Stanford CS224W: Reasoning over Knowledge Graphs

CS224W: Machine Learning with Graphs

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http://cs224w.stanford.edu

Announcements

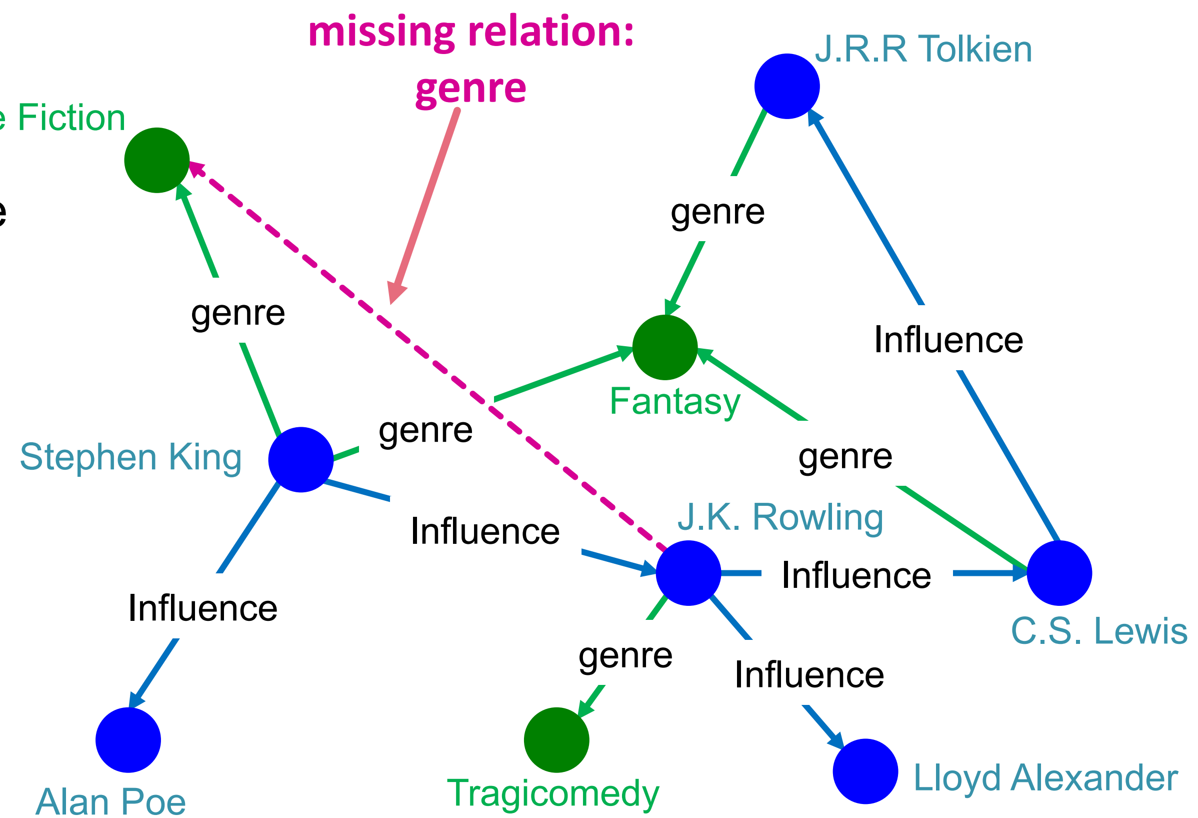
- **Project Proposal** due today
  - Gradescope submissions close at midnight
- **Colab 2** due Thursday

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")

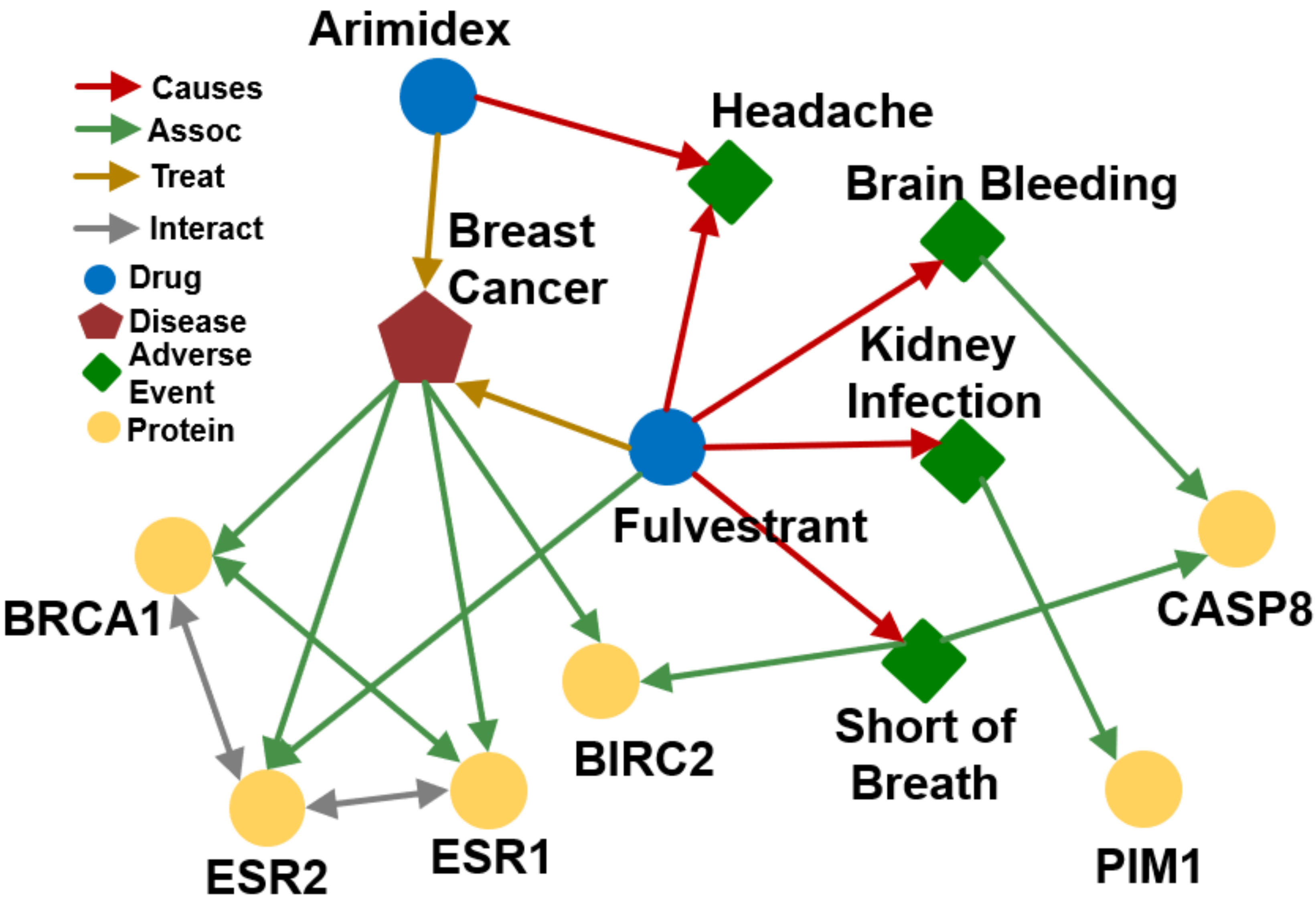


Today: Reasoning over KGs

- **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

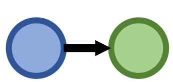


Predictive Queries on KG

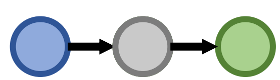
Can we do multi-hop reasoning, i.e., answer complex queries on an incomplete, massive KG?

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))

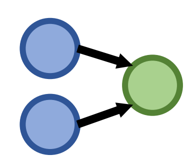
In this lecture, we only focus on answering queries on a KG!
The notation will be detailed next.



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?

$$\Updownarrow$$

- **One-hop query:** Is t an answer to query (h, r)?
  - **For example:** What side effects are caused by drug Fulvestrant?

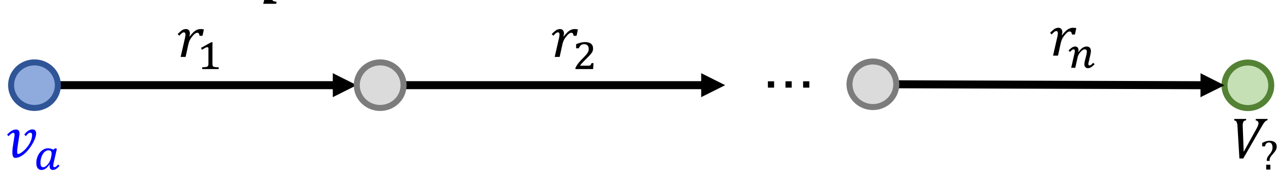
Path Queries

- Generalize one-hop queries to path queries by **adding more relations on the path.**
- An n-hop path query q can be represented by

$$q = (v_a, (r_1, \dots, r_n))$$

  - v_a is an "anchor" entity,
  - Let answers to q in graph G be denoted by $[\![q]\!]_G$.

Query Plan of q:

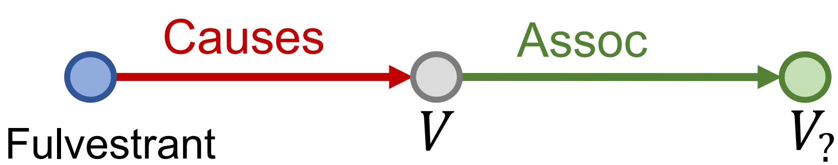


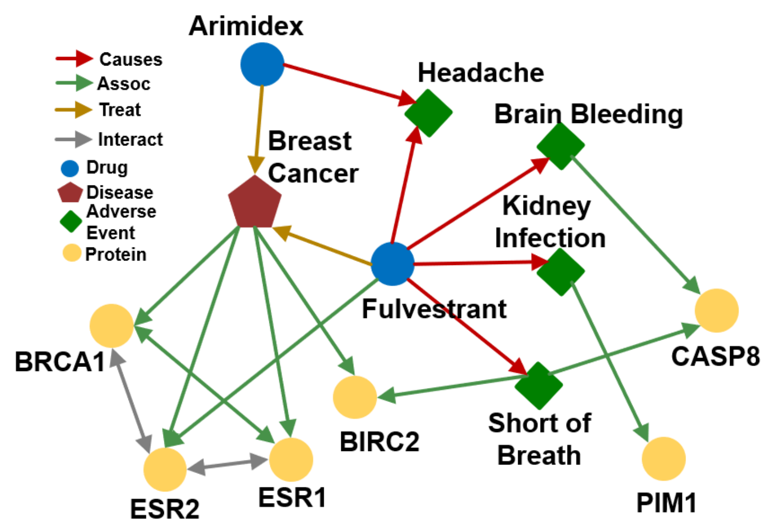
Query plan of path queries is a chain.

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**))



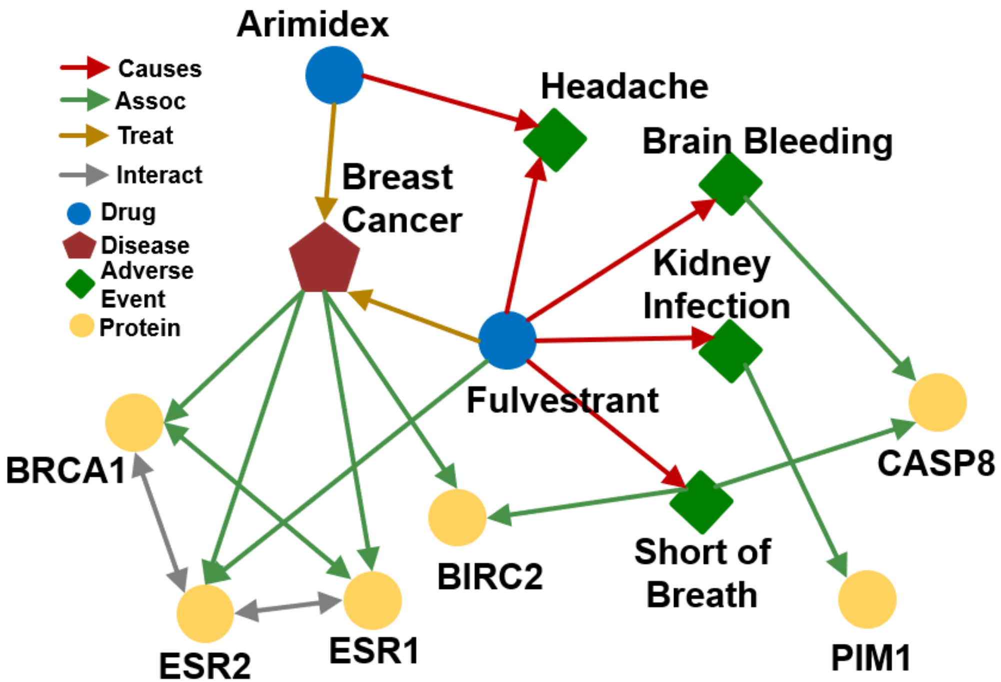


Path Queries

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?



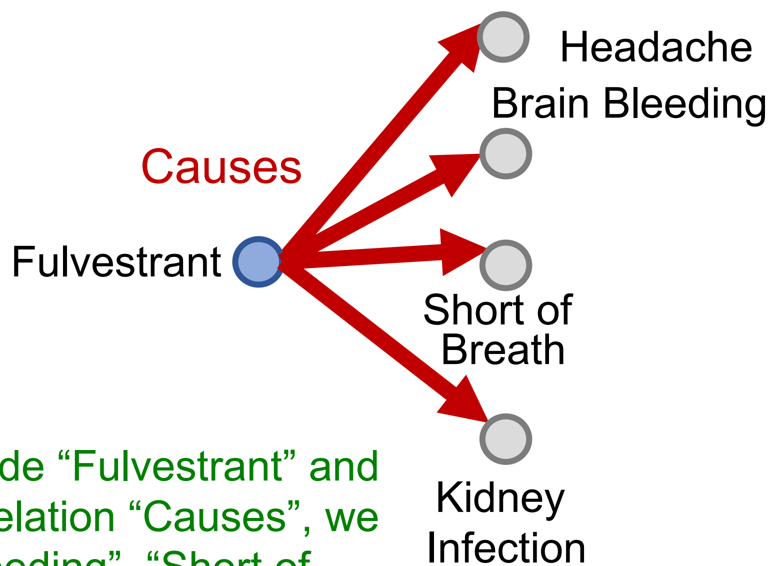
Traversing Knowledge Graphs

- **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

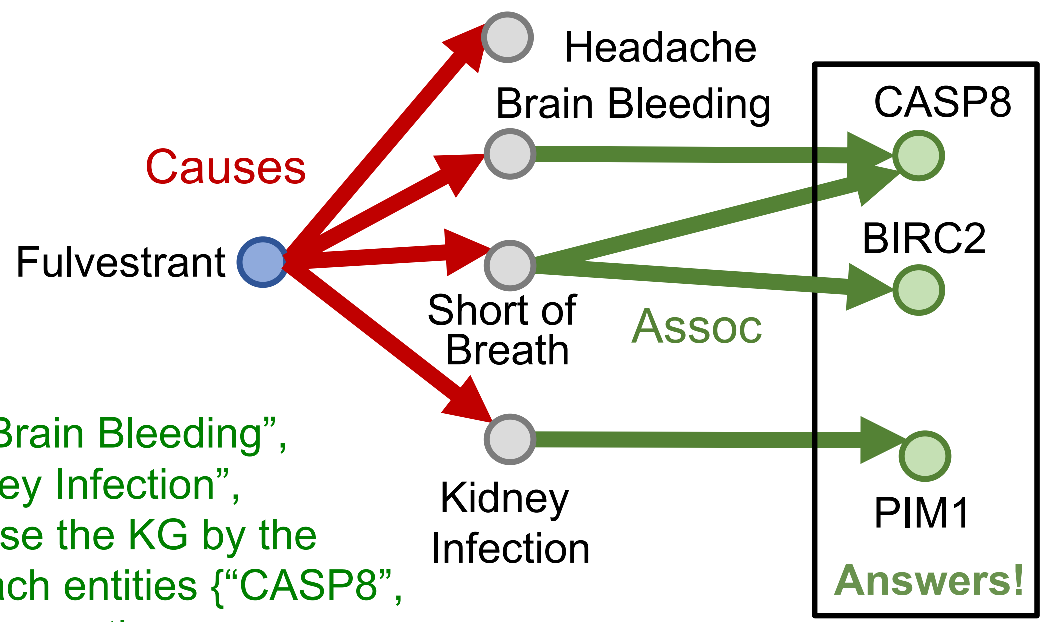
- **We answer path queries by traversing the KG:** *"What proteins are **associated** with adverse events **caused** by **Fulvestrant**?"*
- **Query: (e:Fulvestrant, (r:Causes, r:Assoc))**



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))**



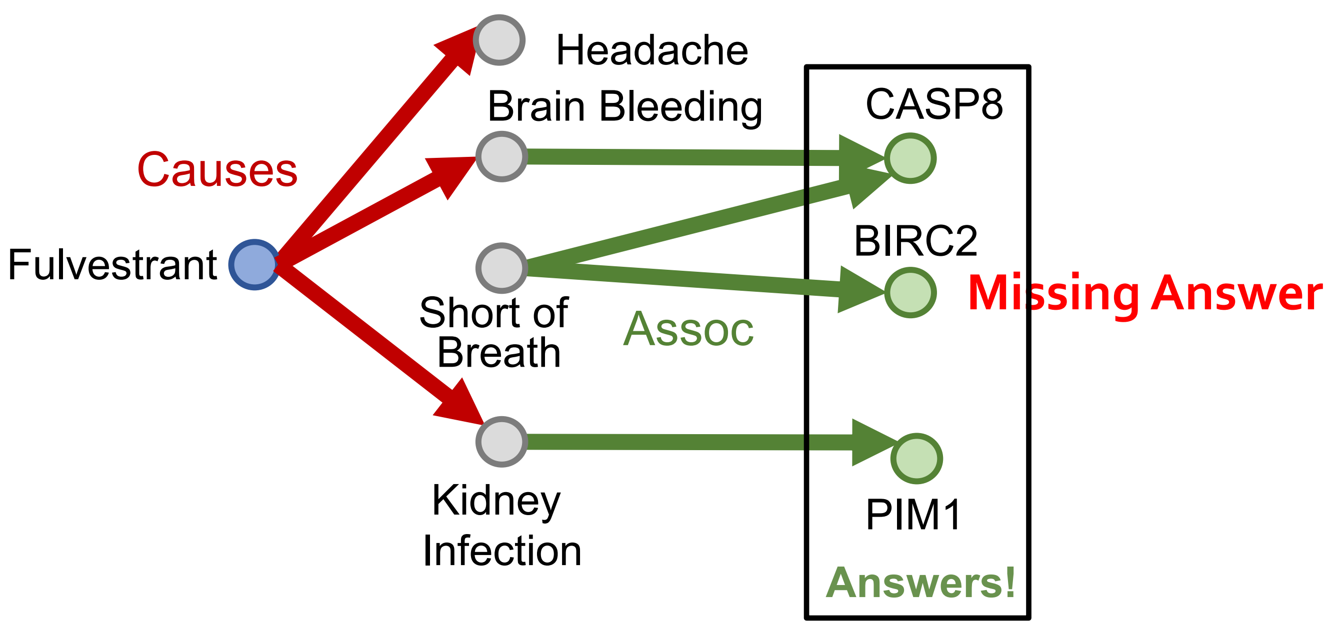
Start from the nodes {"Brain Bleeding", "Short of Breath", "Kidney Infection", "Headache"} and traverse the KG by the relation "Assoc", we reach entities {"CASP8", "BIRC2", "PIM1"}. These are the answers.

