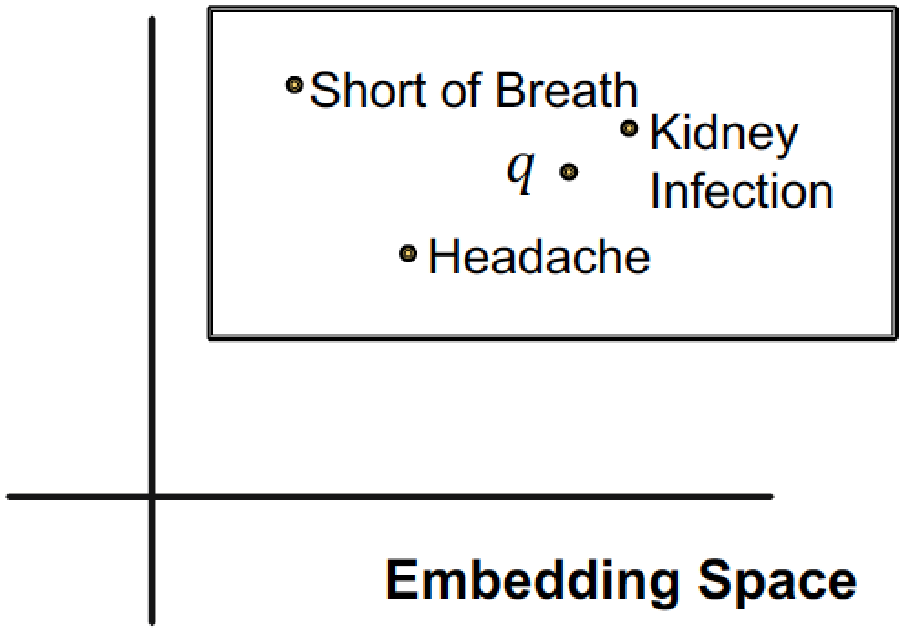


  - (1) Each intermediate node represents a set of entities; how do we represent it?
  - (2) How do we define the intersection operation in the latent space?

Box Embedding

- Embed queries with hyper-rectangles (boxes)

$$q = \big(Center(q), Offset(q)\big)$$

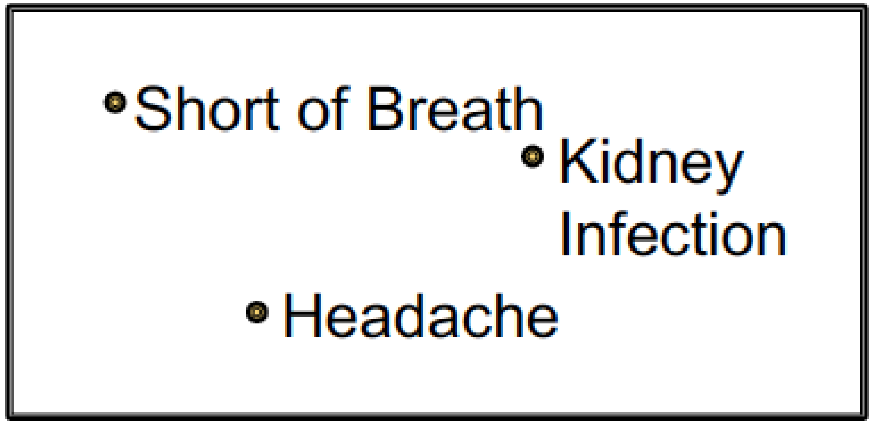


For example, we can embed the adverse events of Fulvestrant with a box that enclose all the answer entities.

Ren et al., [Query2box: Reasoning over Knowledge Graphs in Vector Space Using Box Embeddings](), ICLR 2020.

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



Embed with Box Embedding

- 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 $\boldsymbol{f}$:
    - New operator, inputs are boxes and output is a box
    - Intuitively models intersection of boxes

- Notations:
  - d: out degree
  - $|V|$: # entities
  - $|R|$: # relations

Embed with Box Embedding

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

Query plan

Embedding Space

Projection Operator

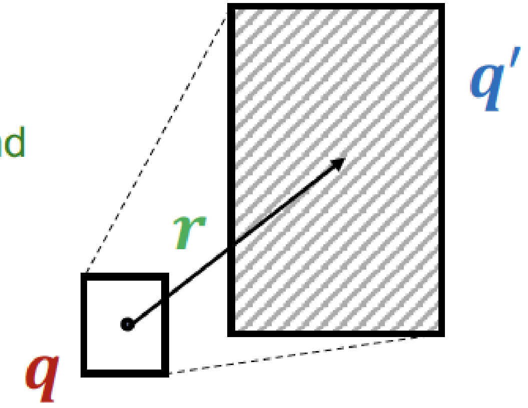
Projection Operator $\mathcal{P}$

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

$$Cen(q') = Cen(q) + Cen(r)$$

$$Off(q') = Off(q) + Off(r)$$

"×" **(cross)** means the projection operator is a **relation** from any box and **relation** to a new box



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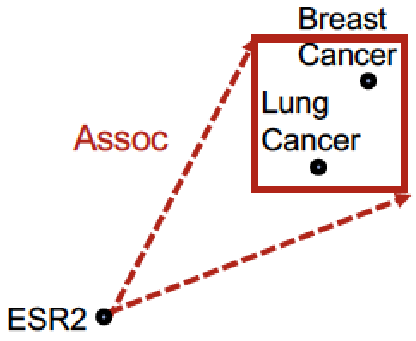
- ((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))
- Use projection operator again following the query plan.

Query Plan

Embedding Space



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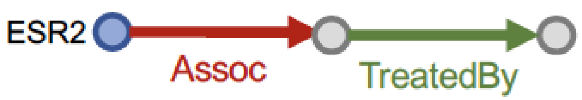
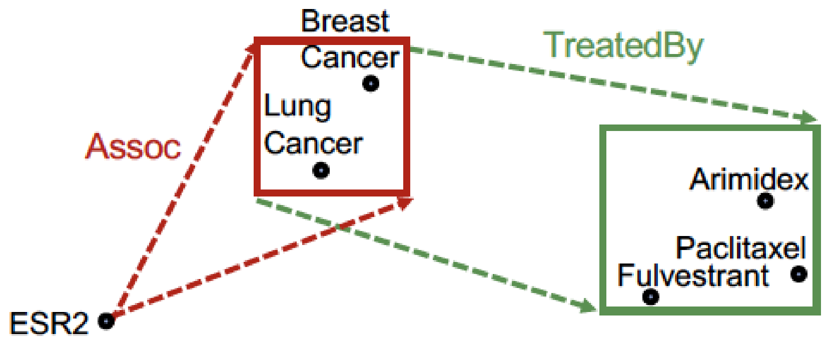


Embedding Space



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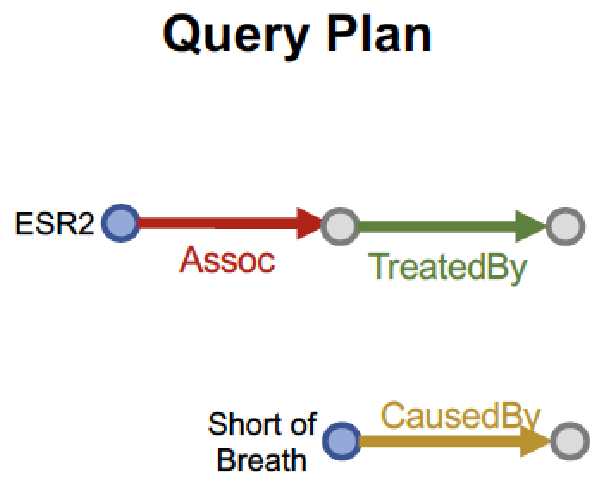

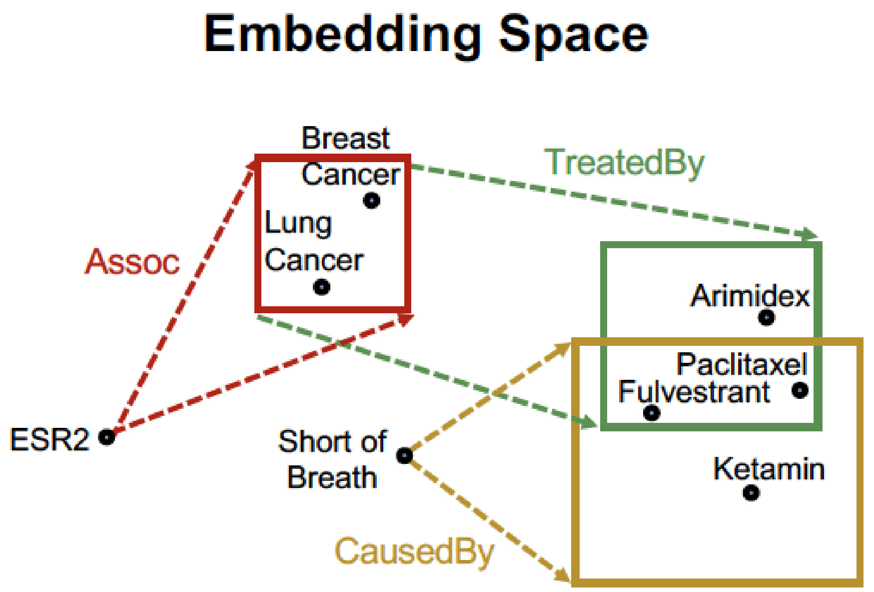

Embed with Box Embedding

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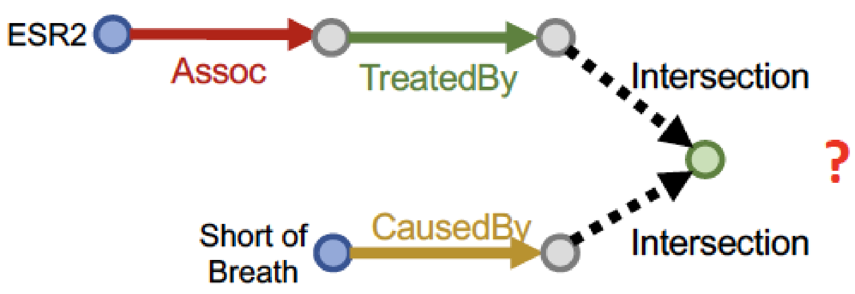
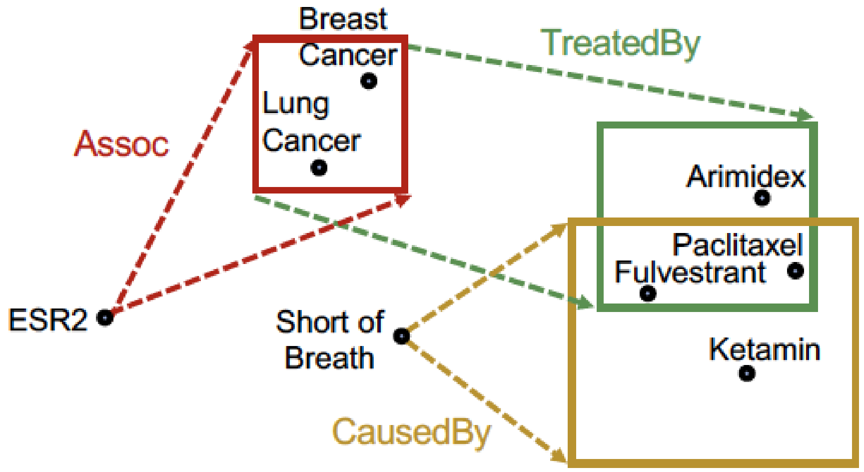
- ((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))
- How do we take intersection of boxes?

