

# Concept Learning in Description Logics

Neurosymbolic Concept Learning

Axel Ngonga



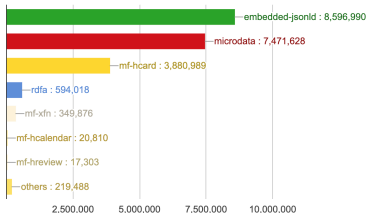
August 14, 2023

## Section 1

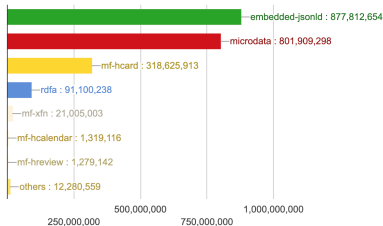
# Motivation

## Data Web

Domains with Triples



URLs with Triples

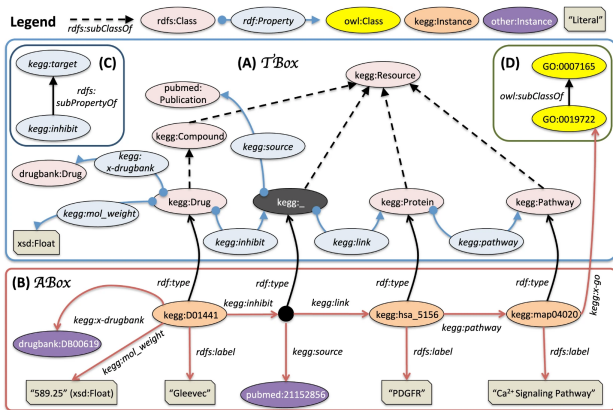


- ▶ RDF knowledge bases are now **first-class citizens** of the Web
- ▶ Approx. 50% of websites contain RDF<sup>1</sup>
- ▶ 2+ billion URLs contain RDF statements
- ▶ Ca. 100 billion statements in Linked Open Data

<sup>1</sup>See <http://webdatacommons.org/structureddata/#results-2022-1>

# Introduction

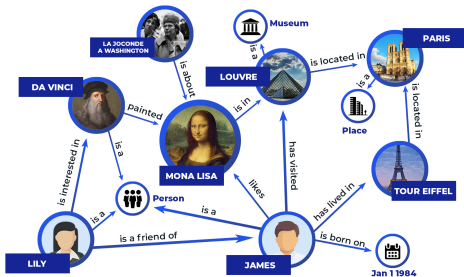
## Description Logics



- ▶ Terminology of RDF datasets in description logics
- ▶ Popular DLs include *ELH* (e.g., for biomedical domain), *ALC* (e.g., for ML-driven applications), and *SROIQ* (e.g., on the Web)

# Motivation

## Example



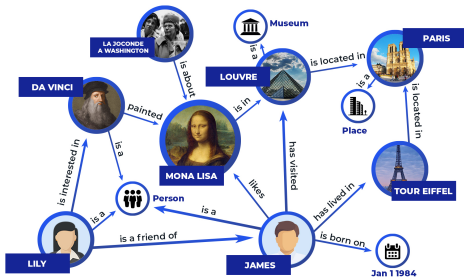
2

►  $E^+ = \{Louvre, TourEiffel\}, E^- = \{Lily, James\}$

<sup>2</sup>Source: <https://bit.ly/3sxCj6e>

# Motivation

## Example



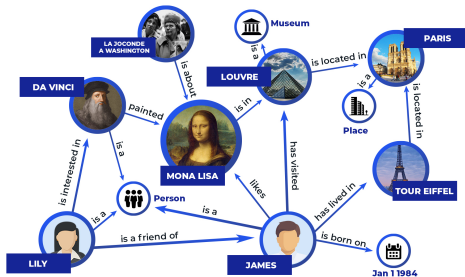
2

- ▶  $E^+ = \{\text{Louvre}, \text{TourEiffel}\}, E^- = \{\text{Lily}, \text{James}\}$
- ▶ **Neural solution:**  $e(v_i) = \varphi \left( \bigoplus_{v_j \in \mathcal{N}_i} e(v_j), e(v_i) \right)$
- ▶ **Pro:** Time-efficient
- ▶ **Contra:** Unintelligible, does not exploits background knowledge