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

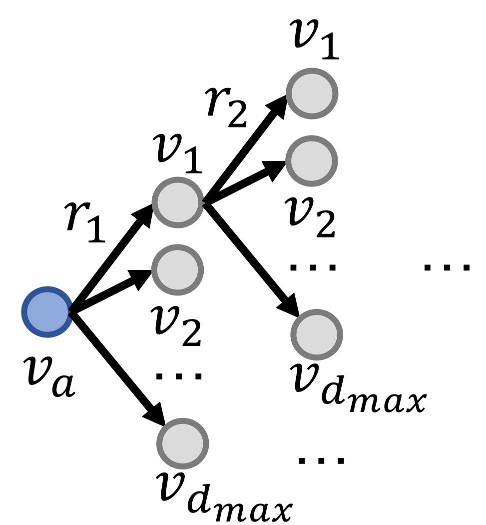
- **We answer path queries by traversing the KG:** *"What proteins are **associated** with adverse events **caused** by **Fulvestrant**?"*
- **Query: (e:Fulvestrant, (r:Causes, r:Assoc))**



Can KG Completion Help?

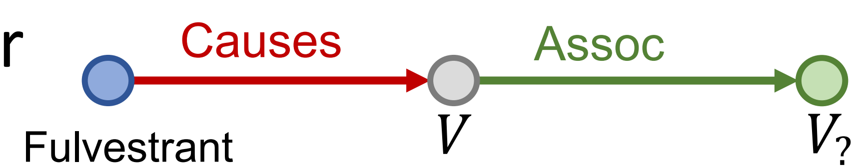
Can we first do KG completion and then traverse the completed (probabilistic) KG?

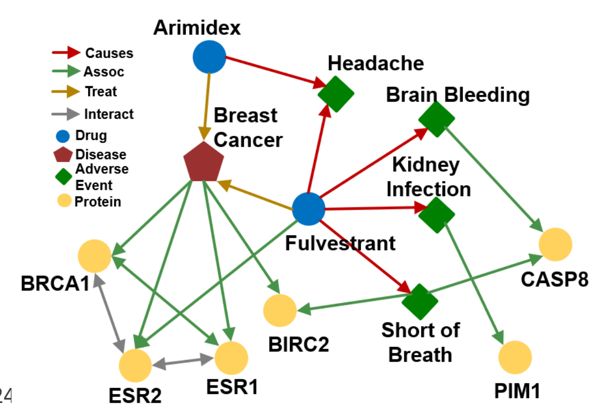
- **No!** The "completed" KG is a **dense graph**!
  - Most (h, r, t) triples (edge on KG) will have some non-zero probability.
- Time complexity of traversing a dense KG is exponential as a function of the path length L: $O(d_{max}^L)$



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 of the Lecture

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.

Stanford CS224W: Answering Predictive Queries on Knowledge Graphs

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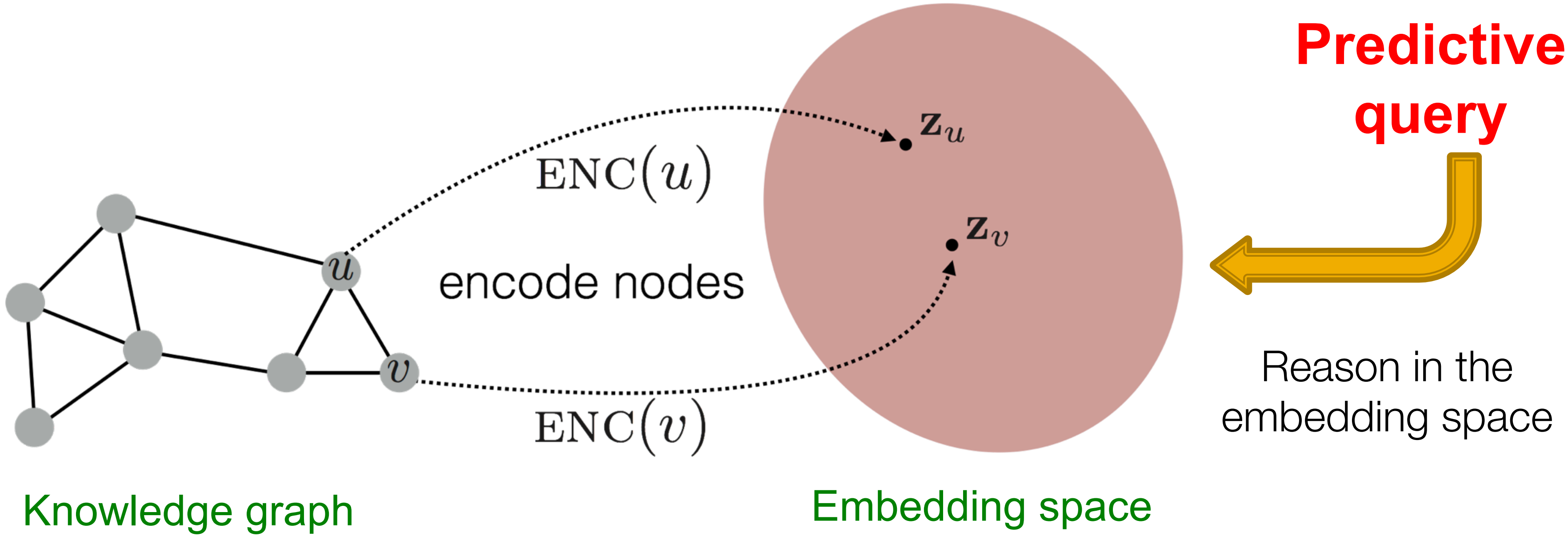
General Idea



Map queries into embedding space. **Learn to reason in that space**

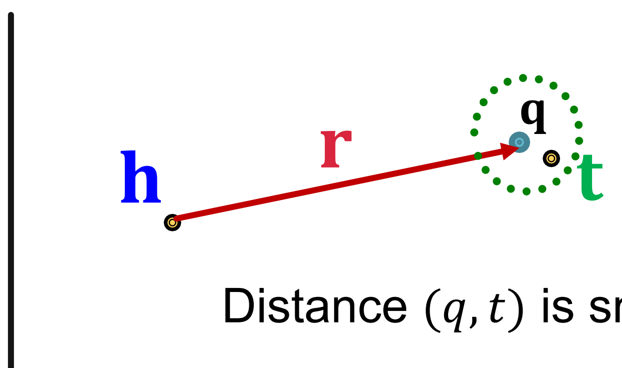
- Embed query into a single **point** in the Euclidean space: answer nodes are close to the query.
- **Query2Box:** Embed query into a hyper-rectangle (**box**) in the Euclidean space: answer nodes are enclosed in the box.

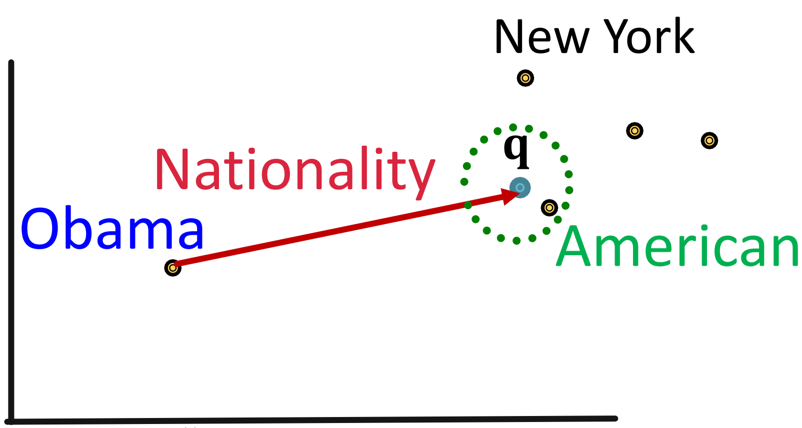
[Embedding Logical Queries on Knowledge Graphs. Hamilton, et al., NeurIPS 2018]
[Query2box: Reasoning over Knowledge Graphs in Vector Space Using Box Embeddings. Ren, et al., ICLR 2020]

Idea: Traversing KG in Vector Space

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

$$f_q(t) = -\|\mathbf{q} - \mathbf{t}\|$$

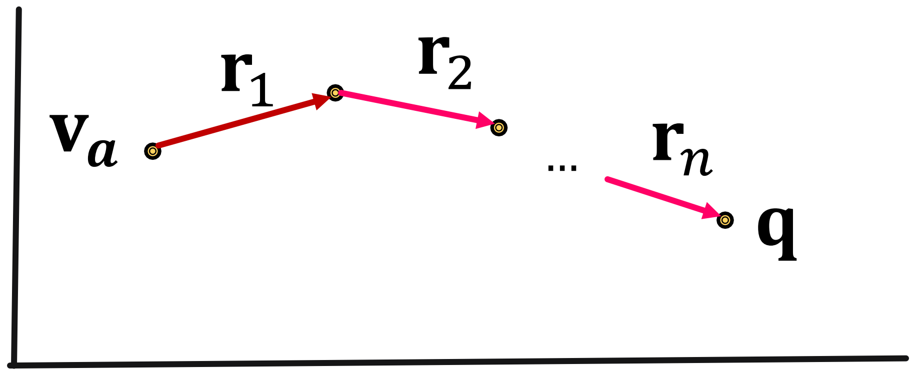




Traversing KG in Vector Space

- **Key idea: Embed queries!**
  - Generalize **TransE** to multi-hop reasoning.

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



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

- 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:

Query Plan

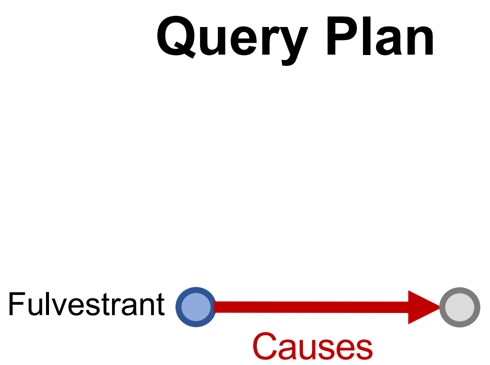
Embedding Process

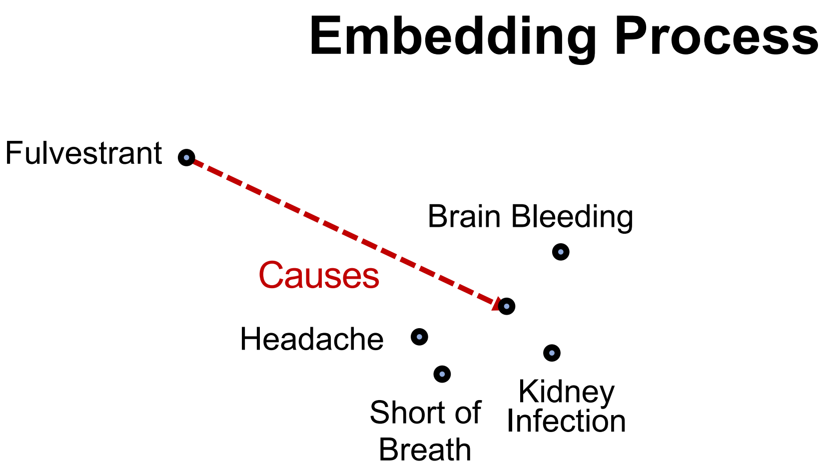
Traversing KG in Vector Space (2)

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:





Traversing KG in Vector Space (3)

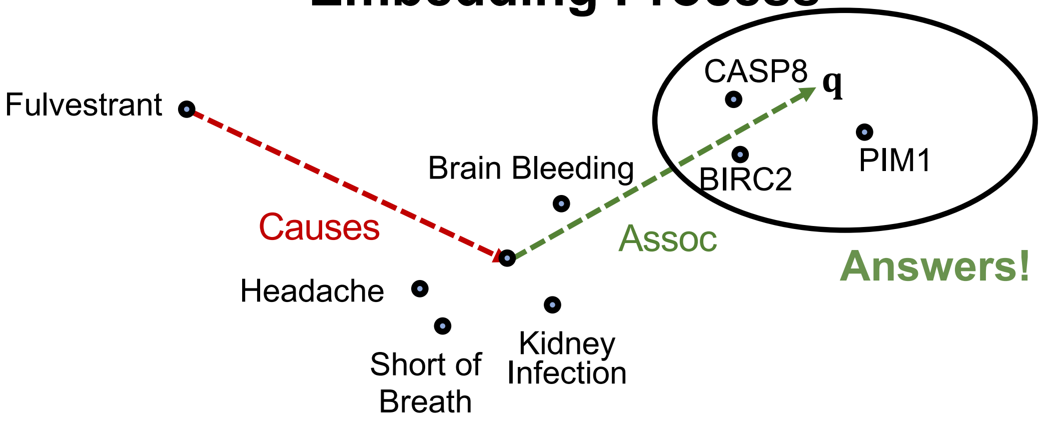
Embed path queries in vector space.