Query Plan

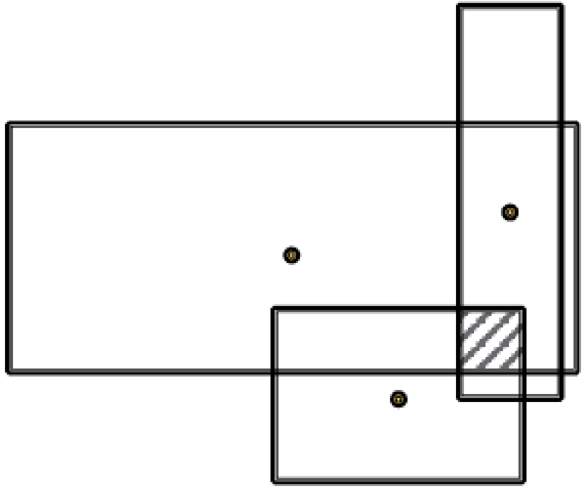


Embedding Space



Intersection Operator

- Geometric Intersection Operator $\mathcal{J}$
  - 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)
  - $\mathcal{J}: Box \times Box \times \cdots \times Box \rightarrow Box$



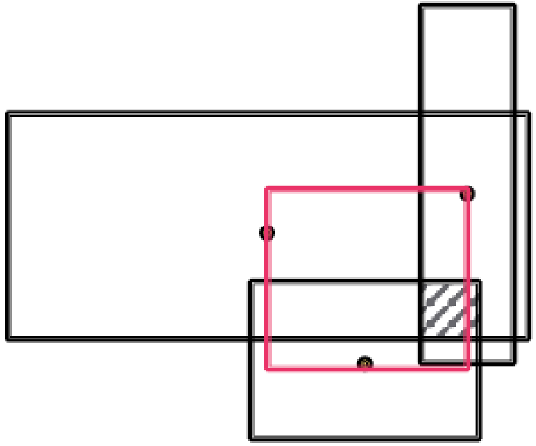
Intersection Operator

- Geometric Intersection Operator $\mathcal{I}$
  - $\mathcal{J}: Box \times Box \times \cdots \times Box \rightarrow Box$

$$\boxed{Cen(q_{inter}) = \sum_i w_i \odot Cen(q_i)}$$

$\odot$: Hadamard product (element-wise product)

$$w_i = \frac{\exp\left(f_{cen}\left(Cen(q_i)\right)\right)}{\sum_j \exp\left(f_{cen}\left(Cen(q_j)\right)\right)}, Cen(q_i) \in \mathbb{R}^d, w_i \in \mathbb{R}^d$$



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 $Cen(q_i)$

Intersection Operator

- Geometric Intersection Operator $\mathcal{J}$
  - $\mathcal{T}: Box \times Box \times \cdots \times Box \to Box$

guarantees shrinking

$$\boxed{\begin{aligned} Off(q_{inter}) = \min\big(Off(q_1), Off(q_2), \cdots, Off(q_n)\big) \\ \odot \sigma\left(f_{off}\big(Off(q_1), Off(q_2), \cdots, Off(q_n)\big)\right) \end{aligned}}$$

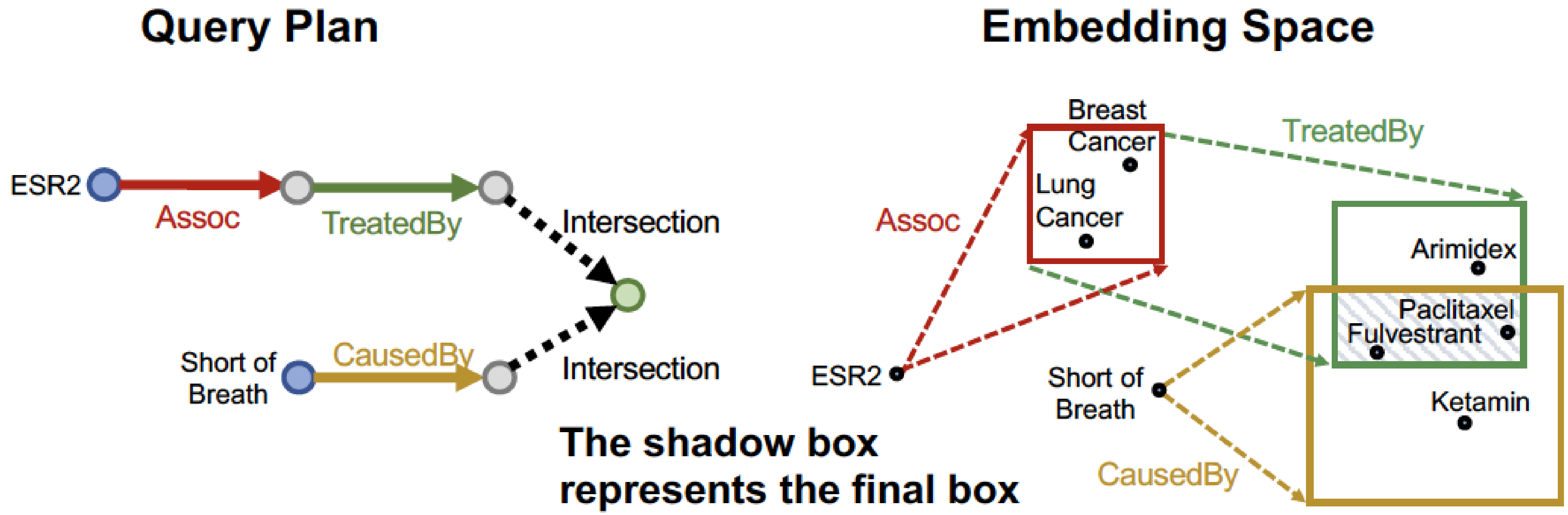
Sigmoid function: squashes output in (0,1)

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

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_{off} to extract the representation of the input boxes with a sigmoid function to guarantee shrinking.

Embed with Box Embedding

- 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))
- Use box intersection operator



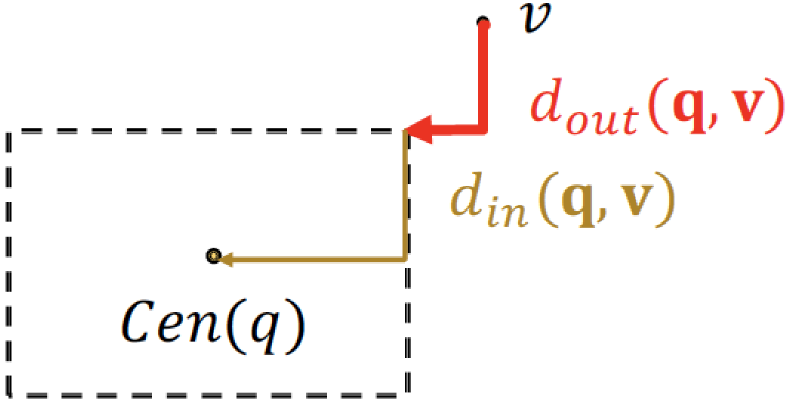
The shadow box represents the final box embedding of the query

Entity-to-Box Distance

- How do we define the score function $f_q(v)$(negative distance)?
- ($f_q(v)$ captures inverse distance of a node $\boldsymbol{v}$ as answer to $\boldsymbol{q}$)
- Given a query box **q** and entity embedding (box) **v**,

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

- where $0 < \alpha < 1$
- Intuition: if the point is enclosed in the box, the distance should be **down-weighted**.
- $f_q(v) = -d_{box}(q,v)$



Extending to Union Operation

- 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?

Embedding AND-OR Queries

- Can we embed AND-OR queries in a lowdimensional 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?

Embedding AND-OR Queries

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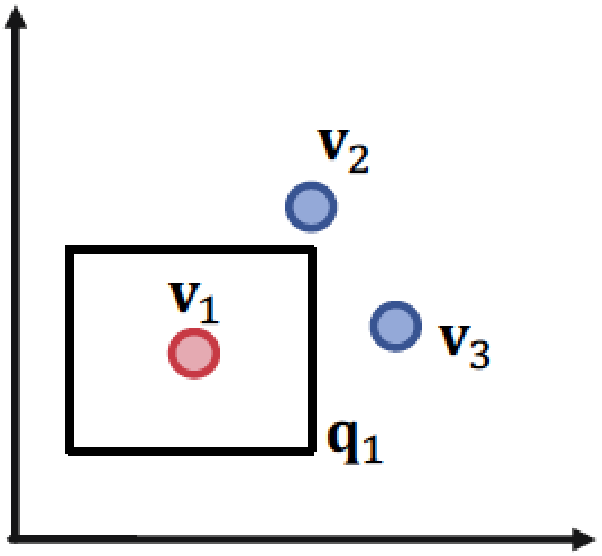

We want red dots (answers) to be in the box while the blue dots (negative answers) to be outside the box

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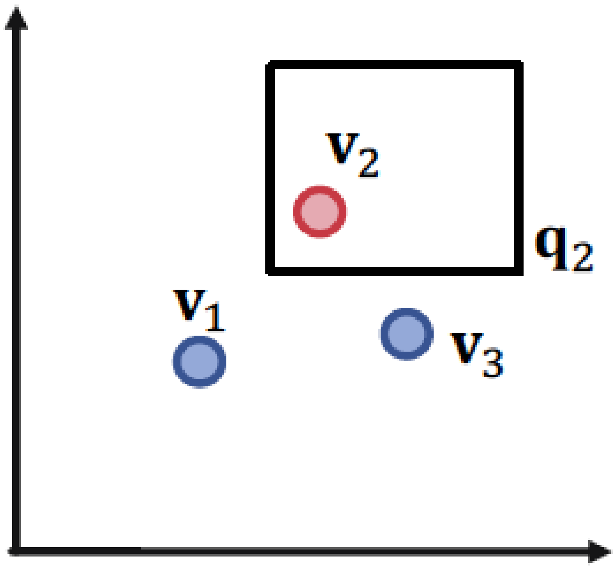