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## Example



3

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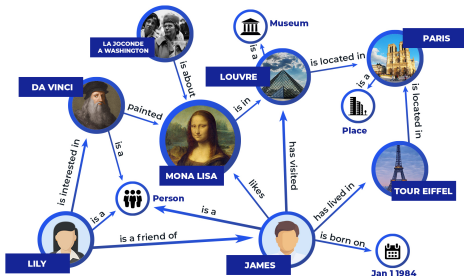
<sup>3</sup>Source: <https://bit.ly/3sxCj6e>





# Motivation

## Example



3

- ▶  $E^+ = \{\text{Louvre}, \text{TourEiffel}\}, E^- = \{\text{Lily}, \text{James}\}$
- ▶ Solution in *ALCO*:  $\mathcal{H} = \{\exists \text{ isLocatedIn.}\{\text{Paris}\}\}$
- ▶ Pro: explainable, exploits background knowledge
- ▶ Contra: slow :-)

<sup>3</sup>Source: <https://bit.ly/3sxCj6e>

## Goal

### Goal

- ▶ Attempt **neuro-symbolic learning** on knowledge graphs
- ▶ Exploit **time efficiency** of neural approaches
- ▶ Keep **explainability** of symbolic approaches



## Section 2

# Class Expression Learning

## Formal definition

- ▶ **Supervised learning** with background knowledge (adapted from [?])
- ▶ **Given:**
  - ▶ Formal logic  $\mathcal{L}$ , e.g.  $\mathcal{ALC}$
  - ▶ Background knowledge in form of knowledge base  $\mathcal{K} = \langle \mathcal{T}, \mathcal{A} \rangle$
  - ▶ Set of positive examples  $E^+ \subseteq N_I$
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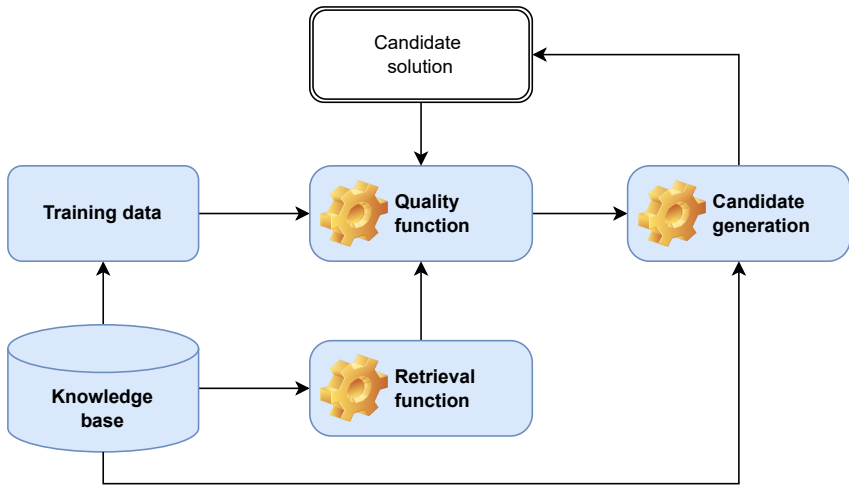
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  1.  $H$  is a class expression in  $\mathcal{L}$ , and (ideally)
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- ▶ Practically, aim to find  $H \in \underset{C \in \mathcal{L}}{\text{argmax}} Q(C)$  [?]

## Common Approach



## Example: Refinement Operator

- ▶ Let  $(S, \sqsubseteq)$  be a space with a quasi-ordering
- ▶ A **top-down refinement operator**  $\rho : S \rightarrow 2^S$  is a mapping with  $\rho(x) \sqsubseteq x$  [?]