- **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



Traversing KG in Vector Space (4)

Insights:

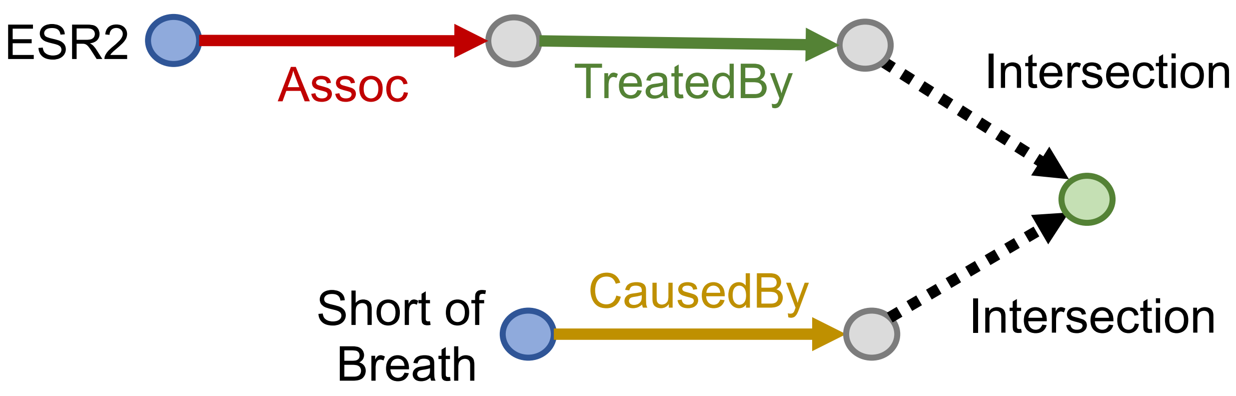
- We can train **TransE** to optimize knowledge graph completion objective (Lecture 11)
- Since **TransE** can naturally handle **compositional relations**, it can handle path queries by translating in the latent space **for multiple hops using addition of relation embeddings**.
- For **DistMult** / **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:

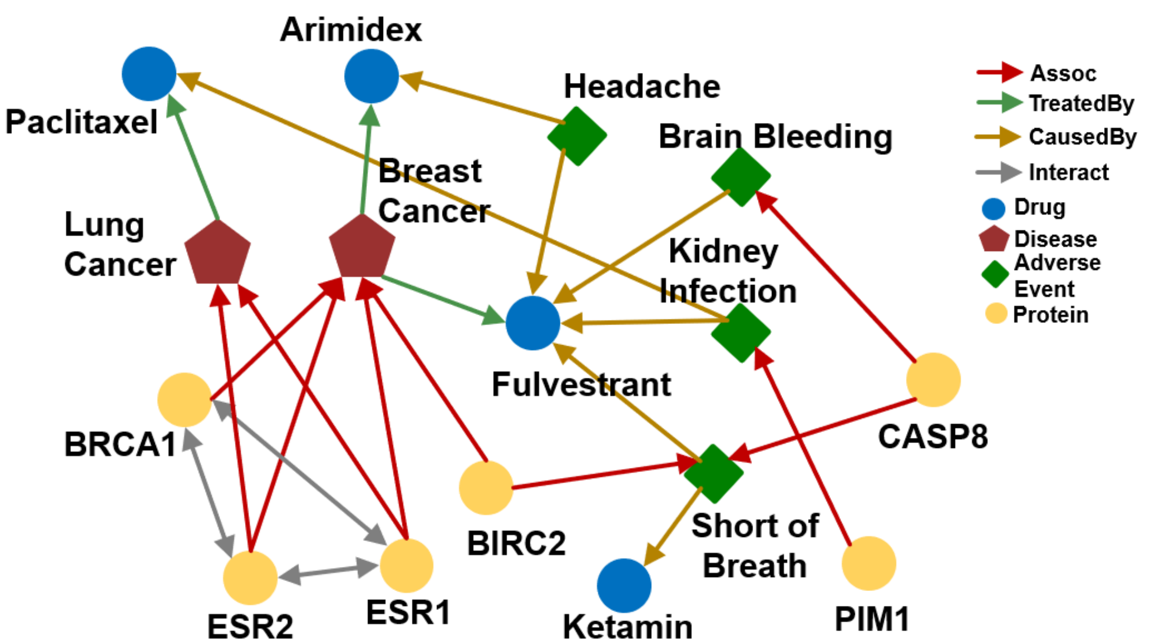


Conjunctive Queries

- *"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?

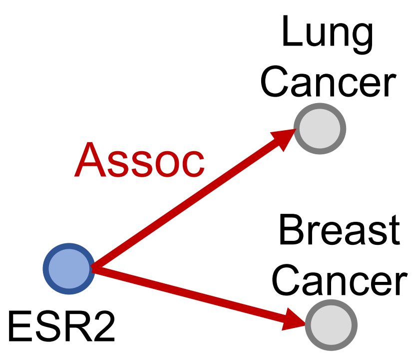


Traversing KG for Conjunctive Queries

- *"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:**



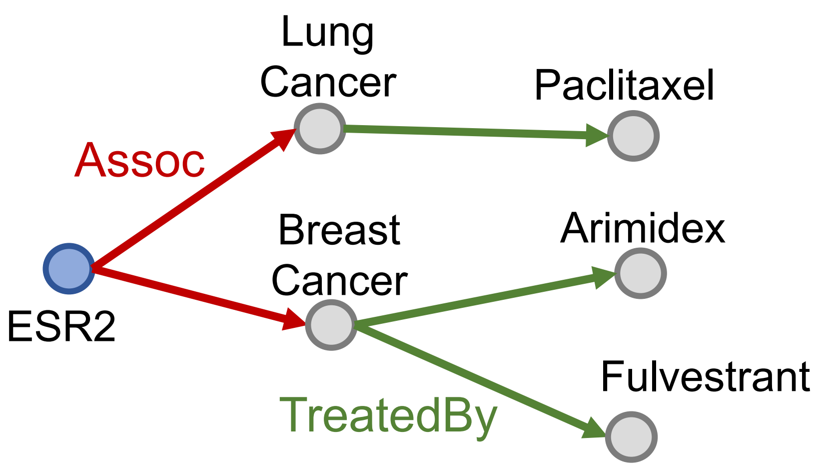
Traverse from the first anchor "ESR2" by relation "Assoc", we reach a set of entities {"Lung Cancer", "Breast Cancer"}

Traversing KG for 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:**



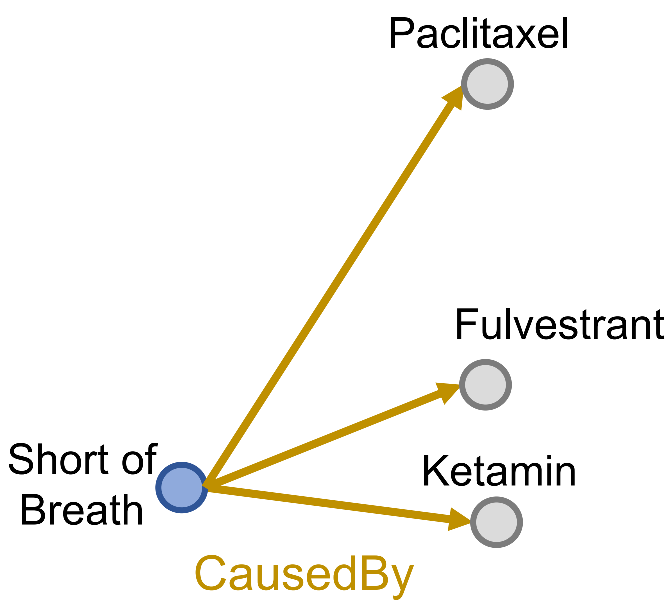
Traverse from the set of entities {"Lung Cancer", "Breast Cancer"} by relation TreatedBy, we reach a set of entities {"Paclitaxel", "Arimidex", "Fulvestrant"}

Traversing KG for Conjunctive Queries

- *"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:**



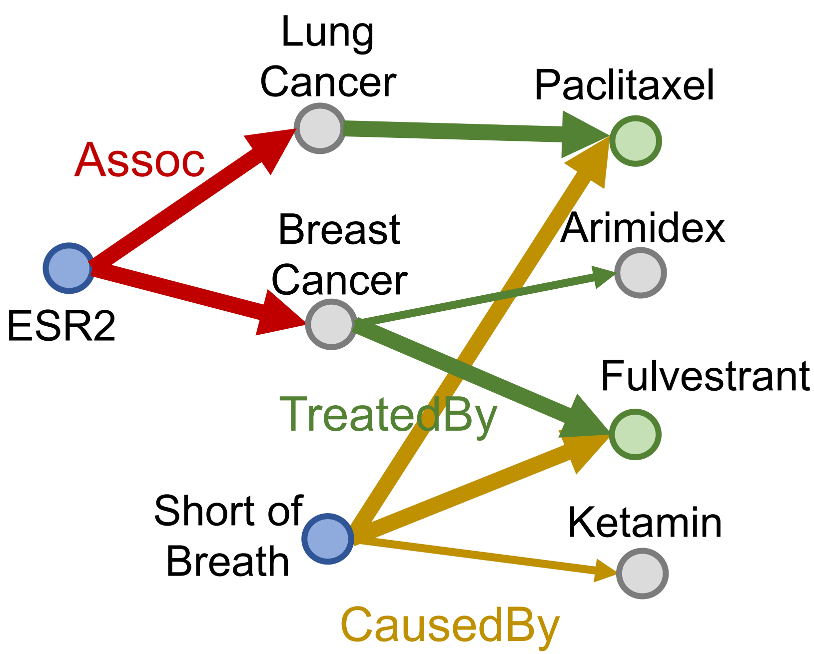
Traverse from the second anchor "Short of Breath" by relation "CausedBy", we reach a set of entities {"Fulvestrant", "Ketamin", "Paclitaxel"}

Traversing KG for 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:**



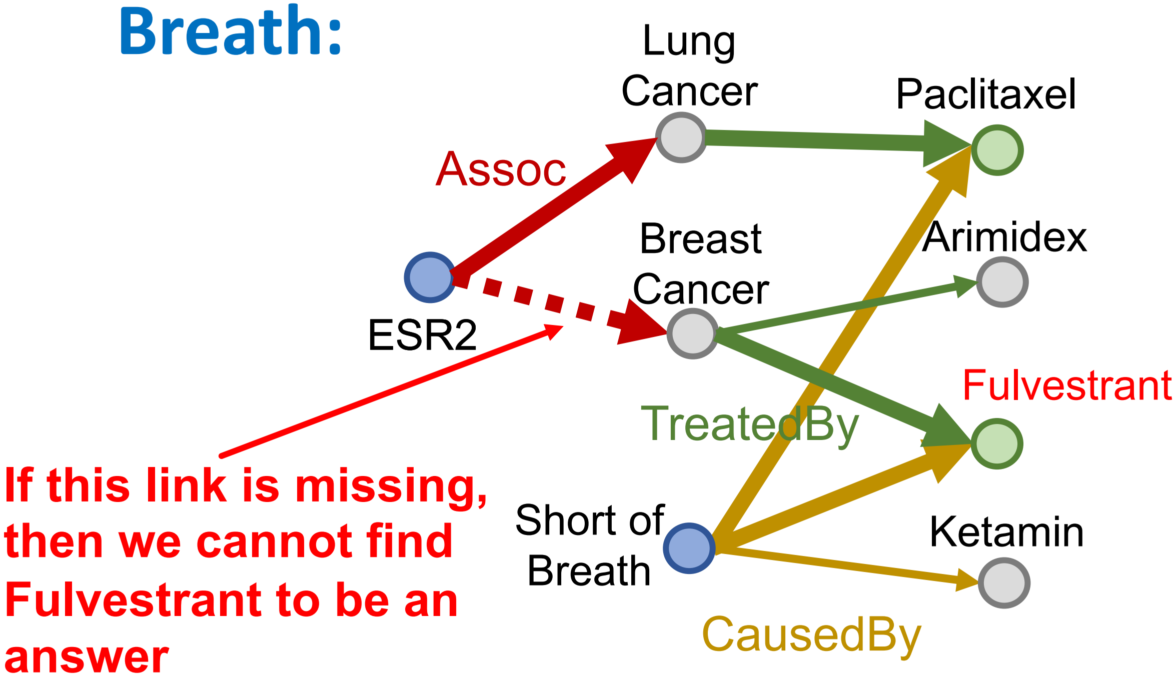
We take intersection between the two sets and get the answers {"Fulvestrant", "Paclitaxel"}

Traversing KG for Conjunctive Queries

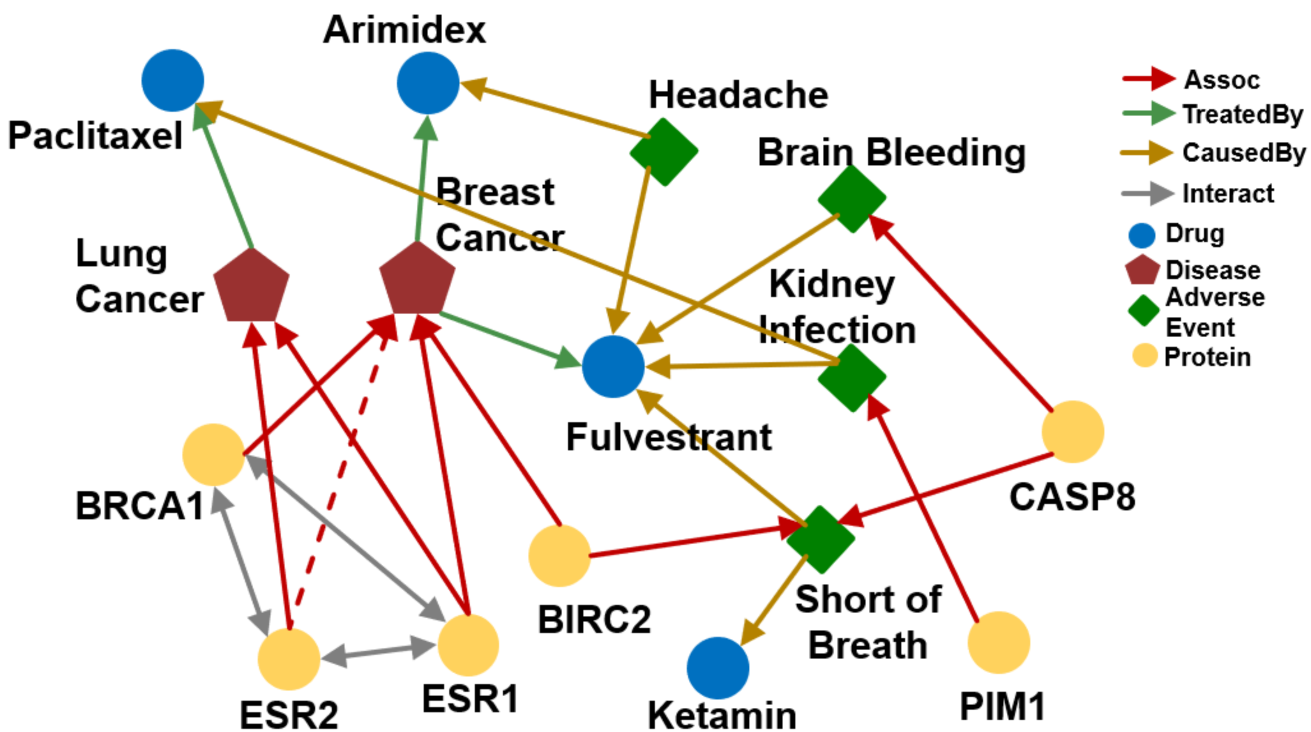
- *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

((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



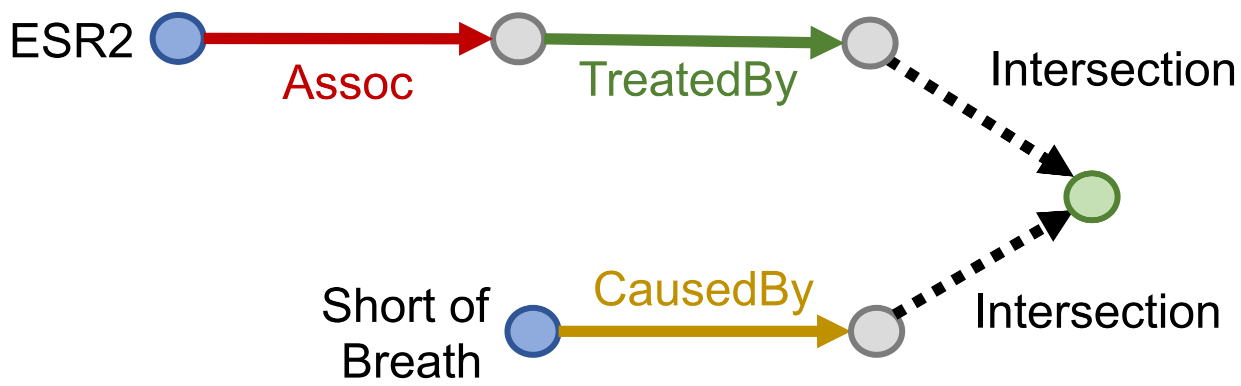
- How can we use embeddings to implicitly impute the **missing (ESR2, Assoc, Breast Cancer)?**
- **Intuition: ESR2** interacts with both **BRCA1** and **ESR1**. Both proteins are associated with **breast cancer**.

Traversing KG in Vector Space

- *“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?

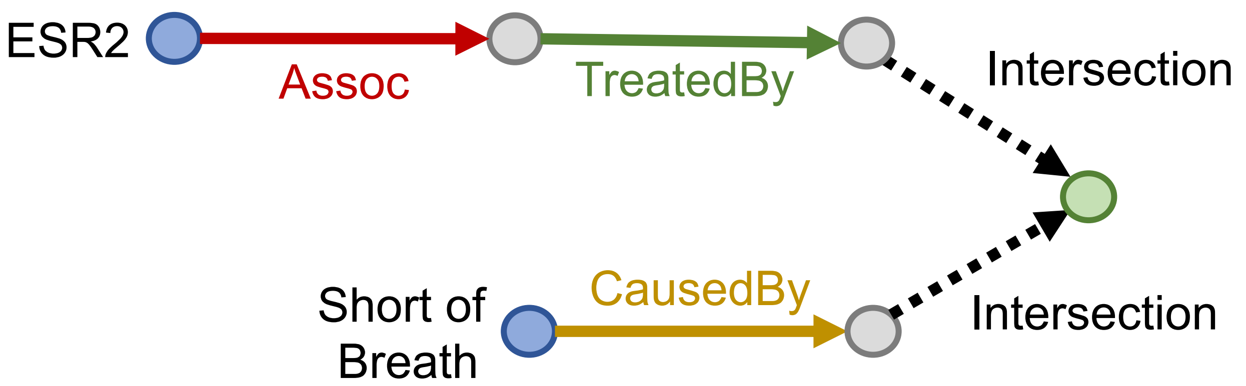
Stanford CS224W: Query2Box: Reasoning over KGs Using Box Embeddings

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

Conjunctive Queries

How can we answer **more complex queries with logical conjunction operation**?