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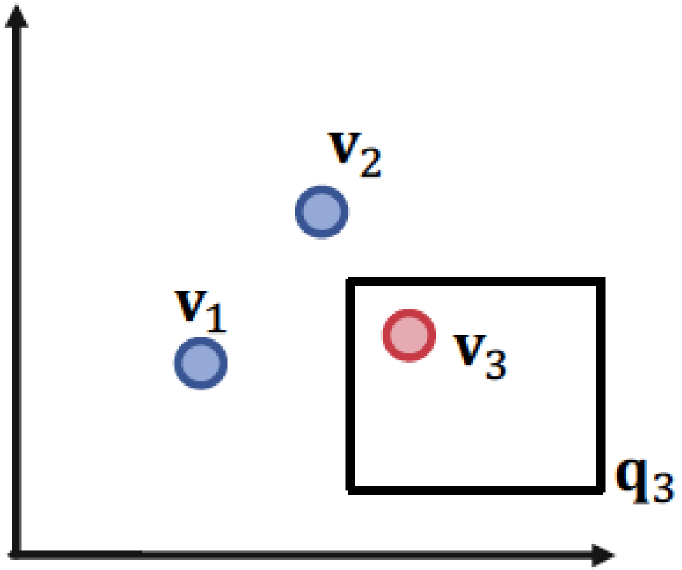

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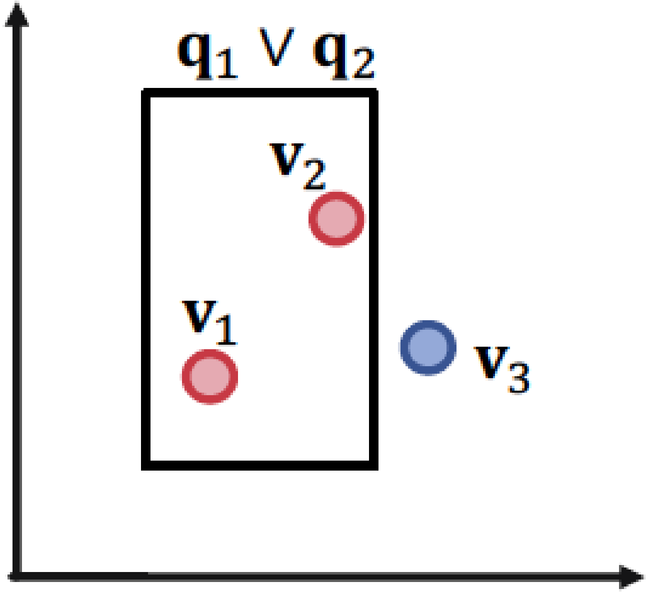

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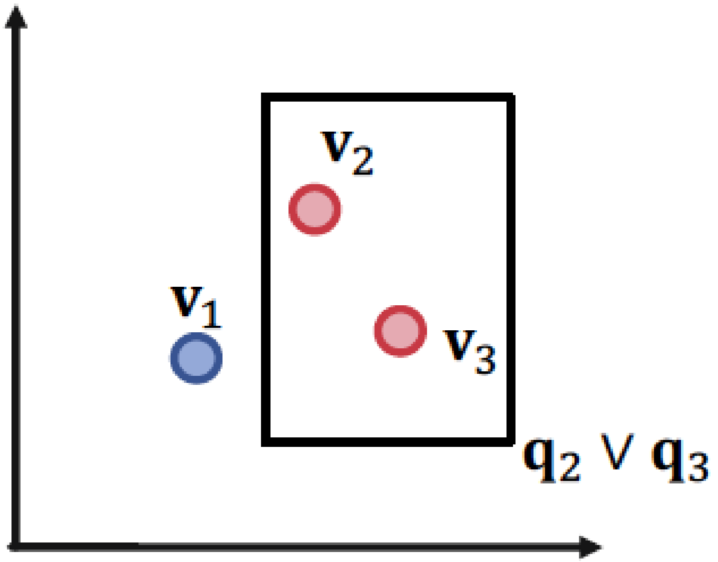

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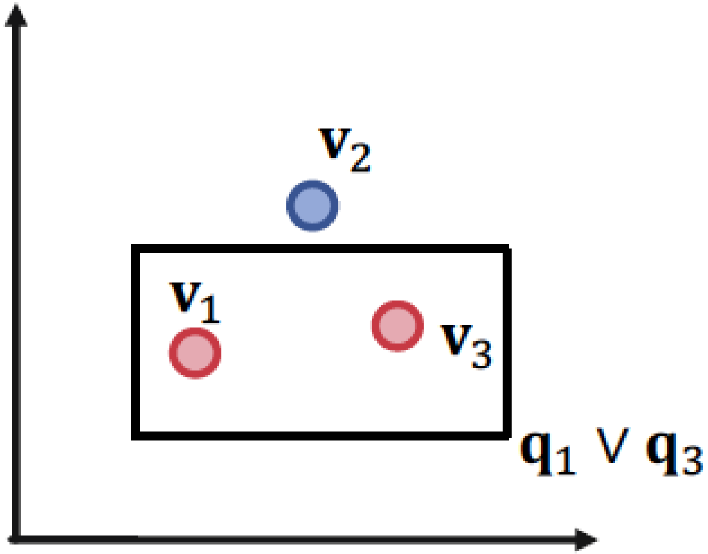

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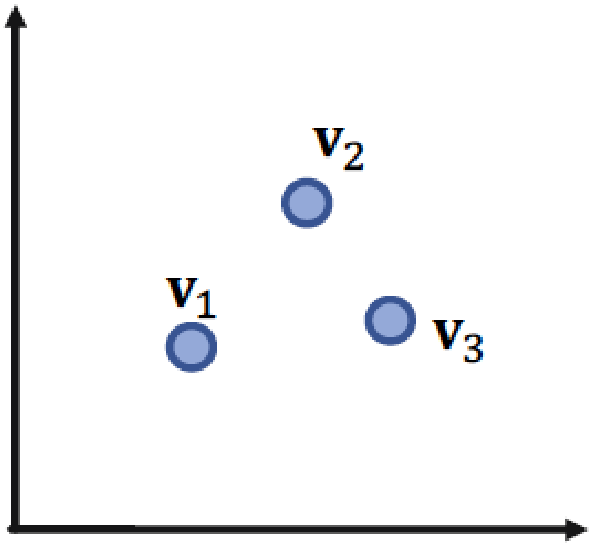
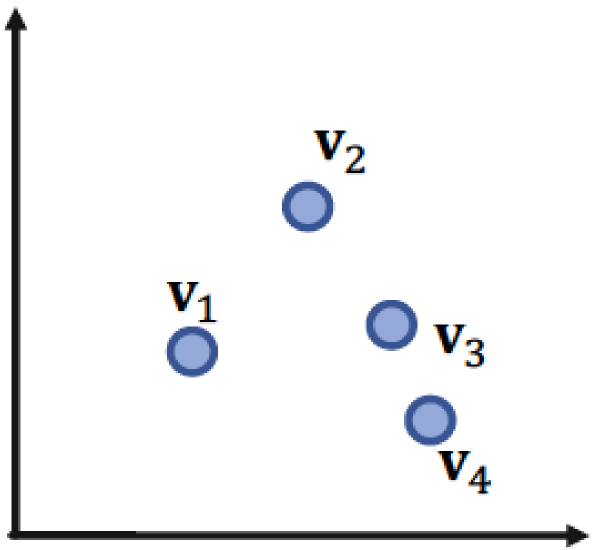


For 3 points, 2-dimension is okay!
How about 4 points?

Embedding AND-OR Queries

- Example:
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}, [\![q_4]\!] = \{v_4\}$
  - If we allow union operation, can we embed them in a two-dimensional plane?



Embedding AND-OR Queries (1)

- Example:
  - Given 3 queries q_1, q_2, q_3, with answer sets:
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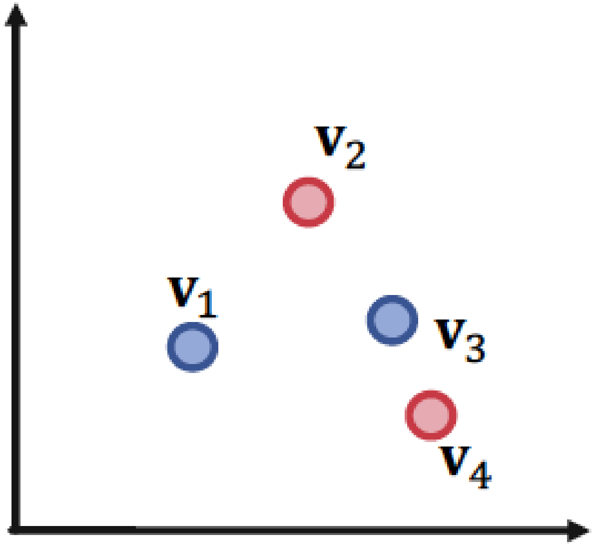


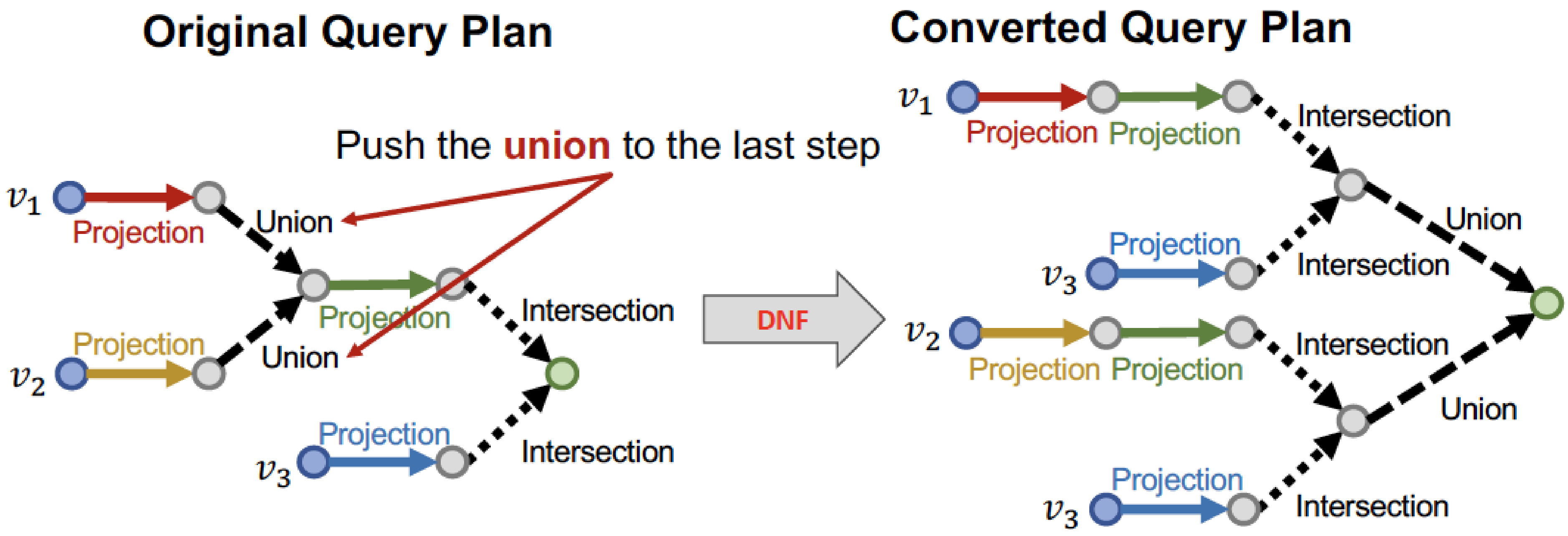
We cannot design a box embedding for $\boldsymbol{q}_2 \vee \boldsymbol{q}_4$, that only v_2, and v_4. are in the box but v_1 and v_3 are outside the box.

Embedding AND-OR Queries (2)

- Can we embed AND-OR queries in low dimensional vector space?
  - **Conclusion**: Given any M conjunctive queries $q_1, q_2, \cdots, q_M$ 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.

Embedding AND-OR Queries (3)

- 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!



Disjunctive Normal Form

- Any AND-OR query can be transformed into equivalent DNF, i.e., disjunction of conjunctive queries.

- Given any AND-OR query $\boldsymbol{q}$,

$$\boxed{q = q_1 \vee q_2 \vee \cdots \vee q_m}$$

  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 $q = q_1 \vee q_2 \vee \cdots \vee q_m$ is defined as:

$$d_{box}(q, v) = \min\left(d_{box}(q_1, v), d_{box}(q_2, v), \cdots, d_{box}(q_m, v)\right)$$

- **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 q and an Entity

- Distance between entity embedding and a DNF $q = q_1 \vee q_2 \vee \cdots \vee q_m$ is defined as:

$$d_{box}(q, v) = \min\left(d_{box}(q_1, v), d_{box}(q_2, v), \cdots, d_{box}(q_m, v)\right)$$

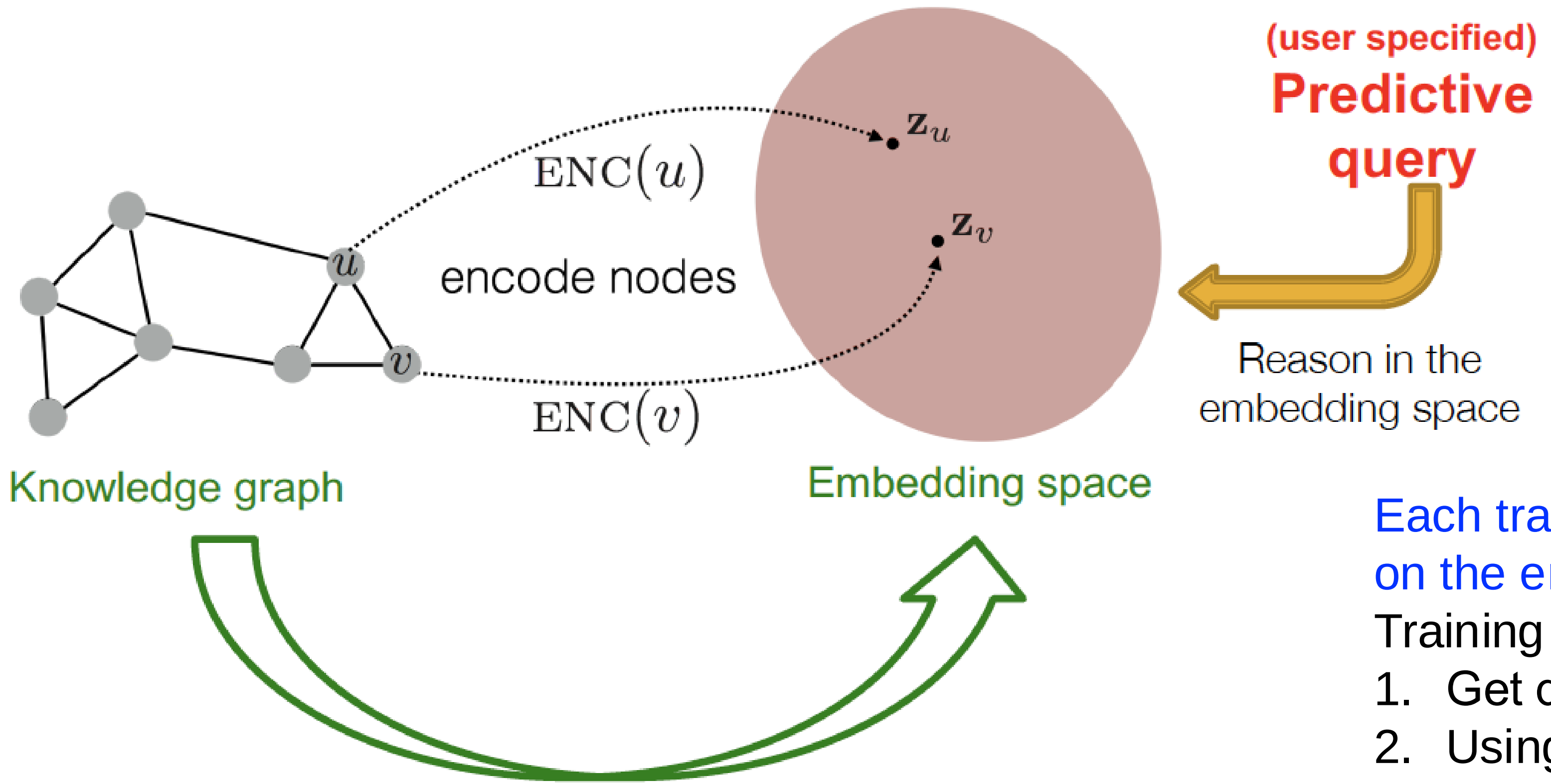
- The process of embedding any AND-OR query $\boldsymbol{q}$
  1. Transform q to equivalent DNF $q_1 \vee q_2 \vee \cdots \vee q_m$
  2. Embed q_1 to q_m
  3. Calculate the (box) distance $d_{box}(q_i, v)$
  4. Take the minimum of all distance
  5. The final score $f_q(v) = -d_{box}(q, v)$

How to Train Query2Box

Training Overview

- Overview and Intuition (similar to KG completion):
  - Given a query embedding $\mathbf{q}$, 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?

Training Overview



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

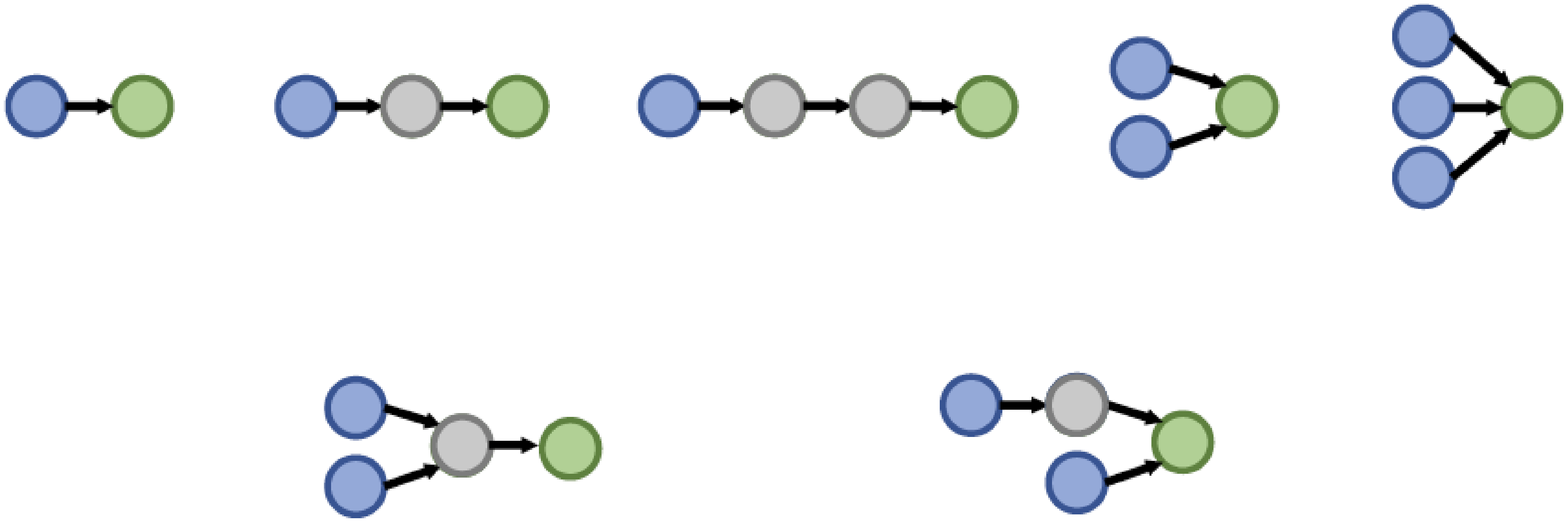
Training: Details

- Training
  1. Sample a query q from the training graph G_{train}, answer $v \in [\![q]\!]_{G_{train}}$ and non-answer $v' \notin [\![q]\!]_{G_{train}}$
  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 l (maximize $f_q(v)$ while minimizing $f_q(v')$)

$$l = -\log \sigma\left(f_q(v)\right) - \log\left(1 - \sigma\left(f_q(v')\right)\right)$$