Query plan:

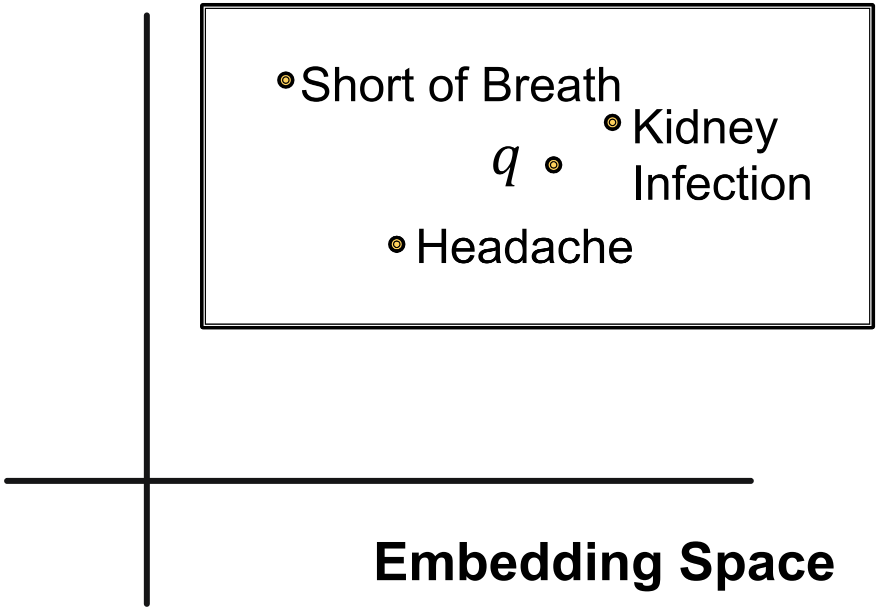


(1) Each intermediate node represents a set of entities; how do we represent it?
(2) How do we define the intersection operation in the latent space?

Box Embeddings

- Embed queries with **hyper-rectangles (boxes)**

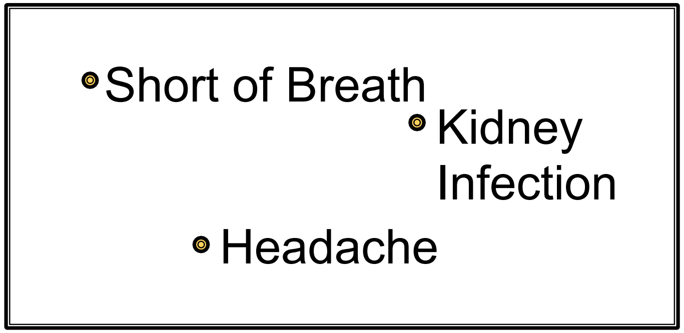
$$\mathbf{q} = (Center(q), Offset(q))$$



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



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 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 with Box Embedding

- **Embed queries in vector space:** *"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:**

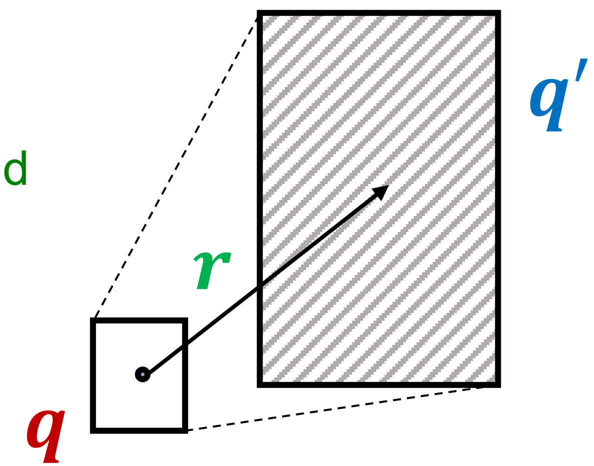
Projection Operator

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 × Relation → 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

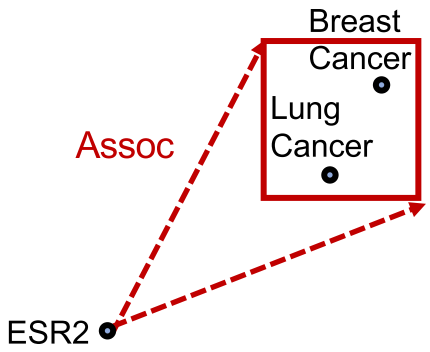


Embed with Box Embedding

- **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



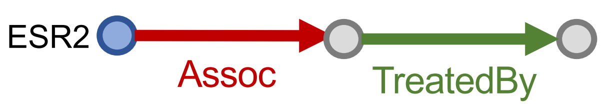
Embed with Box Embedding

"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

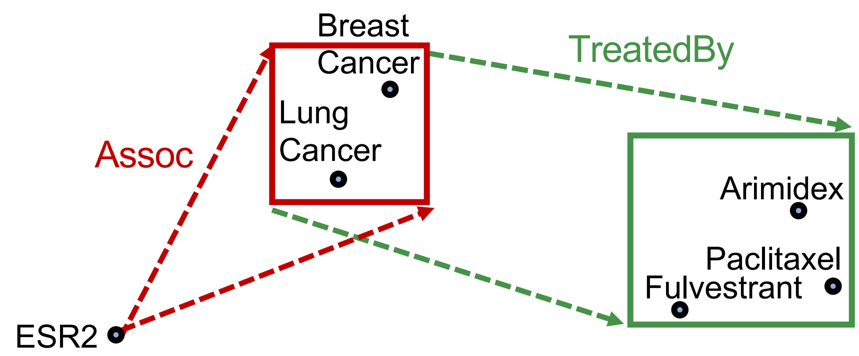
((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

- Use **projection operator** again following the query plan.

Query Plan



Embedding Space



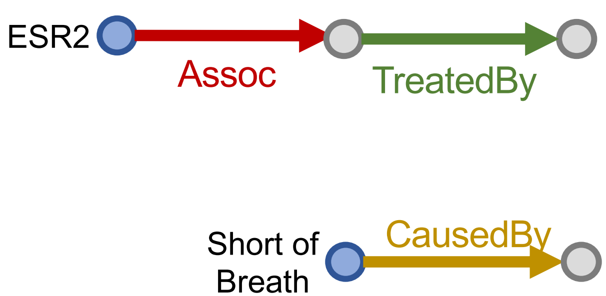
Embed with Box Embedding

"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

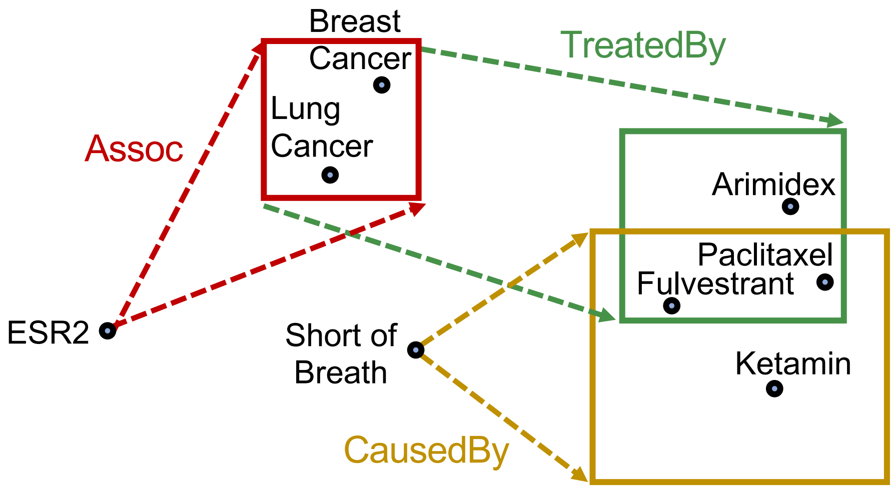
((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

- Use **projection operator** again following the query plan.

Query Plan



Embedding Space



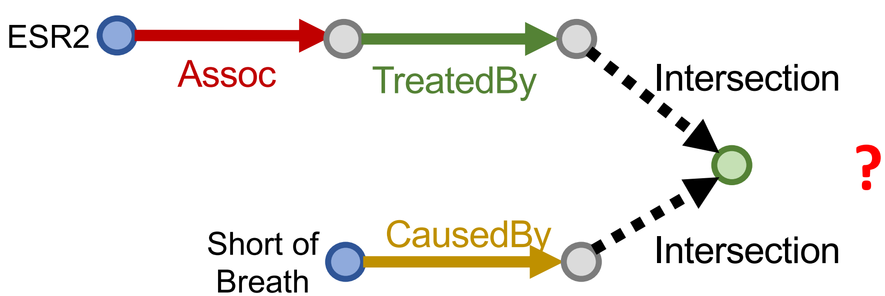
Embed with Box Embedding

"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

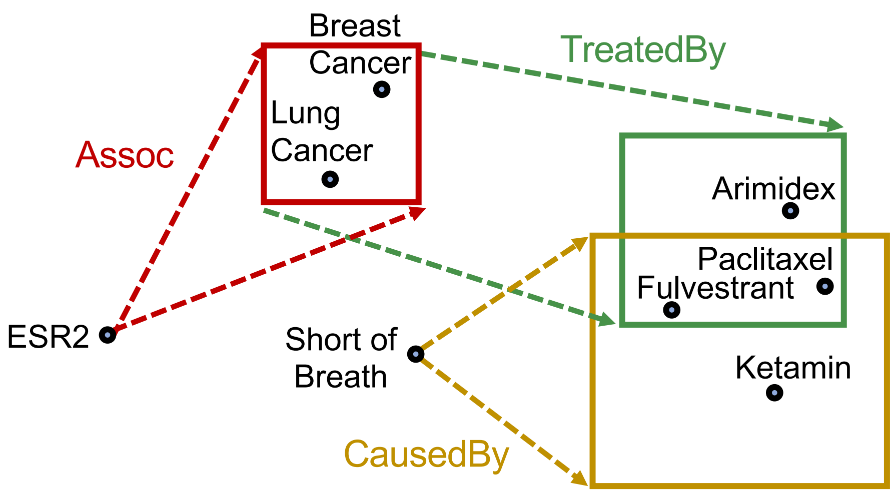
((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

- **How do we take intersection of boxes?**

Query Plan



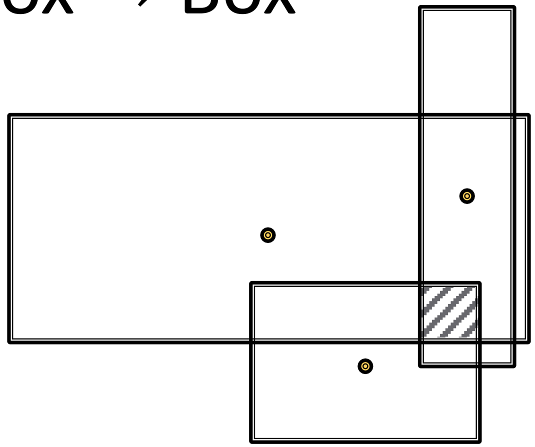
Embedding Space



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 $\times \cdots \times$ Box $\rightarrow$ Box



Intersection Operator

Geometric Intersection Operator $\mathcal{J}$

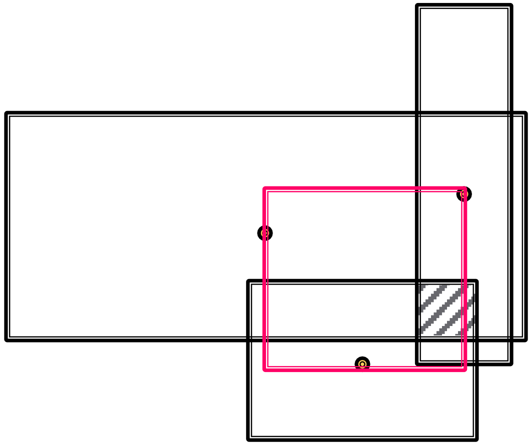
- $\mathcal{J}$: Box $\times \cdots \times$ Box $\rightarrow$ Box

Hadamard product (element-wise product)

$$Cen(q_{inter}) = \sum_i \boldsymbol{w}_i \odot Cen(q_i)$$

$$\boldsymbol{w}_i = \frac{\exp(f_{cen}(Cen(q_i)))}{\sum_j \exp(f_{cen}(Cen(q_j)))}$$

$$Cen(q_i) \in \mathbb{R}^d$$
$$\boldsymbol{w}_i \in \mathbb{R}^d$$



Intuition: The center should be in the red region!
Implementation: The center is a **weighted sum** of the input box centers

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

$\boldsymbol{w}_i$ **represents a "self-attention" score for the center of each input** $Cen(q_i)$.

Intersection Operator

Geometric Intersection Operator $\mathcal{J}$

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

$$Off(q_{inter})$$
$$= \min\big(Off(q_1), \ldots, Off(q_n)\big)$$
$$\odot\, \sigma(f_{off}(Off(q_1), \ldots, Off(q_n)))$$

guarantees shrinking

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**.

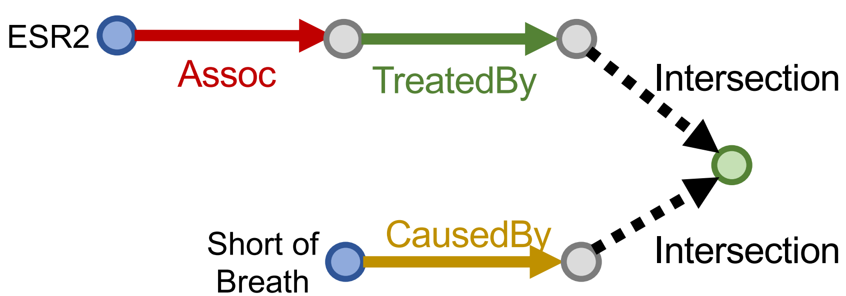
Embed with Box Embedding

"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

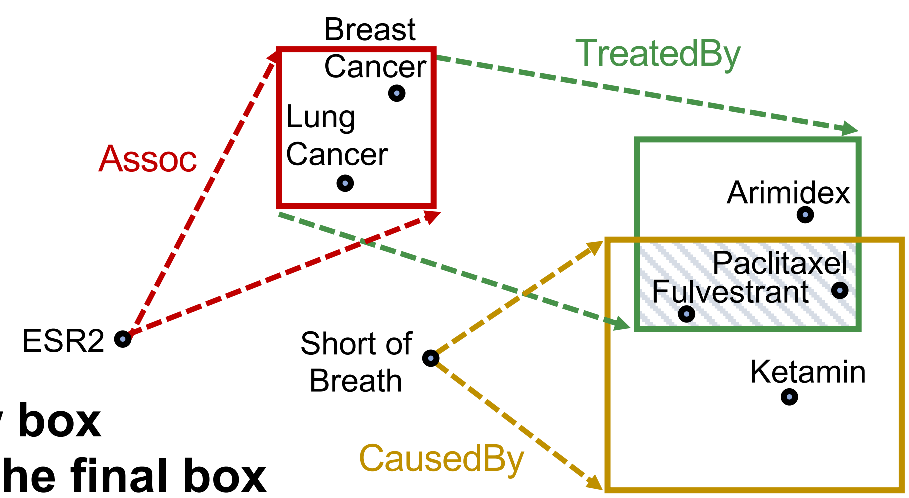
((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

- **Use box intersection operator**

Query Plan



Embedding Space



The shadow box represents the final box embedding of the query

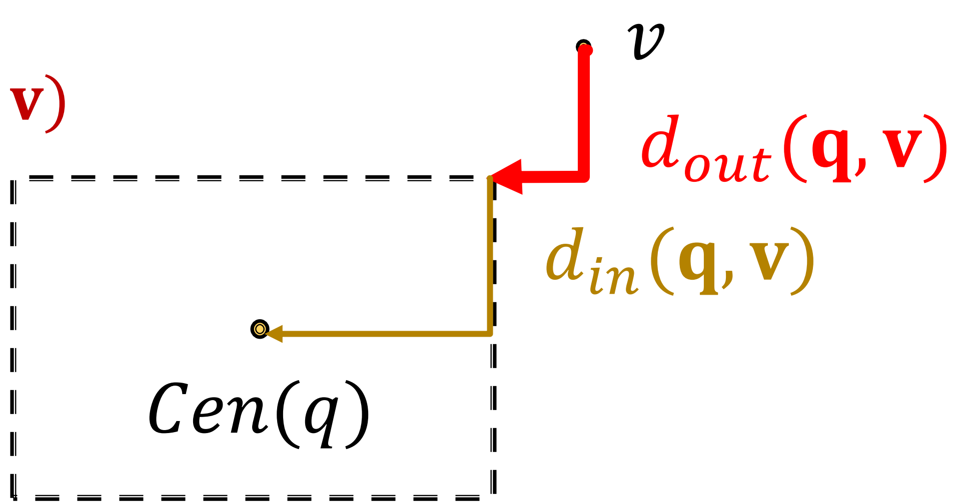
Entity-to-Box Distance

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

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

where $0 < \alpha < 1$.