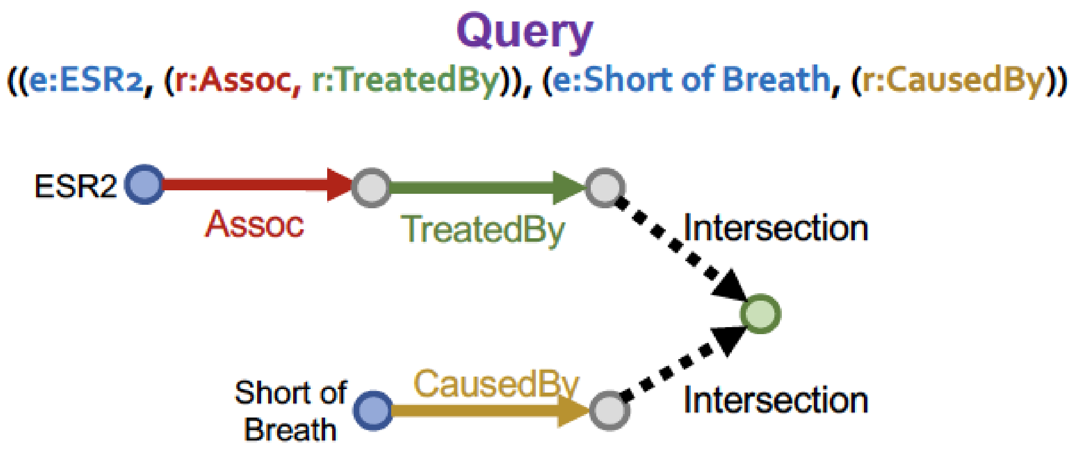
Query Generation from Templates

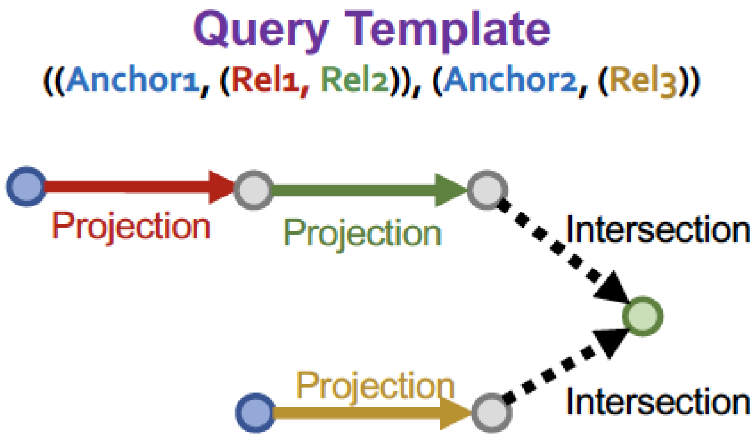
- Generate queries from multiple query templates:



Query Generation from 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 Generation from Templates

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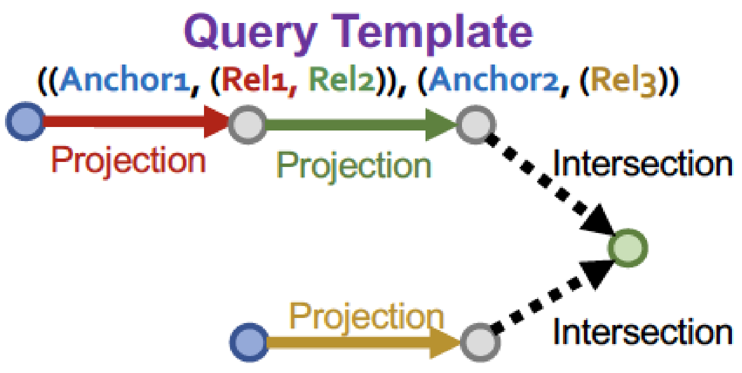
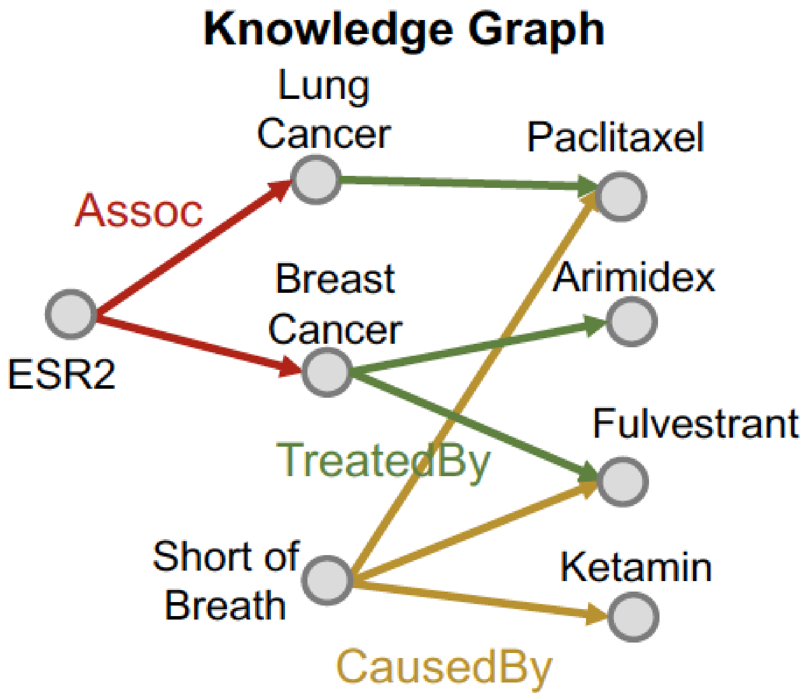
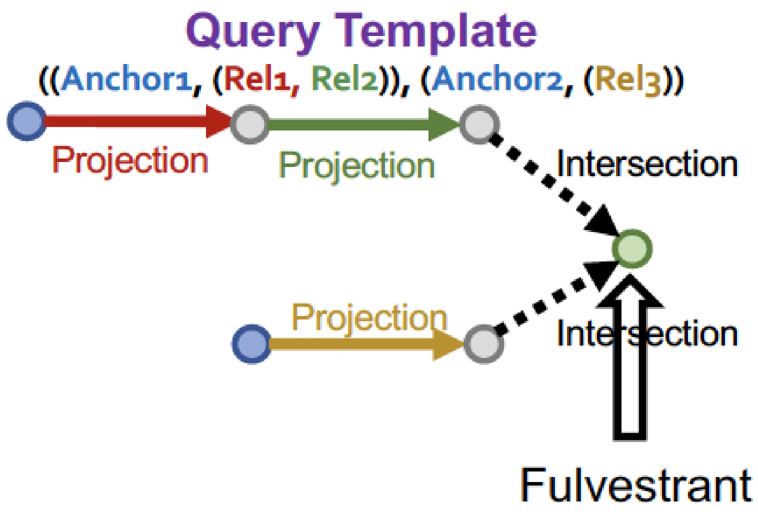




Overview:
Start from instantiating the answer node of the query template and then iteratively instantiate the other edges and nodes until we ground all the anchor nodes

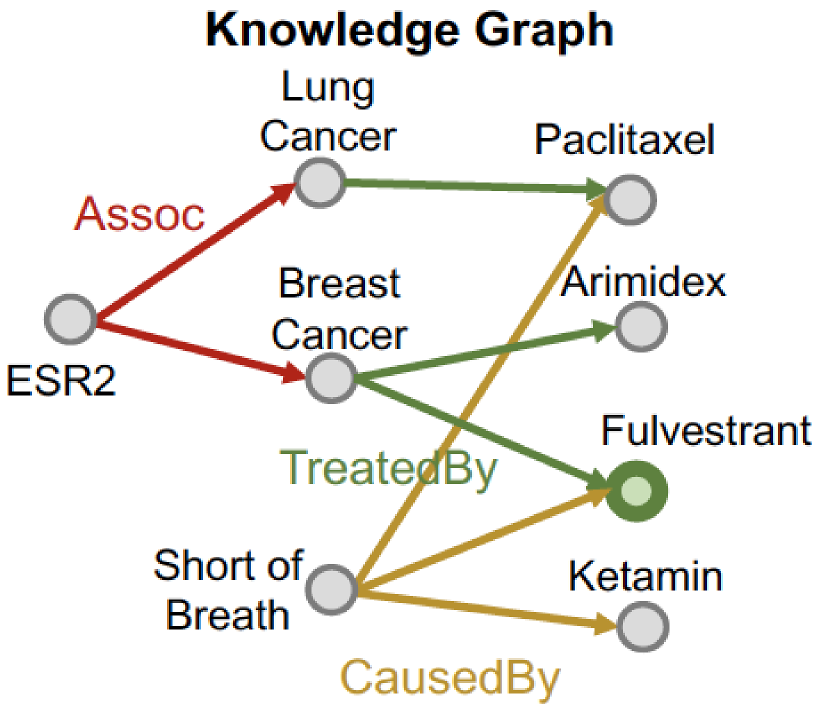
Query Generation from Templates

- How to instantiate a query template given a KG?



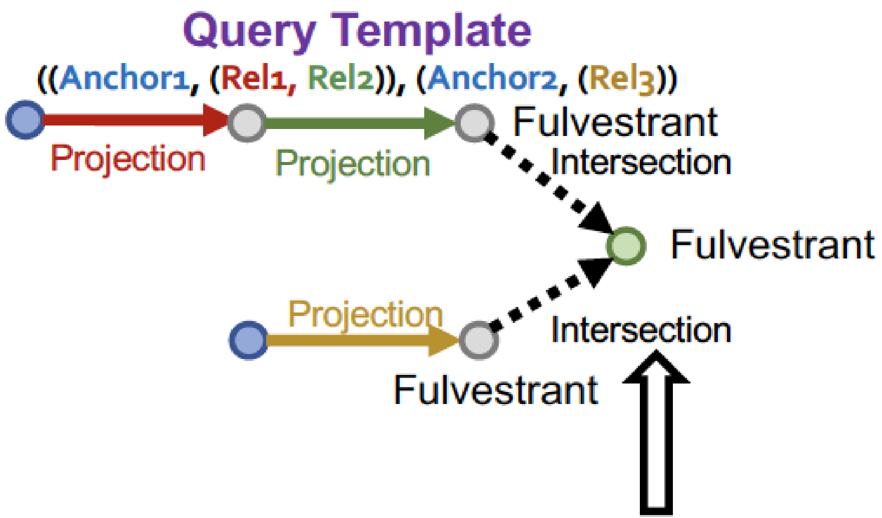
Start from instantiating the root node of the query template.

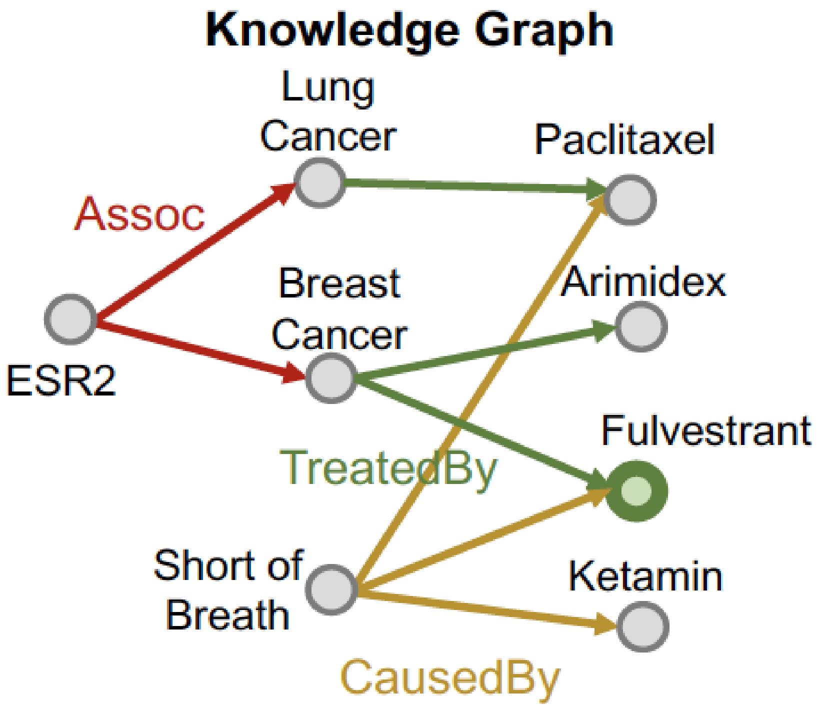
Randomly pick one entity from KG as the root node, e.g., we pick **Fulvestrant**.



Query Generation from Templates

- 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**.

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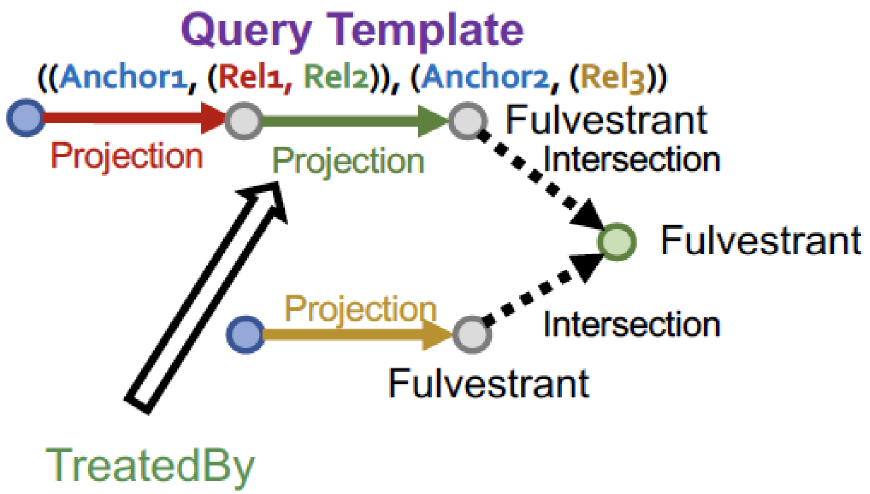

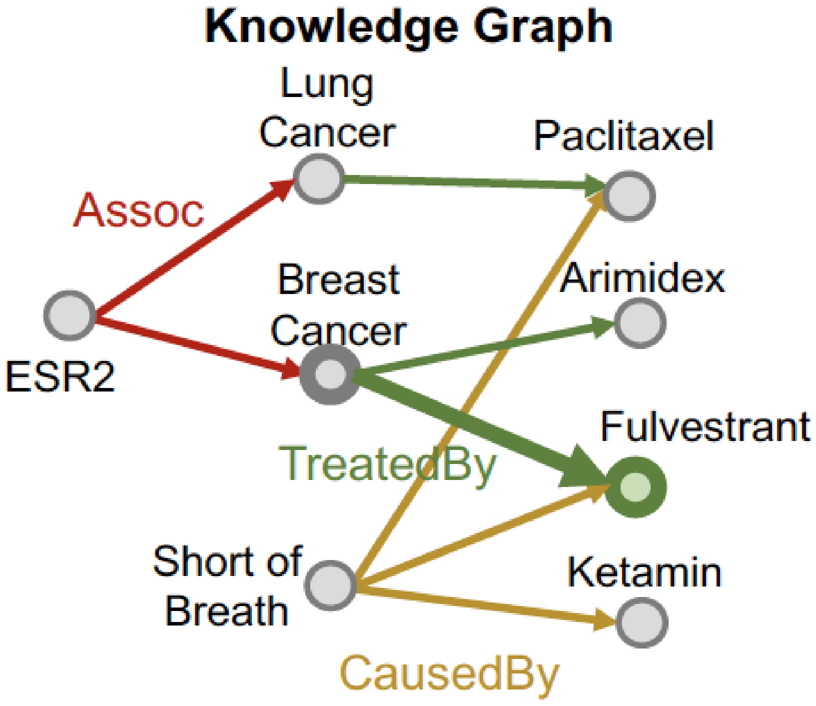

We instantiate the Projection edge in the template by randomly sample one relation associated with the current entity **Fulvestrant**.
For example, we may select relation TreatedBy, and check what entities are connected to **Fulvestrant** with TreatedBy: {Breast Cancer}.

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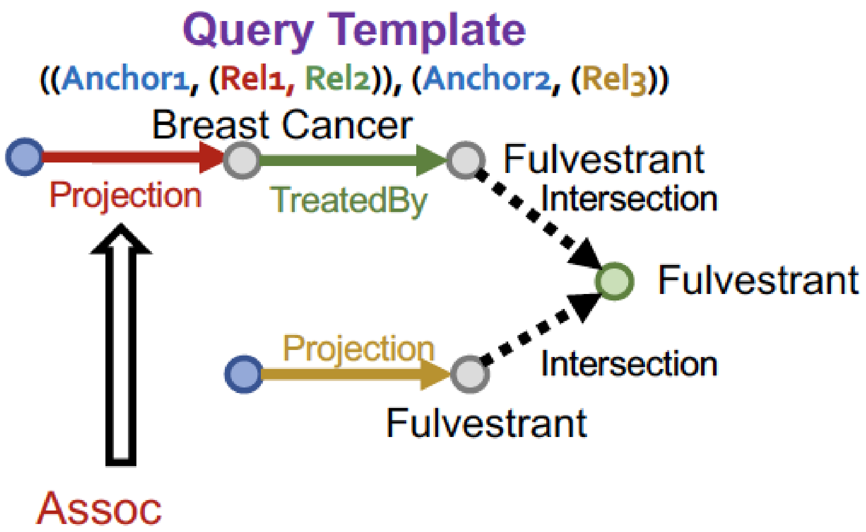
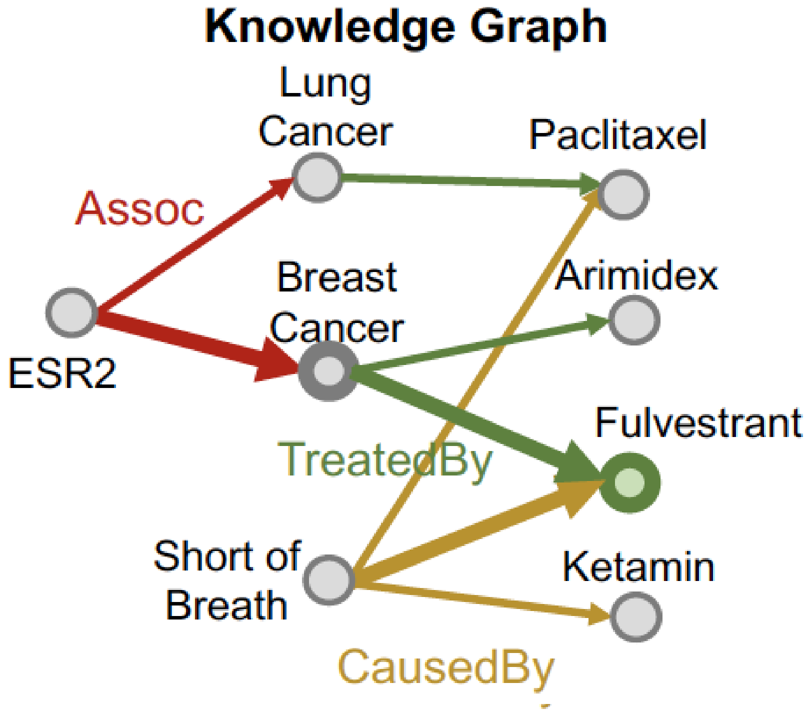


We first look at one branch and ground the Projection edge with the relation associated with **Breast Cancer**, e.g., Assoc. Then we check what entities are connected to **Breast Cancer** with Assoc: {**ESR2**}.



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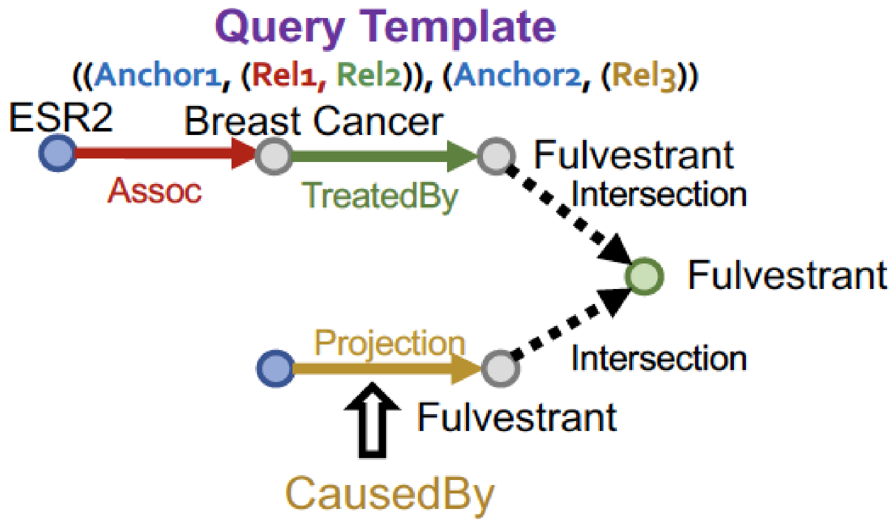

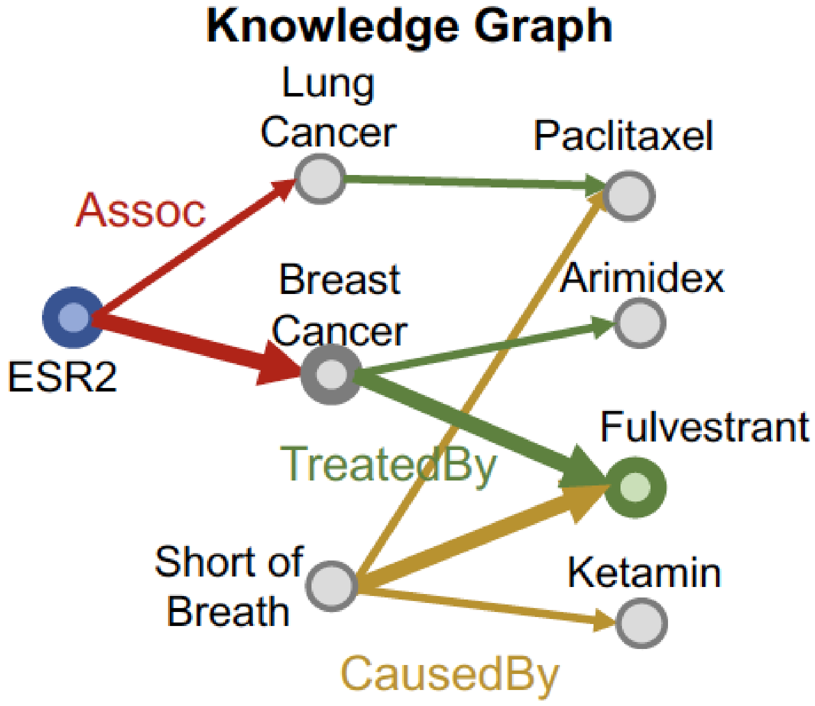

Then we look at the second branch and ground the Projection edge with the relation associated with **Fulvestrant**, e.g., CausedBy. Then we check what entities are connected to **Fulvestrant** with CausedBy: {Short of Breath}.