- **Intuition**: if the point is enclosed in the box, the distance should be **downweighted**.
- $\boldsymbol{f_q(v) = -d_{box}(\mathbf{q}, \mathbf{v})}$



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 **E**xistential **P**ositive **F**irst-**o**rder (**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 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?

Embedding AND-OR Queries

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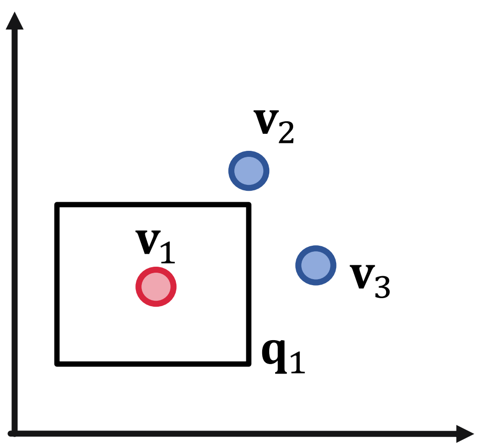

We want **red dots (answers)** to be in the box while the **blue dots (negative answers)** to be outside the box

Embedding AND-OR Queries

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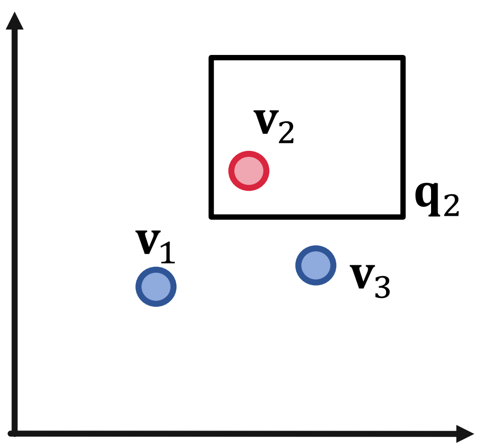

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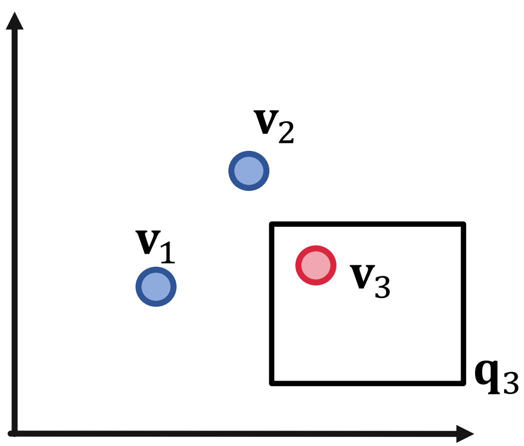

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Embedding AND-OR Queries

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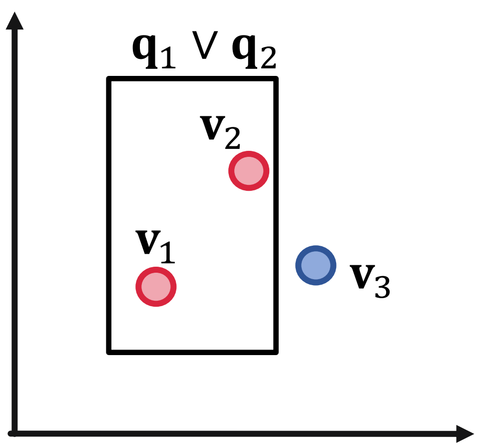

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Embedding AND-OR Queries

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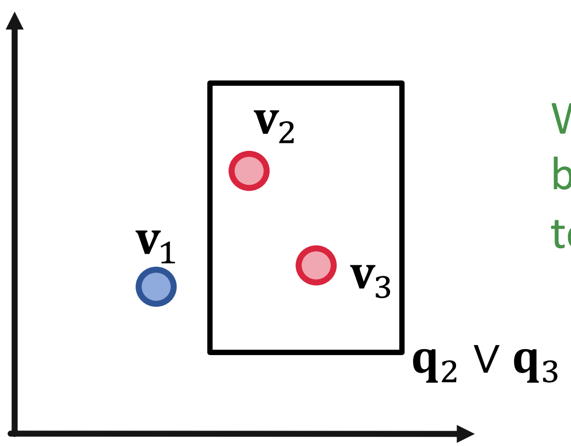

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Embedding AND-OR Queries

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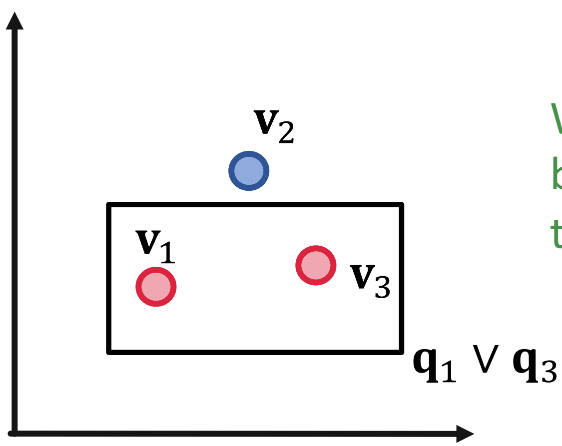

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Embedding AND-OR Queries

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  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
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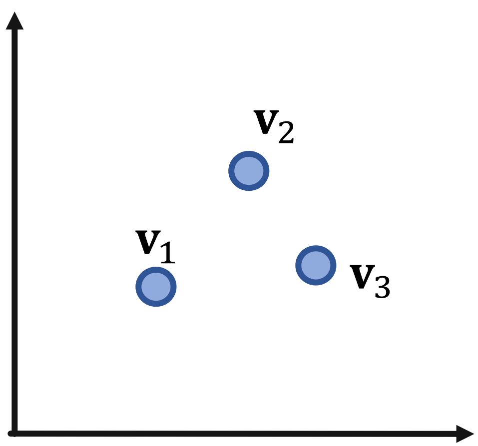
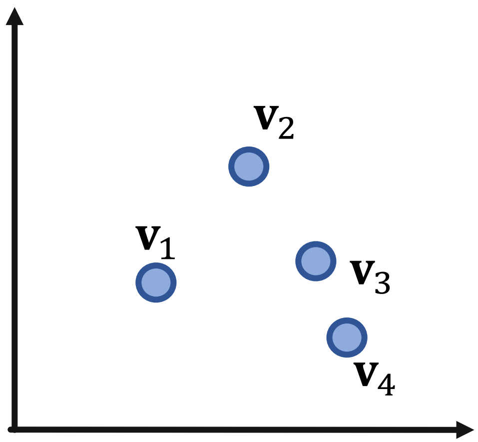


For 3 points, 2-dimension is okay!
How about 4 points?

Embedding AND-OR Queries (2)

- **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?



Embedding AND-OR Queries (2)

- **Example 2:**
  - Given 4 queries q_1, q_2, q_3, q_4 with answers:
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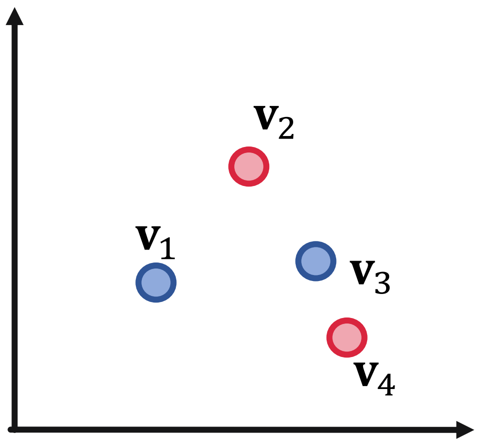
  - If we allow union operation, can we embed them in two-dimensional plane?



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)

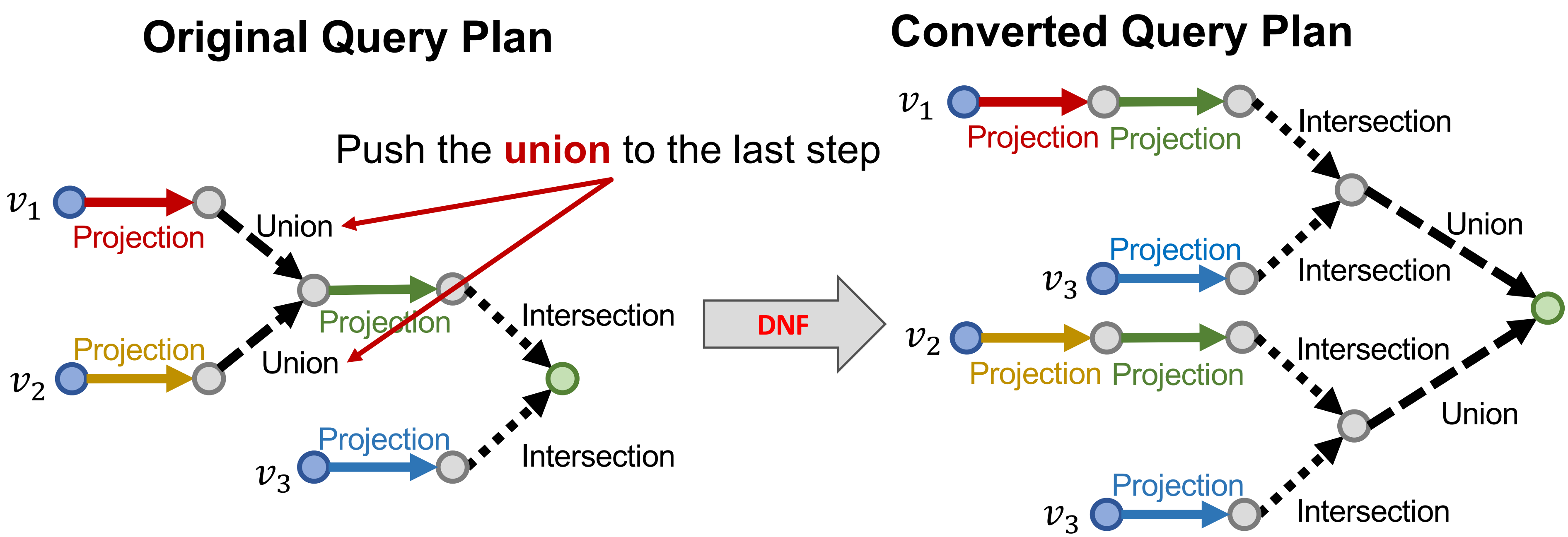
Can we embed AND-OR queries in low-dimensional vector space?

- **Conclusion**: Given any M conjunctive queries $q_1, \dots, q_M$ 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 q,**

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

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:

$$d_{box}(\mathbf{q}, \mathbf{v}) = min(d_{box}(\mathbf{q}_1, \mathbf{v}), \ldots, d_{box}(\mathbf{q}_m, \mathbf{v}))$$

- **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 $\mathbf{v}$ is close to one conjunctive query $\mathbf{q}_i$, then $\mathbf{v}$ should be close to $\mathbf{q}$ **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:

$$d_{box}(\mathbf{q}, \mathbf{v}) = min(d_{box}(\mathbf{q}_1, \mathbf{v}), \ldots, d_{box}(\mathbf{q}_m, \mathbf{v}))$$

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

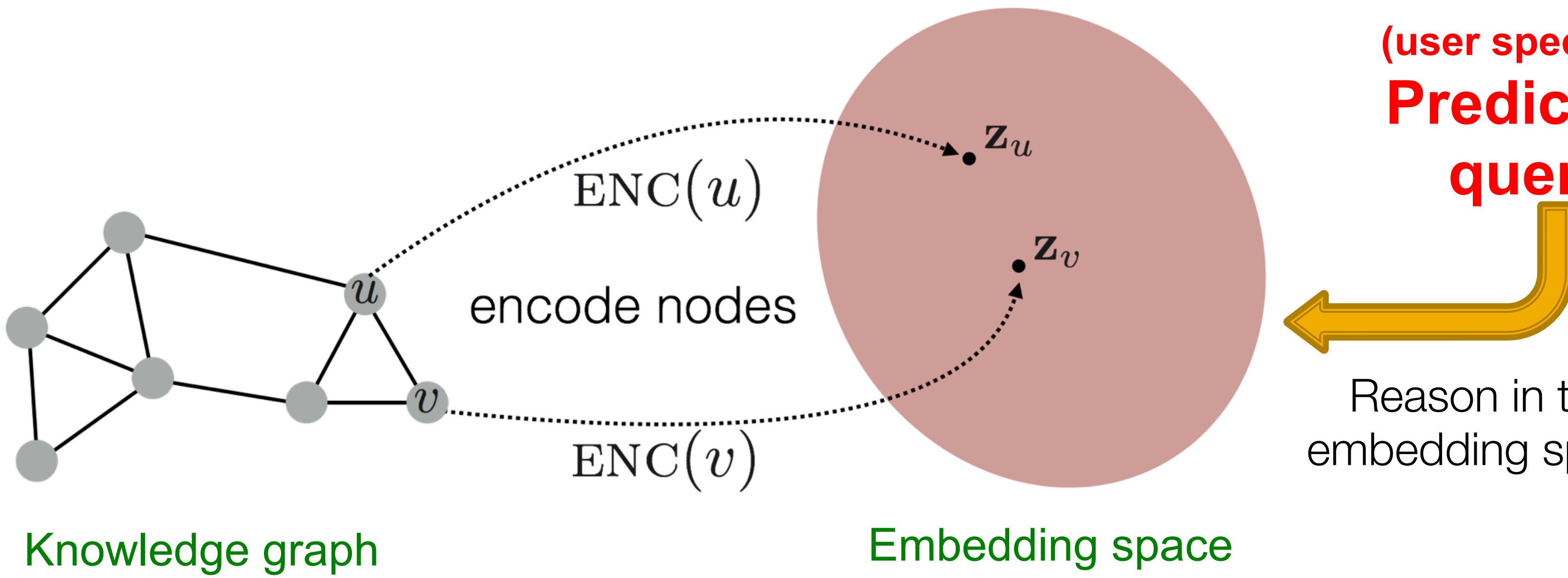
Stanford CS224W: How to Train Query2box

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

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



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

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).

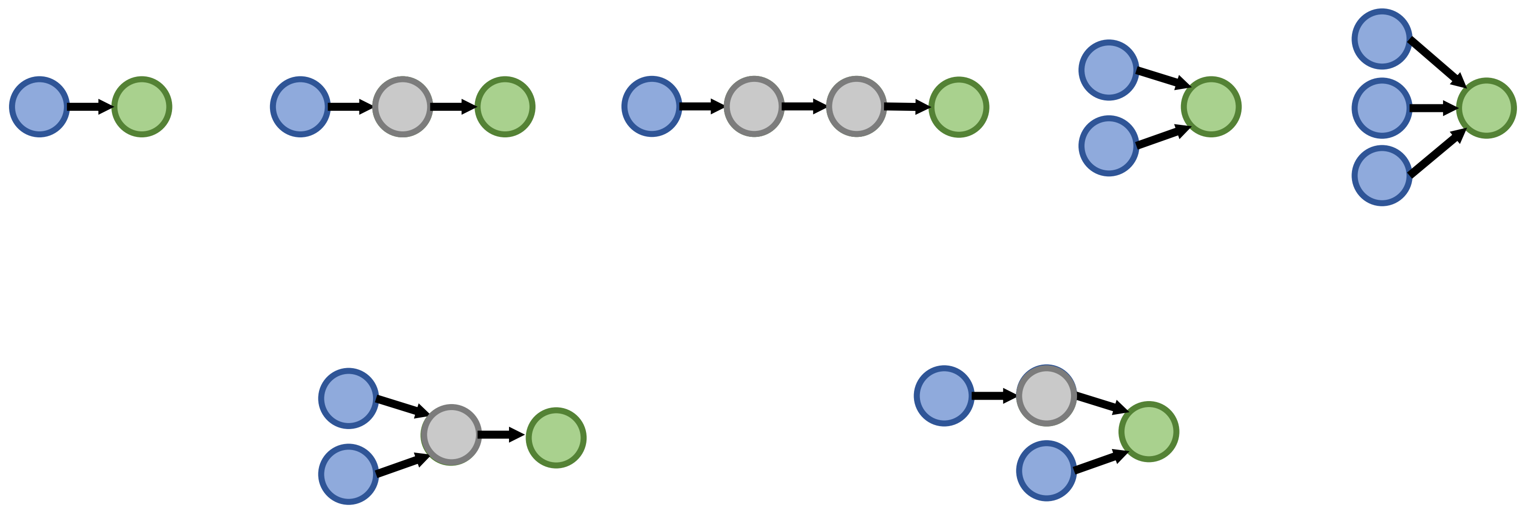
Training: Details

- **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 $\mathbf{q}$.
     - 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 minimize $f_q(v')$):