Query Generation from Templates

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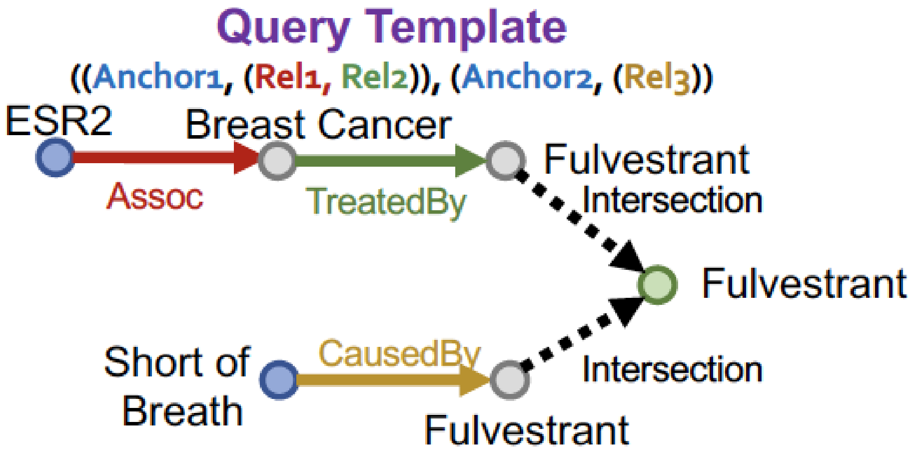
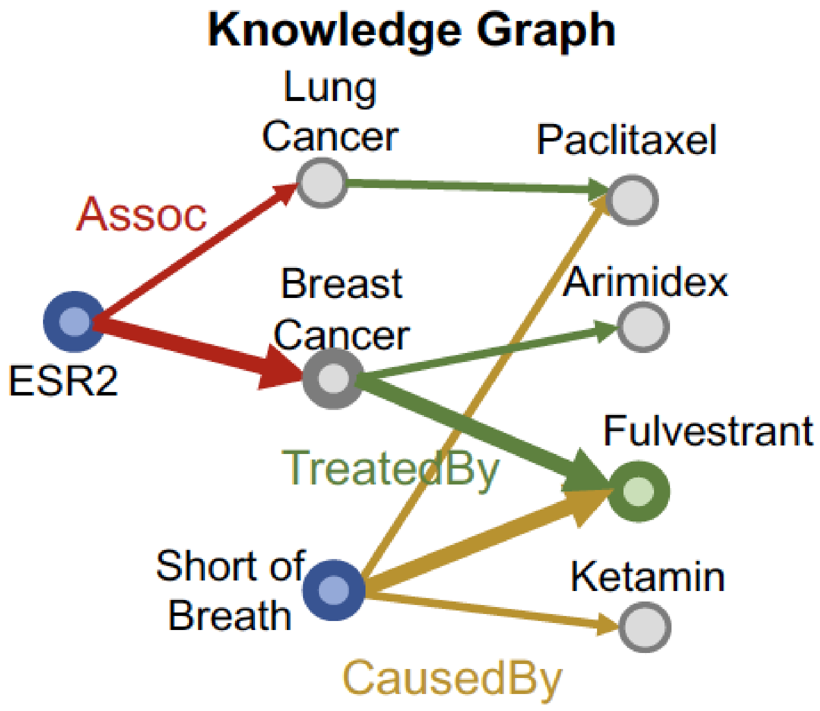
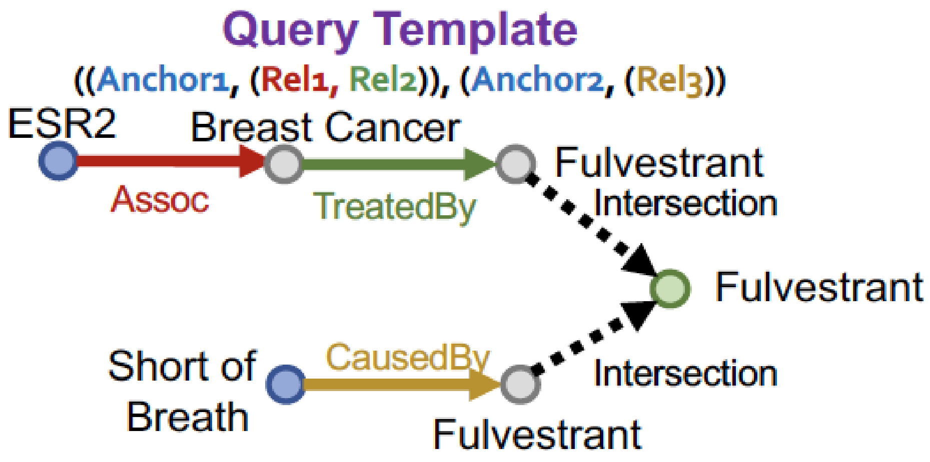


We select entity from {**Short of Breath**}, set it as the anchor node.



Query Generation from Templates

- How to instantiate a query template given a KG?



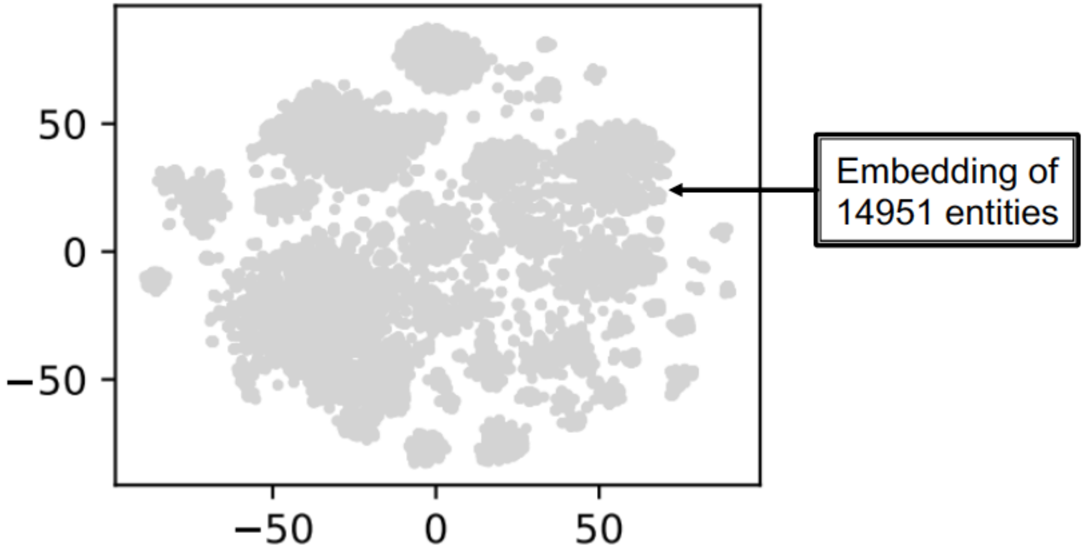
- Now, we instantiated a query ***q***!
- ***q***: ((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))
- The query q must have answers on the KG and one of the answers is the instantiated answer node: **Fulvestrant**.
- We may obtain the full set of answers $[\![q]\!]_G$ by KG traversal.
- We can sample negative answers $v' \notin [\![q]\!]_G$

Example of Query2Box

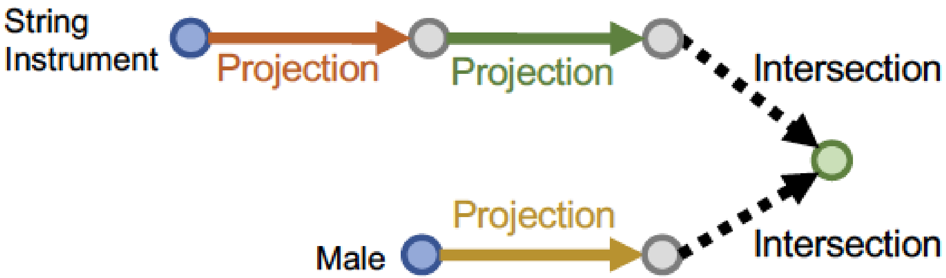
Visualization

- 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

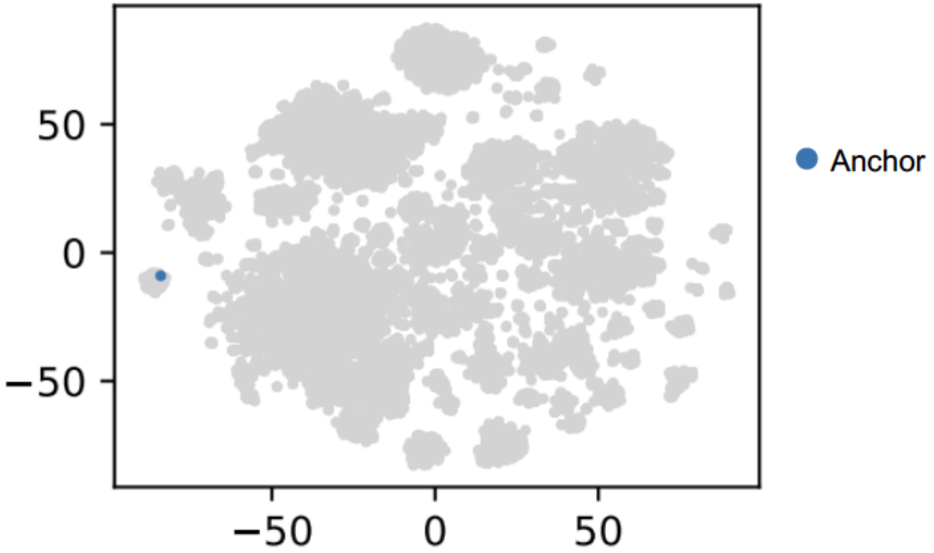
Embedding Space



- “List male instrumentalists who play string instruments”