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

Query Generation from Templates

- **Generate queries from multiple query templates:**

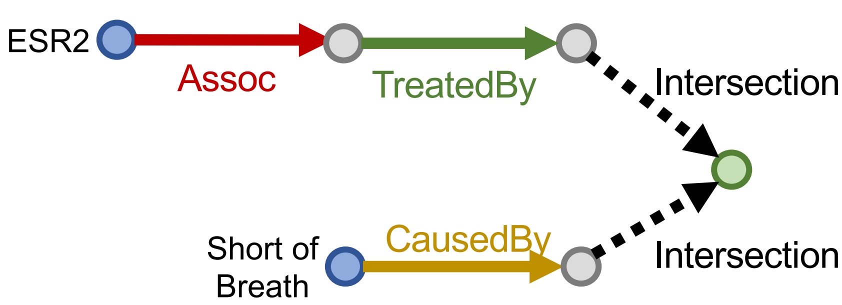


Query Generation from Templates

- 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?**

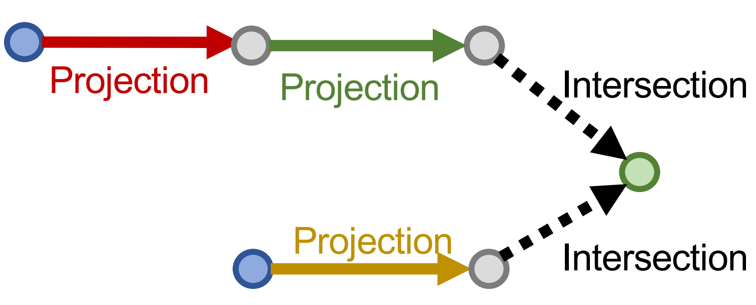
Query

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



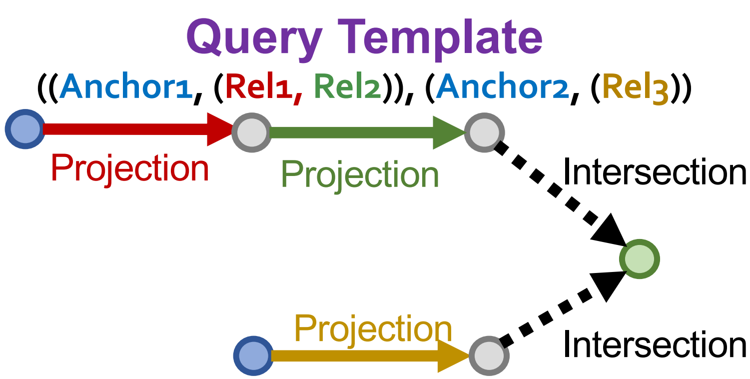
Query Template

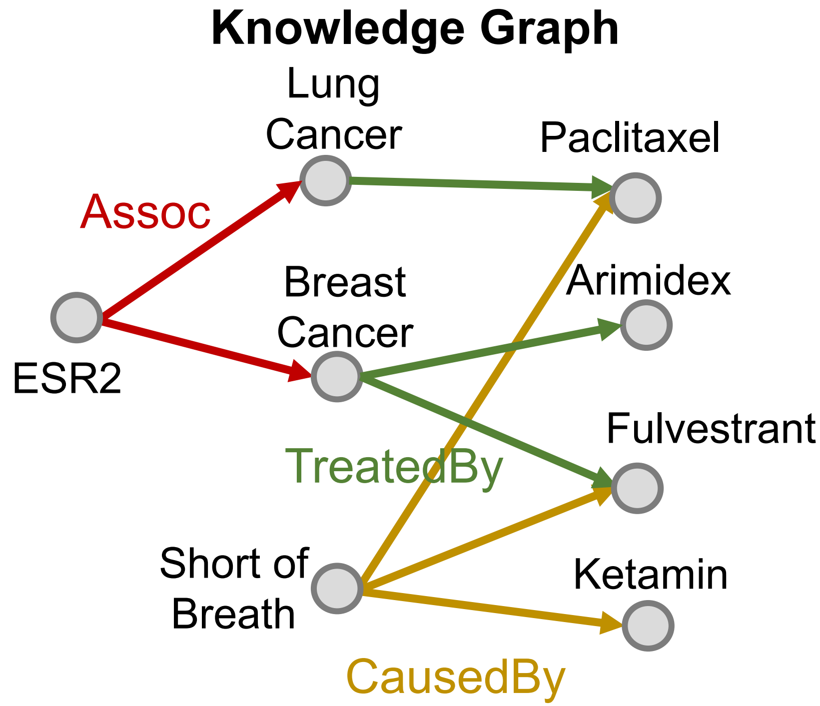
((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3))



Query Generation from Templates

- **How to instantiate a query template given a KG?**

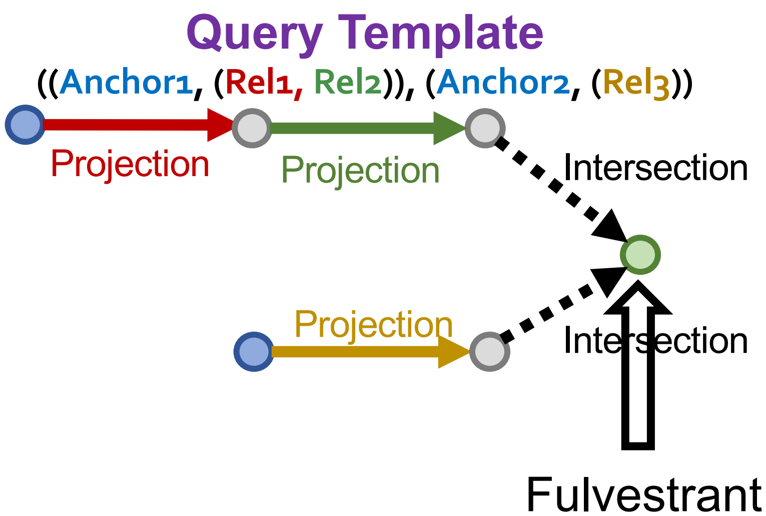


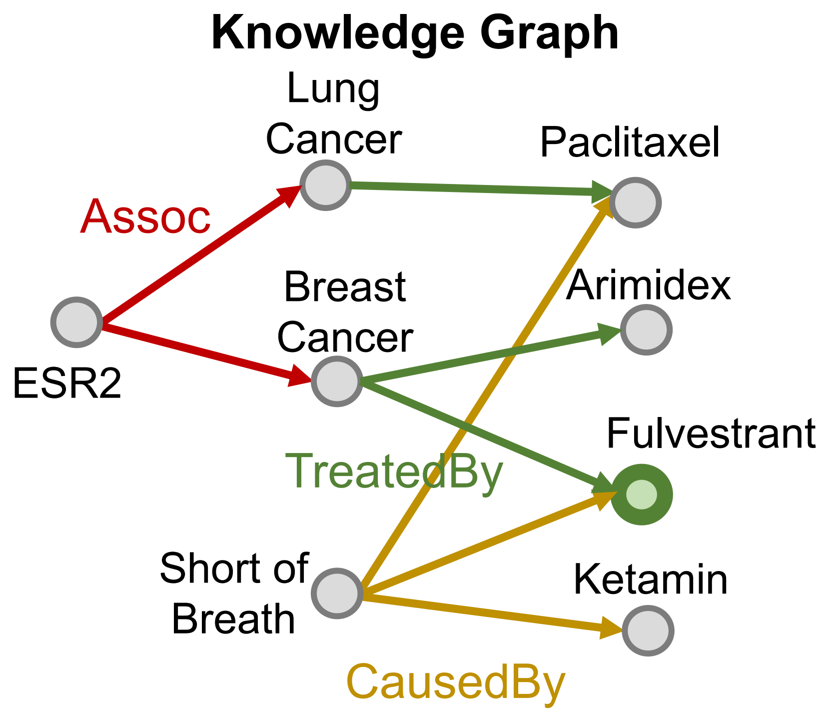


Overview:
Start from instantiating the **answer node** of the query template and then iteratively instantiate the other edges and nodes until we ground **all the anchor nodes**

Query Generation from Templates

- **How to instantiate a query template given a KG?**



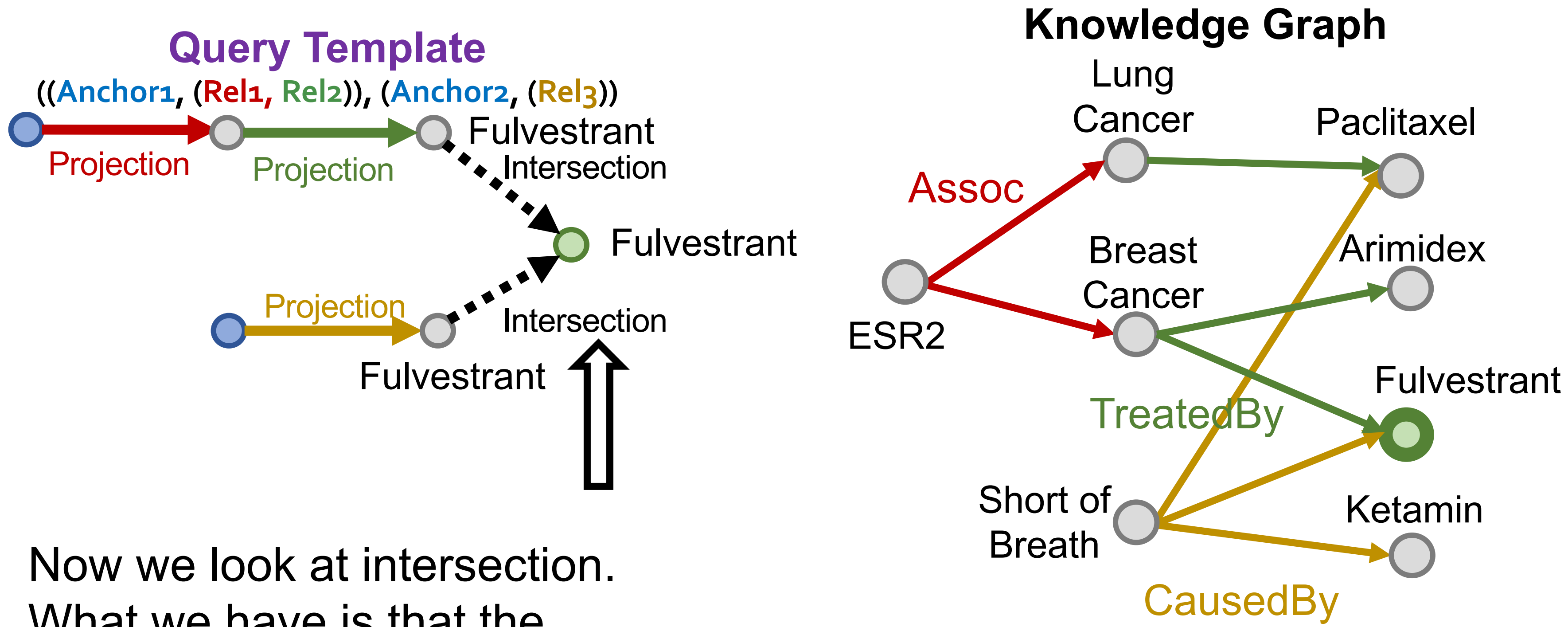


Start from instantiating the **root node** of the query template.

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

Query Generation from Templates

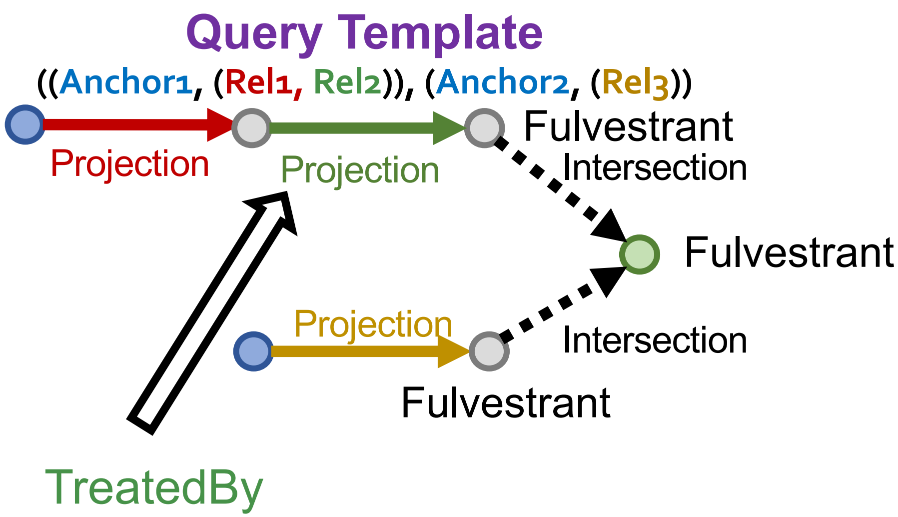
- **How to instantiate a query template given a KG?**

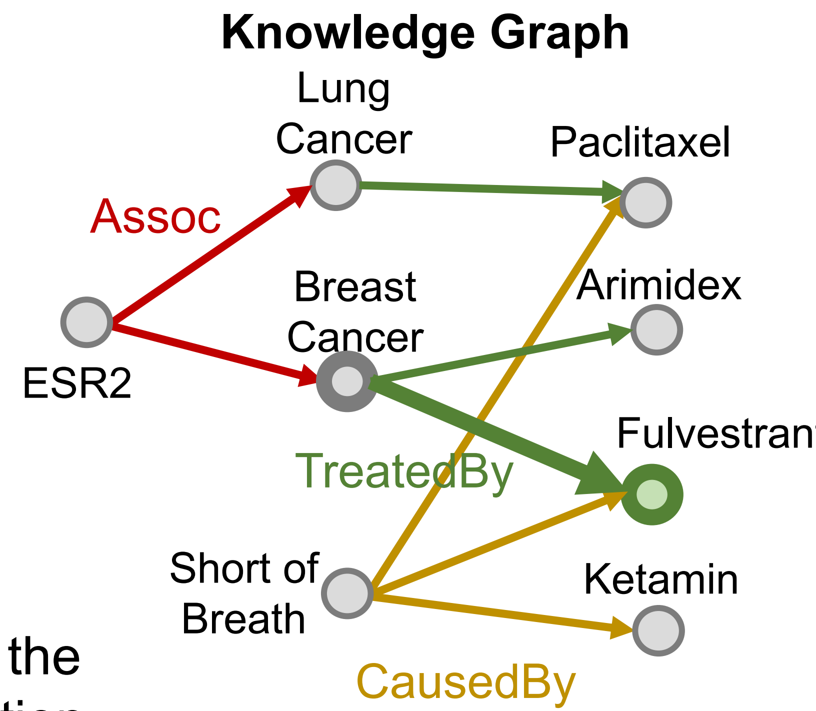


Now we look at intersection. What we have is that the intersection of the sets of entities is **Fulvestrant**, then naturally the two sets should also contain **Fulvestrant**.

Query Generation from Templates

- **How to instantiate a query template given a KG?**





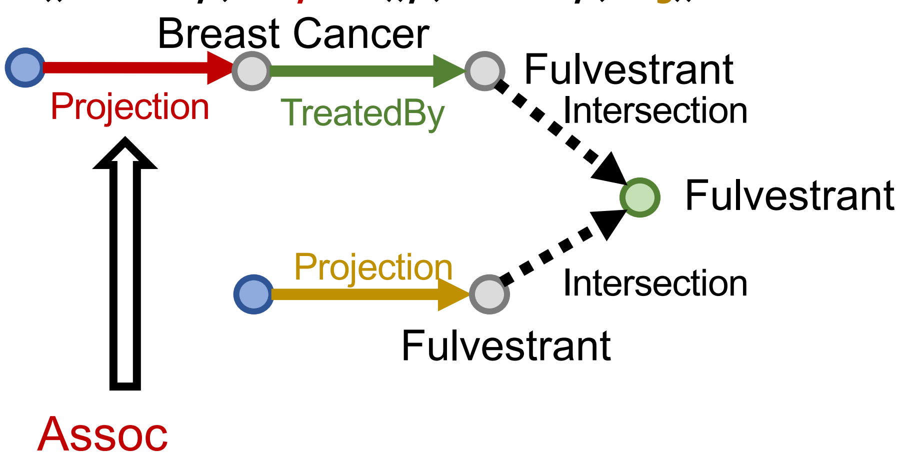
We instantiate the **Projection edge** in the template by randomly sample one relation associated with the current entity **Fulvestrant**. For example, we may select relation **TreatedBy**, and check what entities are connected to **Fulvestrant** with **TreatedBy**: {**Breast Cancer**}.