Embedding Space



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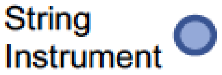
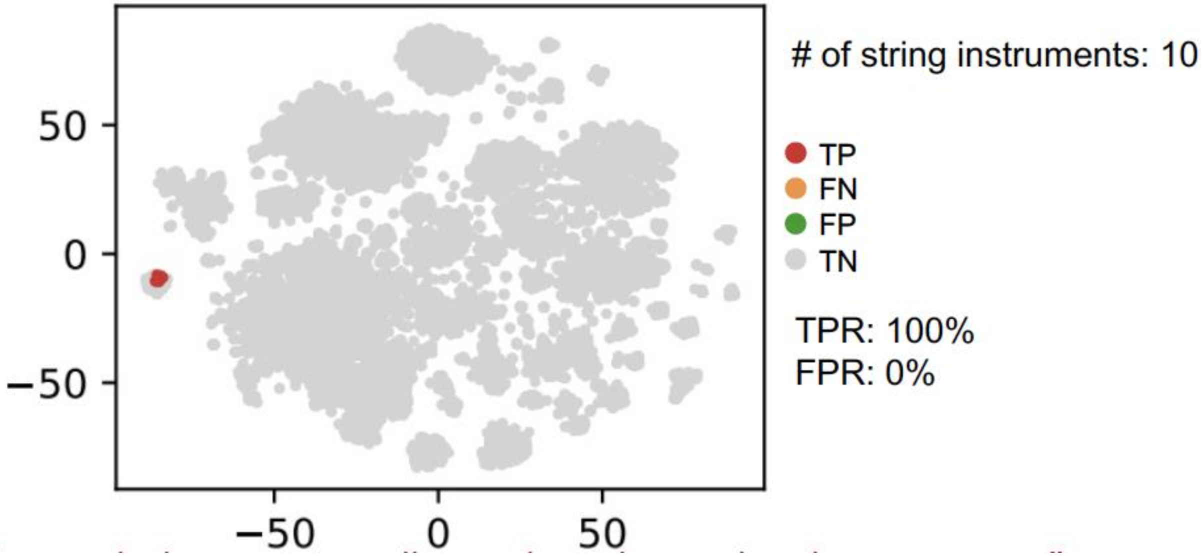
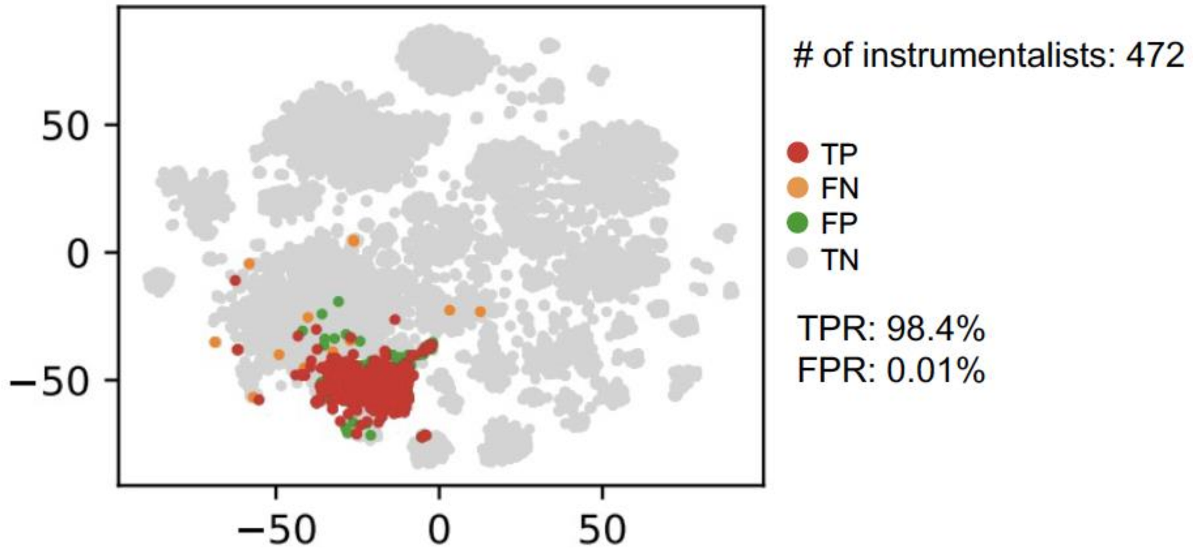


Embedding Space



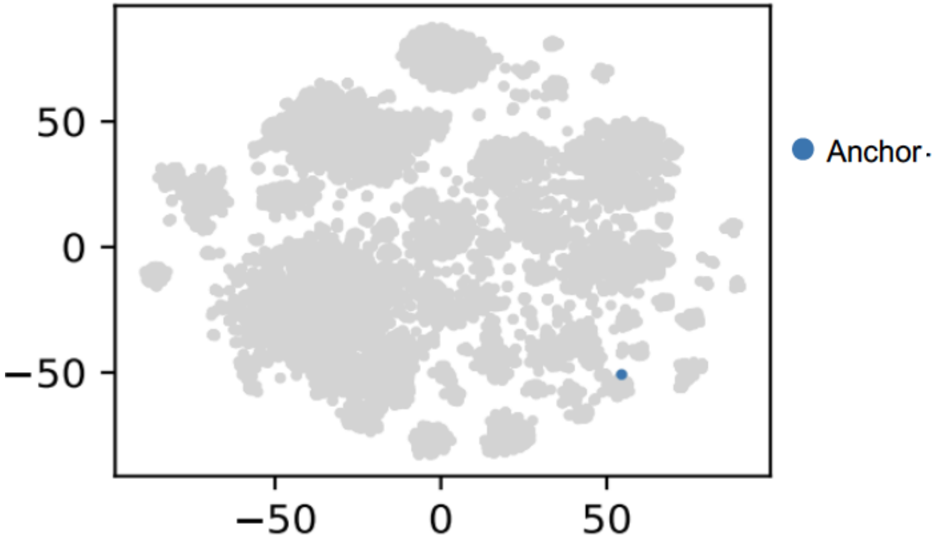
- "List male instrumentalists who play string instruments"

Embedding Space



- "List male instrumentalists who play string instruments"

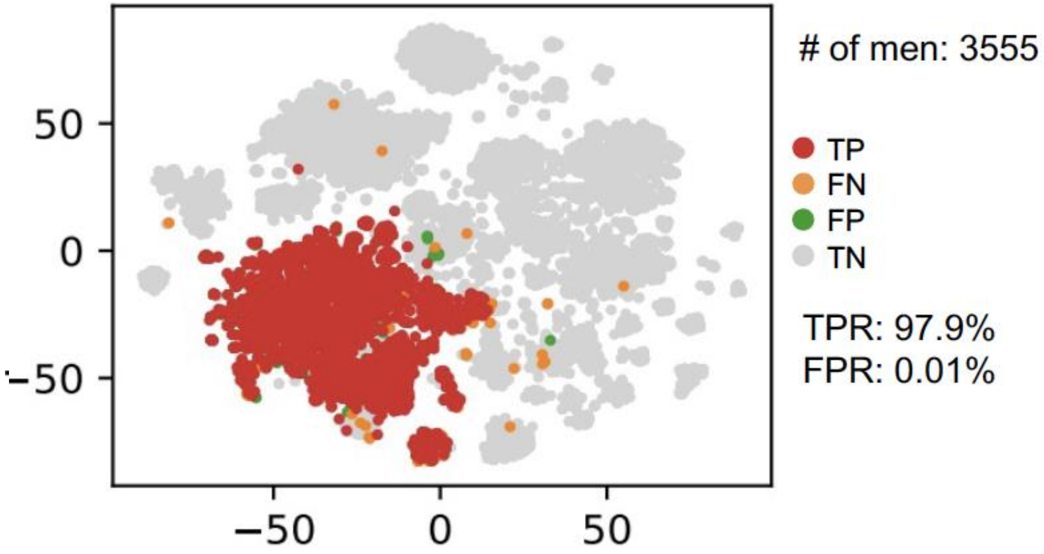
Embedding Space



- “List male instrumentalists who play string instruments”

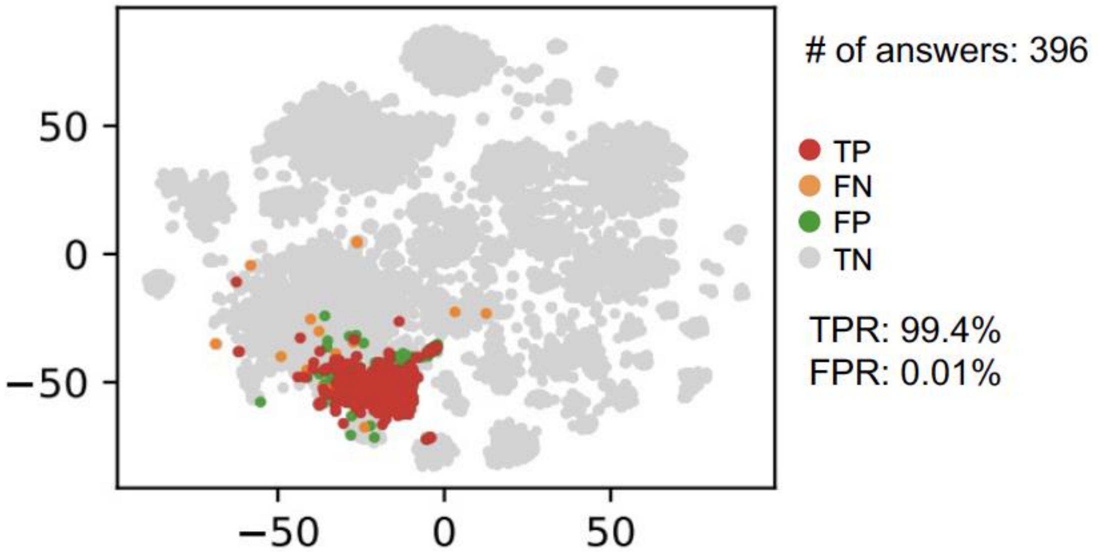
Male

Embedding Space

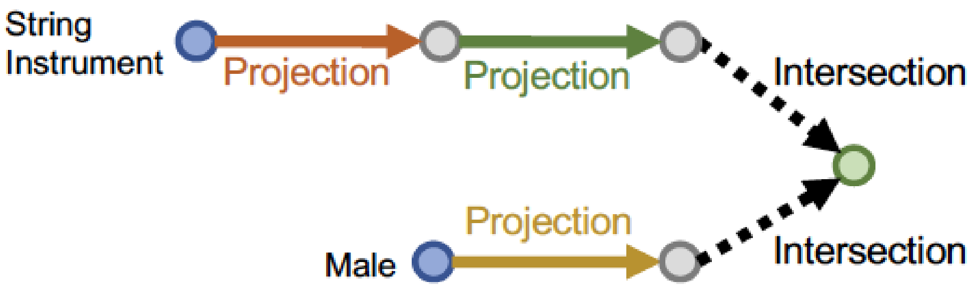


- “List <u>male</u> instrumentalists who play string instruments”

Embedding Space



- "List male instrumentalists who play string instruments"



Summary

- 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