Query Generation from Templates

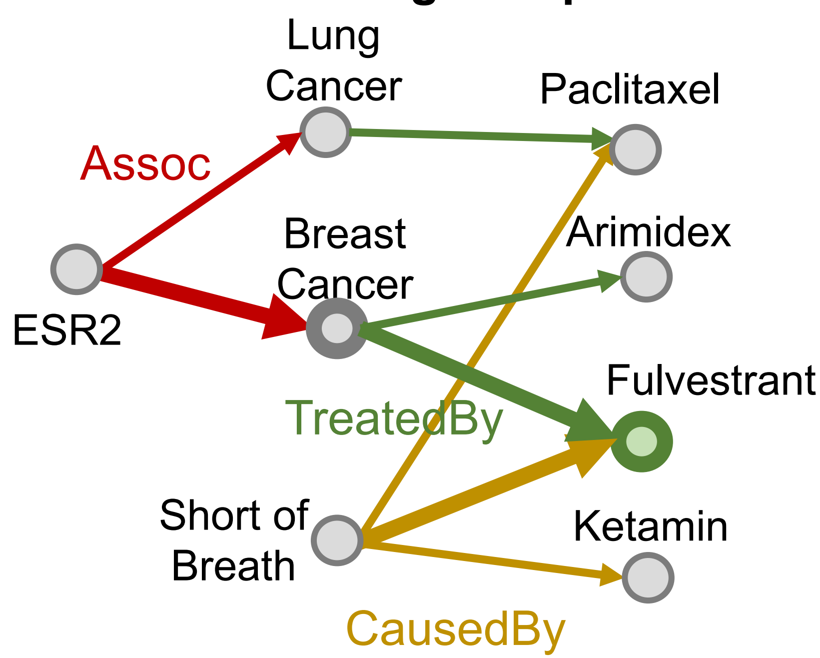
- **How to instantiate a query template given a KG?**

Query Template

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



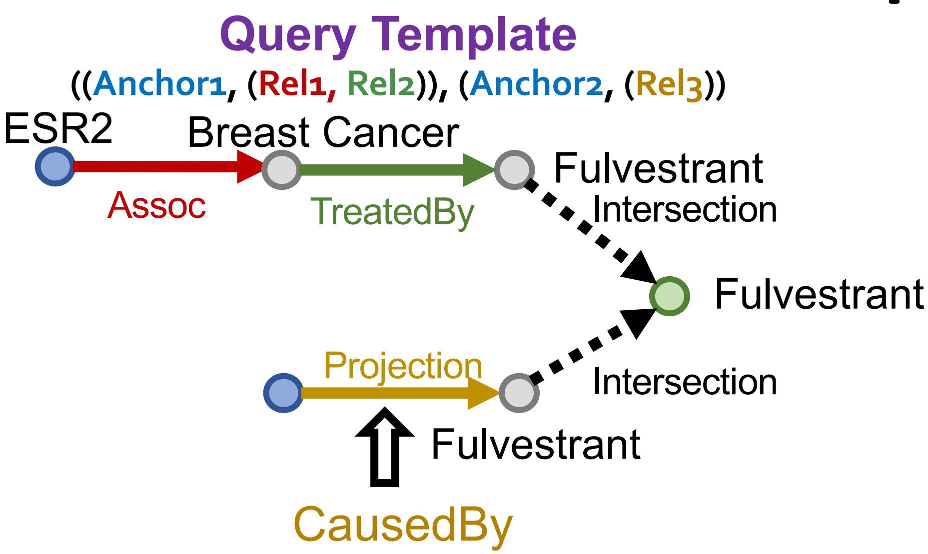
Knowledge Graph

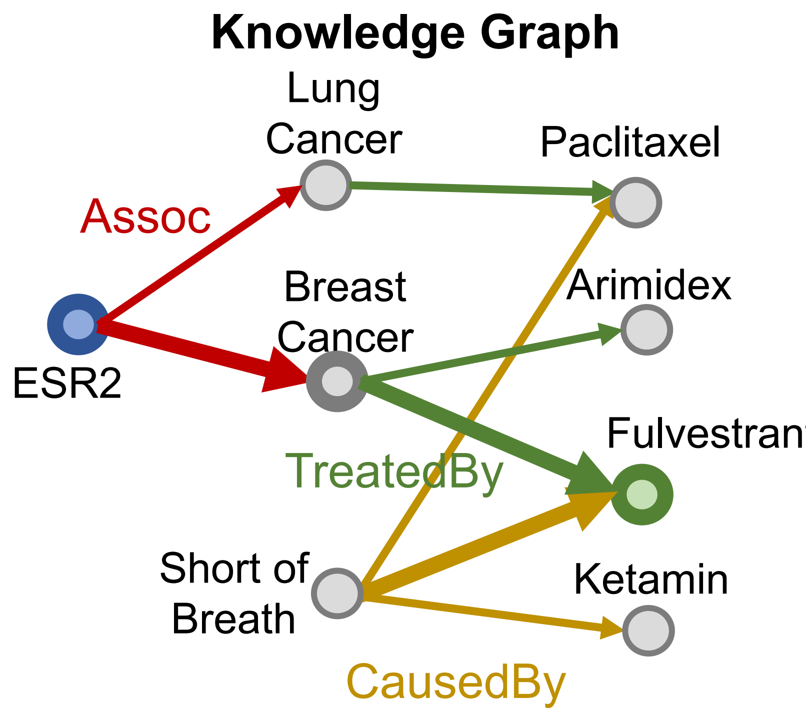


We first look at one branch and ground the **Projection edge** with the relation associated with **Breast Cancer**, e.g., **Assoc**. Then we check what entities are connected to **Breast Cancer** with **Assoc**: {**ESR2**}.

Query Generation from Templates

- **How to instantiate a query template given a KG?**

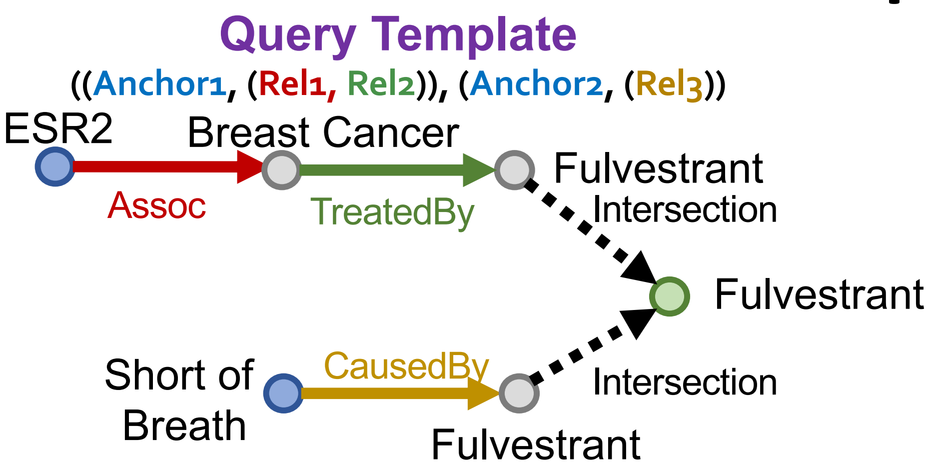


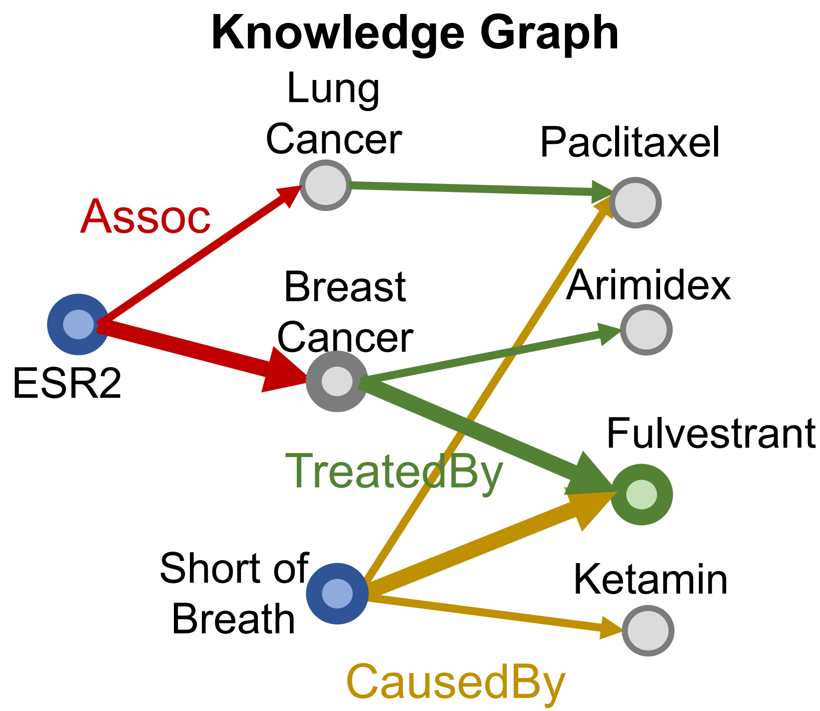


Then we look at the second branch and ground the **Projection edge** with the relation associated with **Fulvestrant**, e.g., **CausedBy**. Then we check what entities are connected to **Fulvestrant** with **CausedBy**: {**Short of Breath**}.

Query Generation from Templates

- **How to instantiate a query template given a KG?**

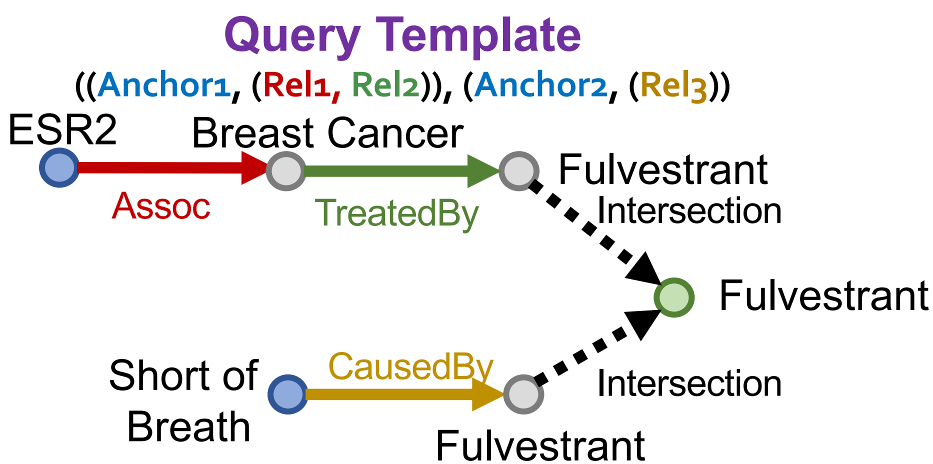




We select entity from {**Short of Breath**}, set it as the anchor node.

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 $v' \notin [\![q]\!]_G$

Stanford CS224W: Example of Query2box

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

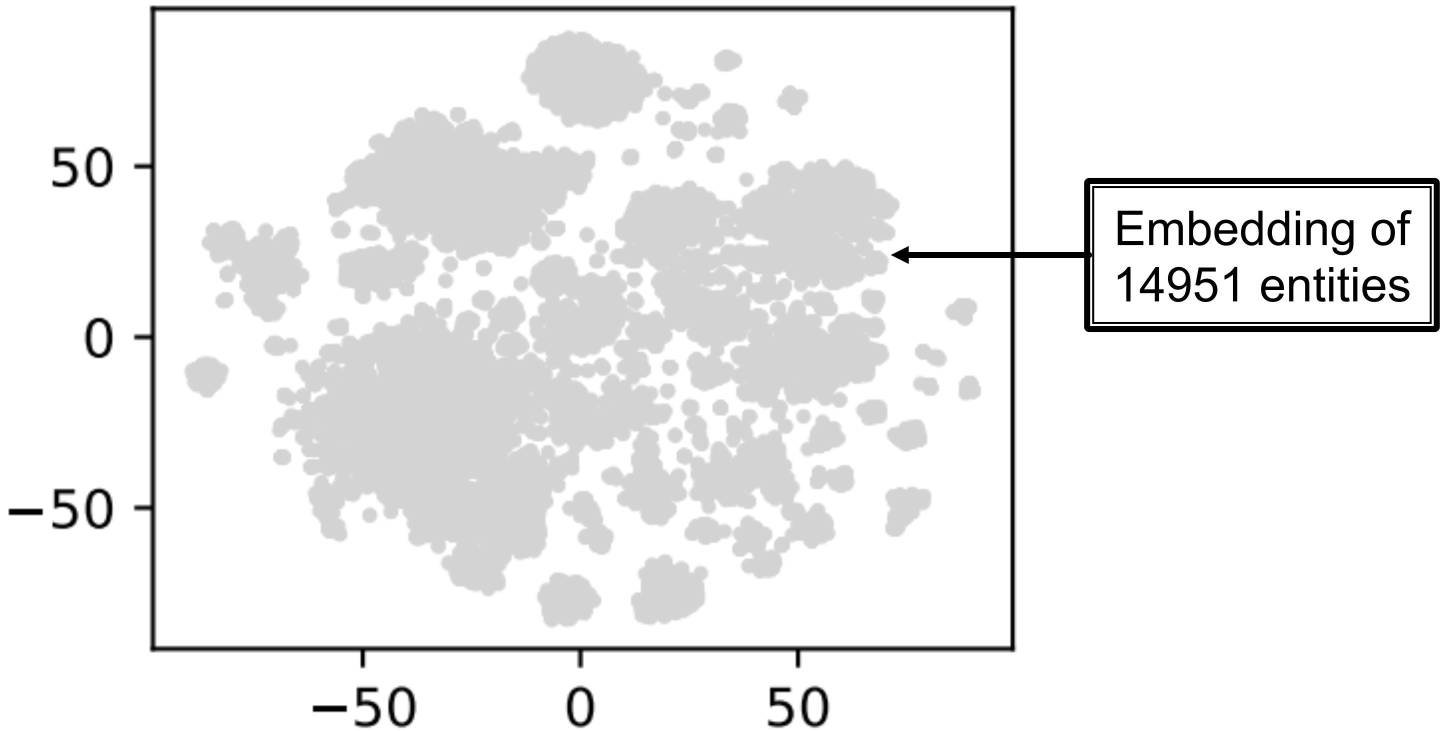
Visualization

- **What do box embeddings actually learn?**

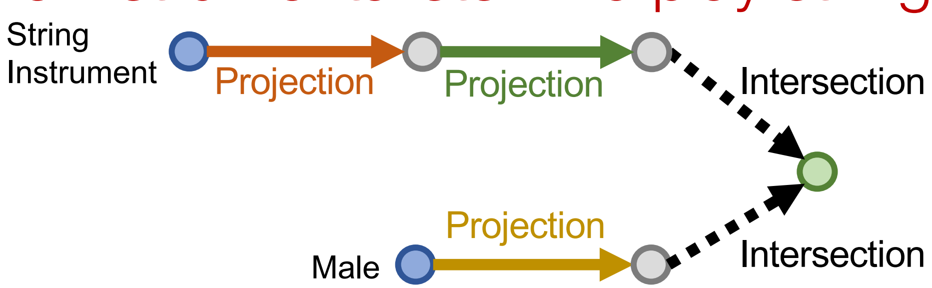
Example: “*List male instrumentalists who play string instruments*”

- We use t-SNE to reduce the embedding space to a 2-dimensional space, in order to visualize the query results

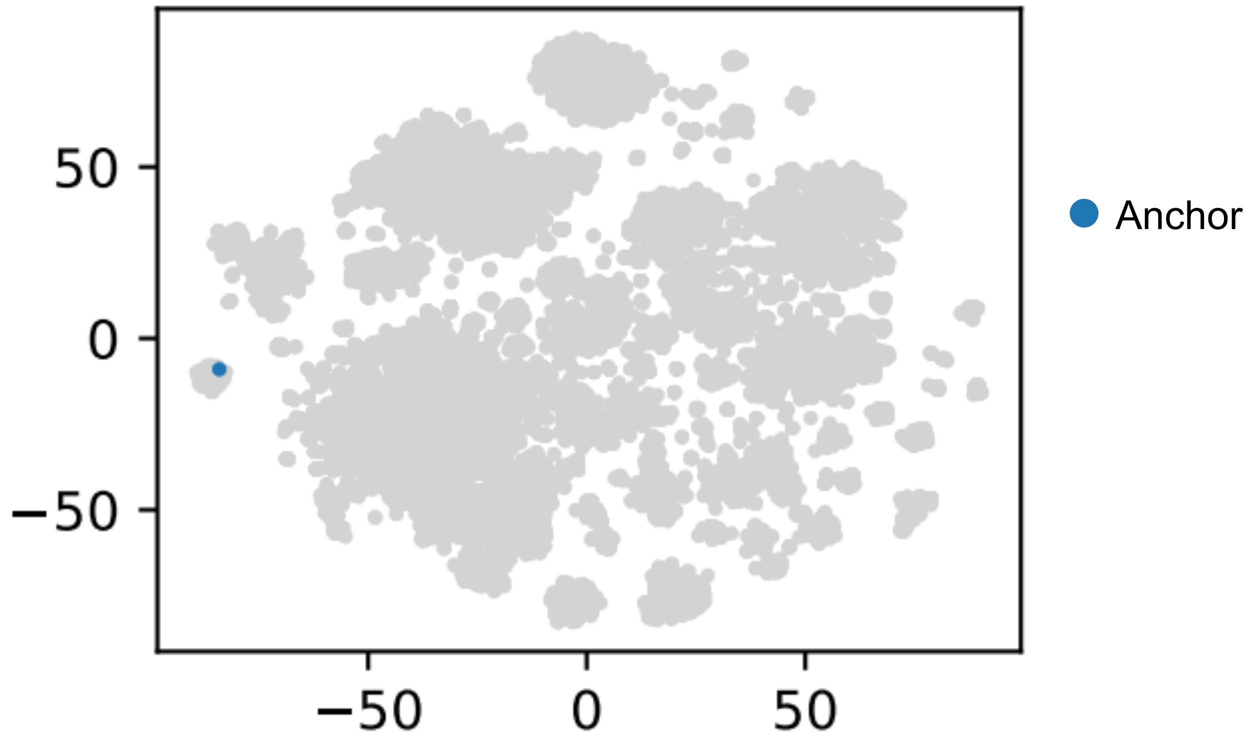
Embedding Space



"List male instrumentalists who play string instruments"

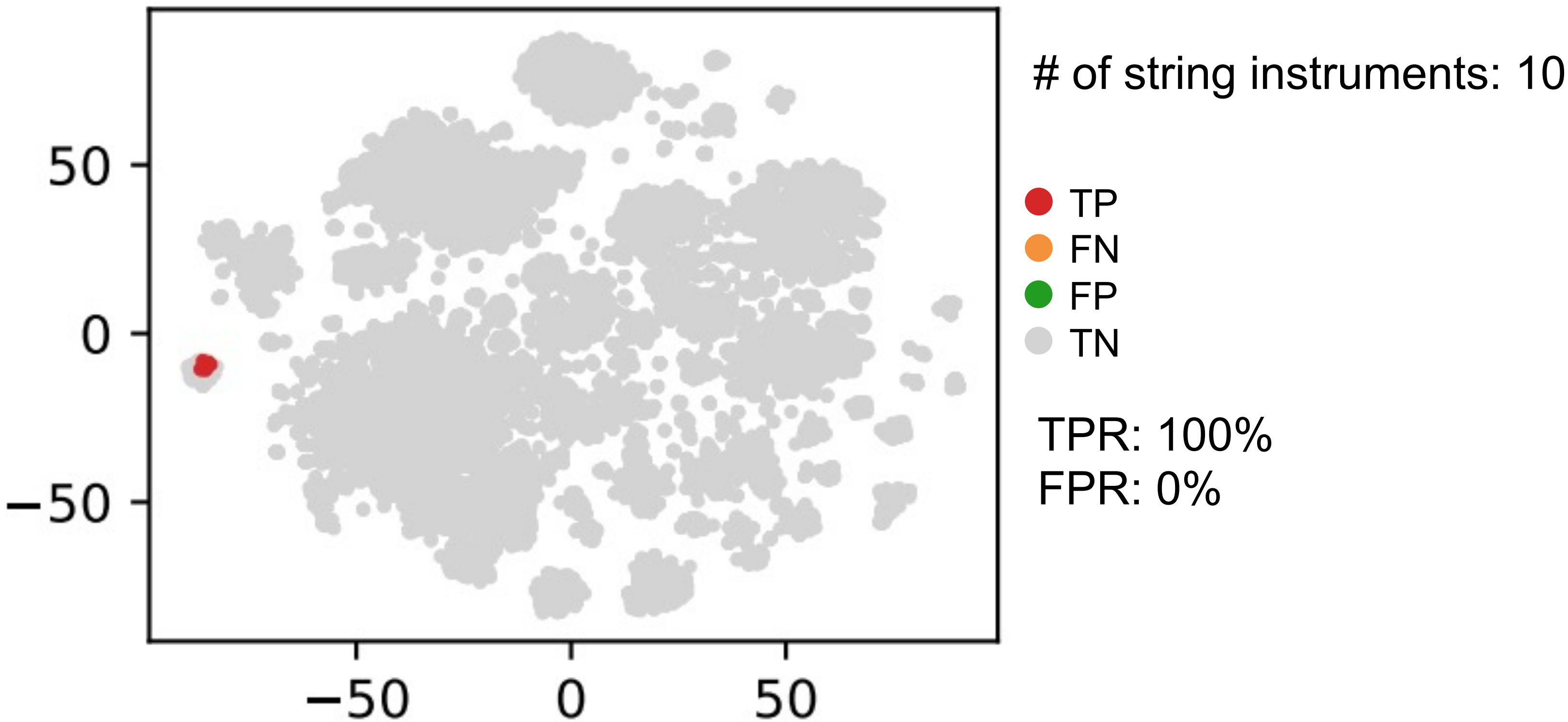


Embedding Space



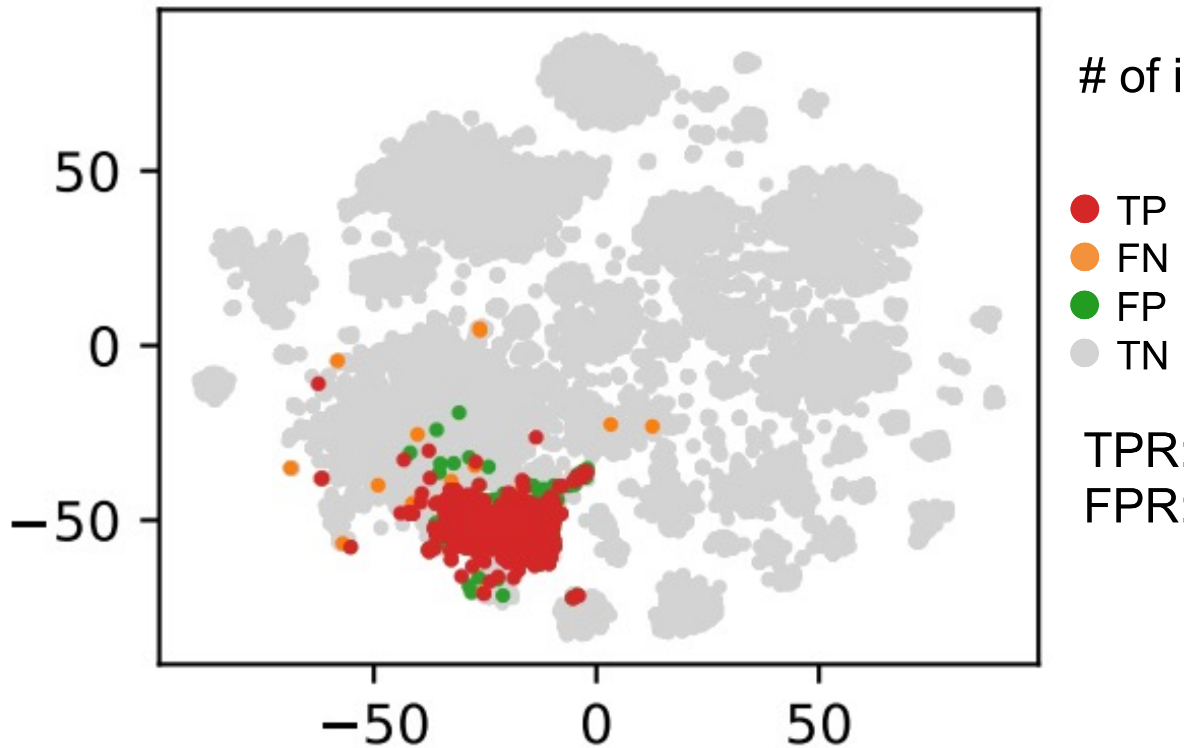
"List male instrumentalists who play string instruments"

Embedding Space



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

Embedding Space

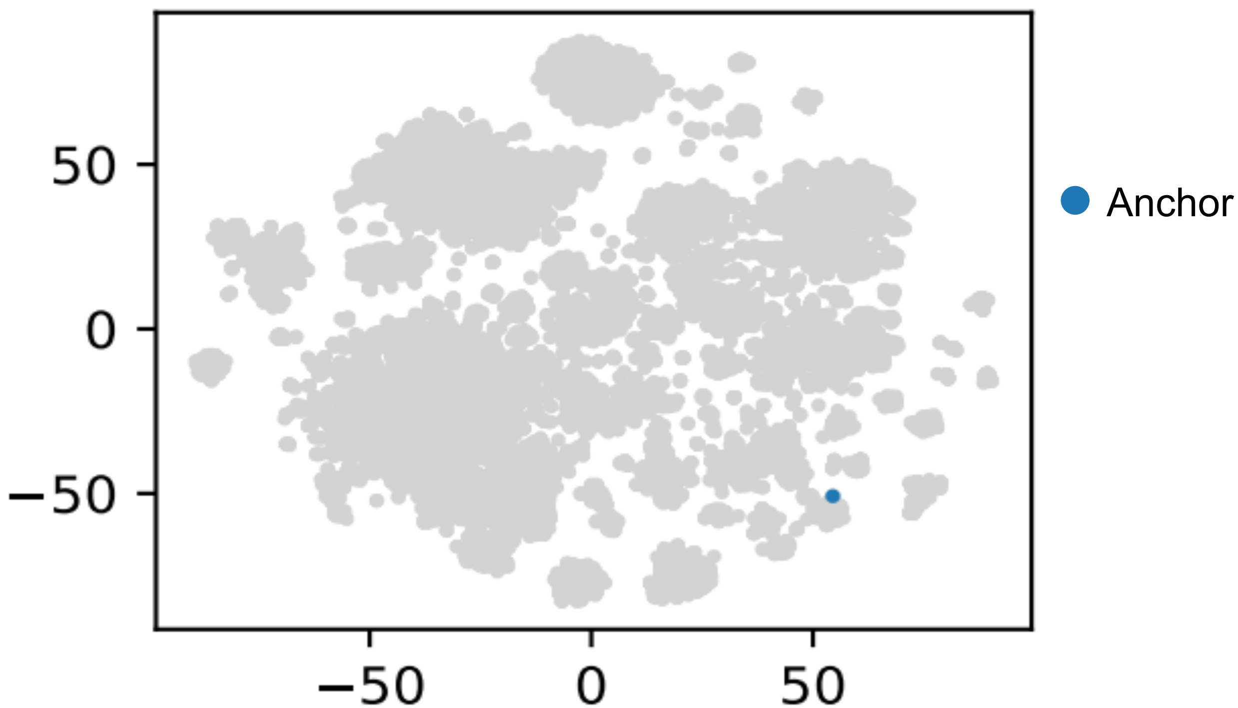


# of instrumentalists: 472

TPR: 98.4%
FPR: 0.01%

“List male instrumentalists who play string instruments”

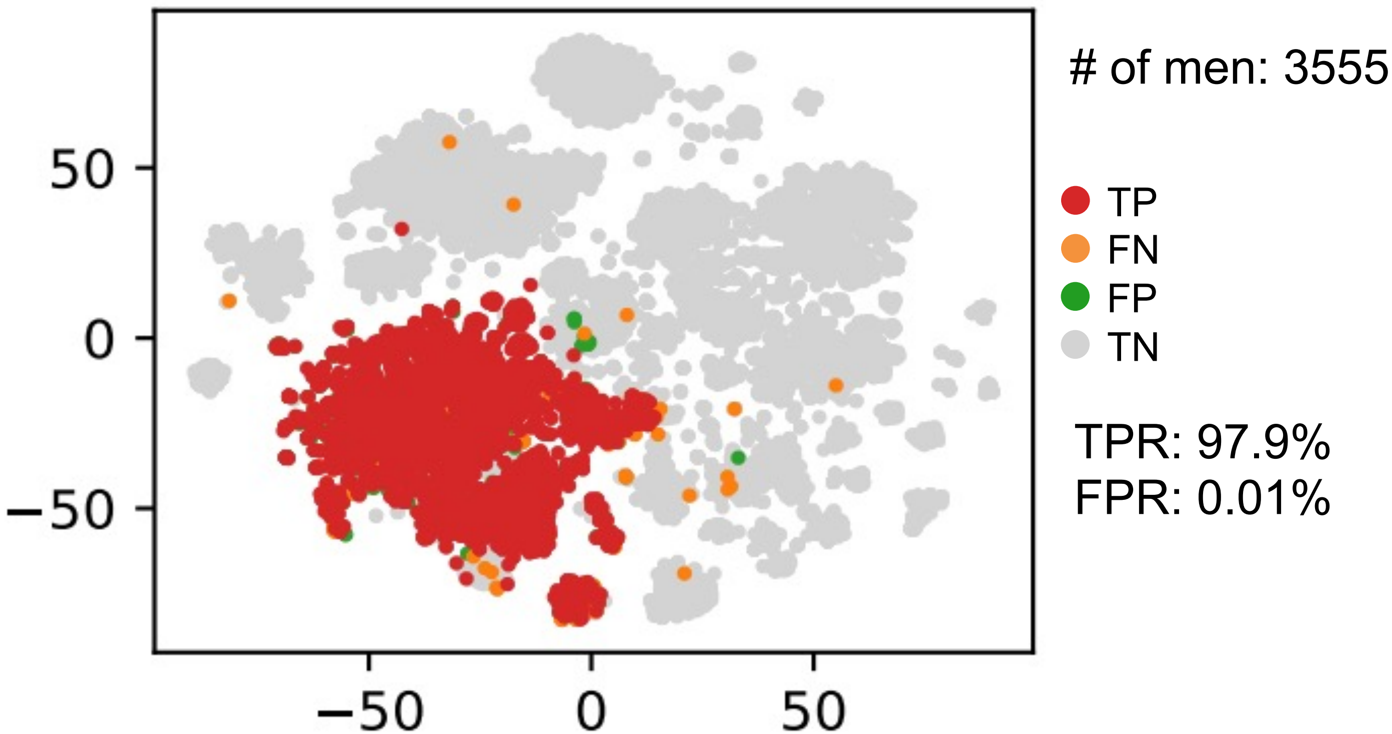
Embedding Space



“List male instrumentalists who play string instruments”

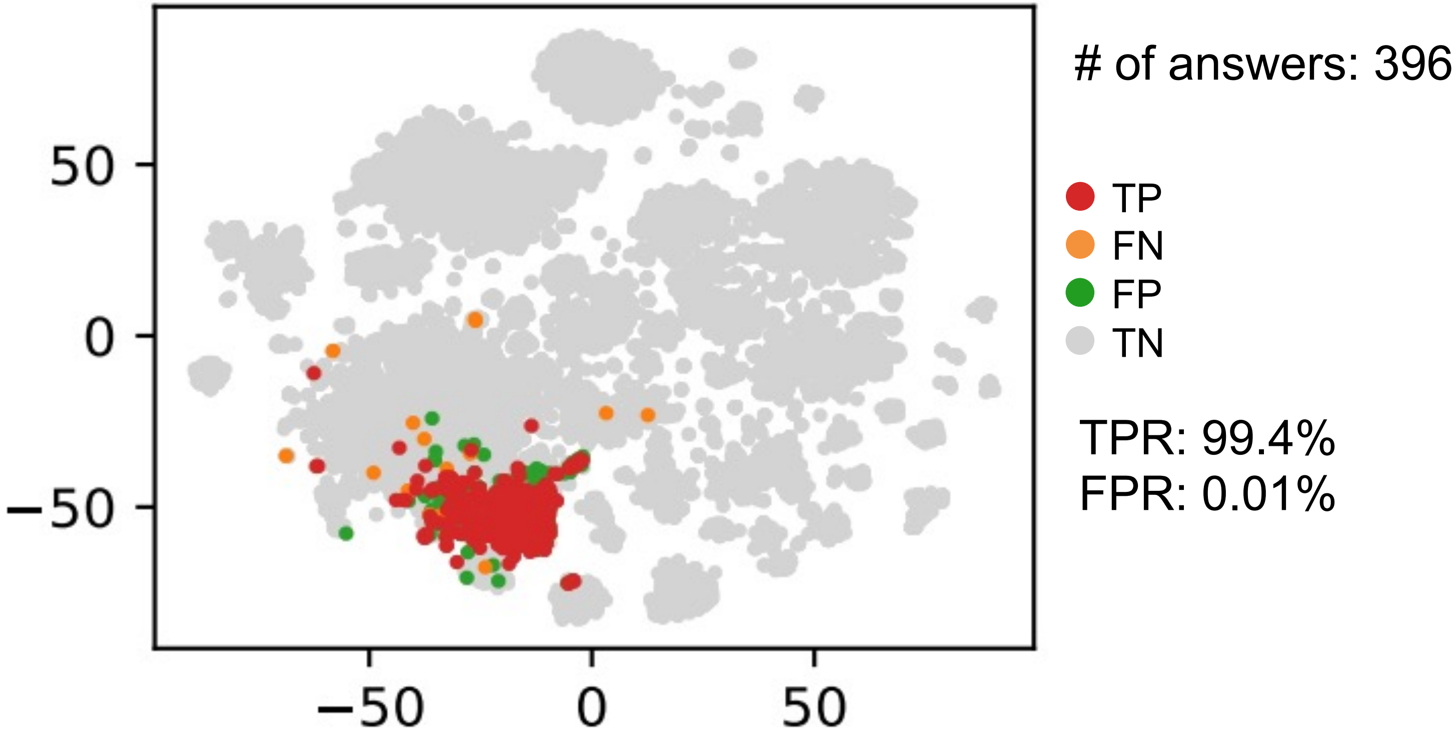
Male

Embedding Space

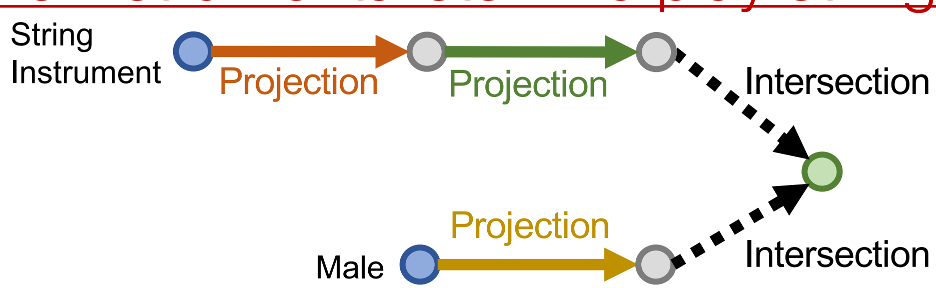


"List <u>male</u> instrumentalists who play string instruments"

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**