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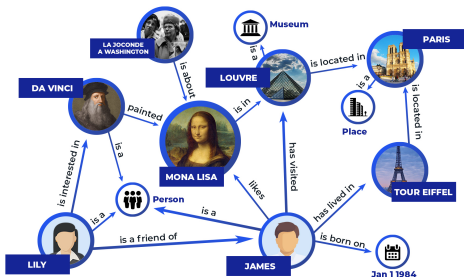
### Example

- ▶ Let  $S$  be the set of all concepts in our language  $\mathcal{L} = \mathcal{ALC}$
- ▶ The following operator  $\rho$  is a top-down refinement operator

$$\rho(C) = \begin{cases} C & \\ N_C \cup \neg N_C \cup \{\exists r_j. \rho(C_i)\} & \text{if } C = \top \\ \rho(D) & \text{if } D \sqsubseteq C \\ C \sqcap D & \text{with } D \in N_C \\ C \sqcap \exists r. \rho(D) & \text{with } D \in N_C \end{cases}$$

# Class Expression Learning

## Example



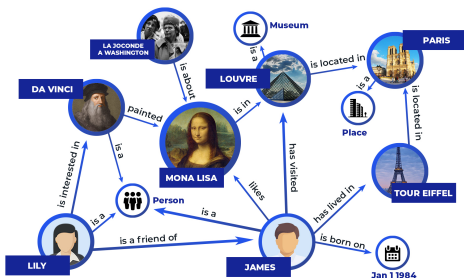
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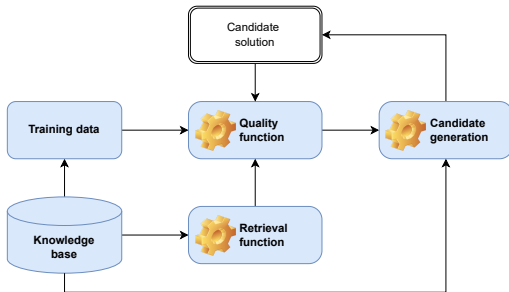
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- ▶  $E^+ = \{\text{Louvre}, \text{TourEiffel}\}, E^- = \{\text{Lily}, \text{James}\}$
- ▶  $\rho(\top) = \{\text{Person}, \text{Museum}, \text{Place}, \exists \text{is\_located\_in}.\top, \dots\}$

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# Learning problem

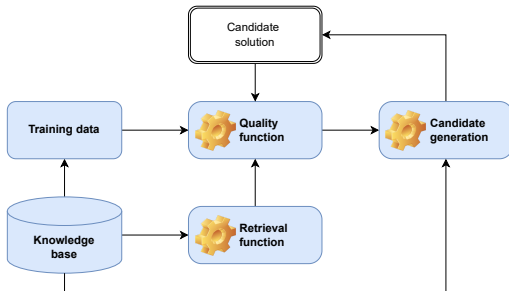
## Challenges



- ▶ **Retrieval** is expensive

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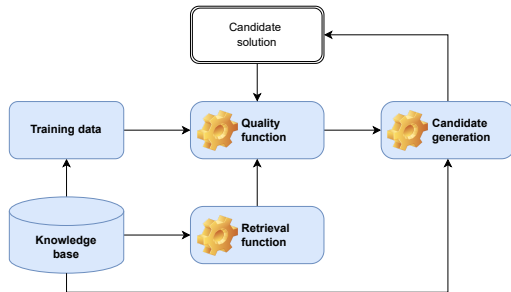
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- ▶ **Retrieval** is expensive  $\Rightarrow$  Exploit SPARQL
- ▶ **Quality functions** are often myopic

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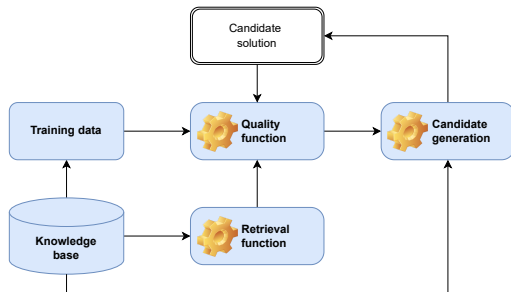
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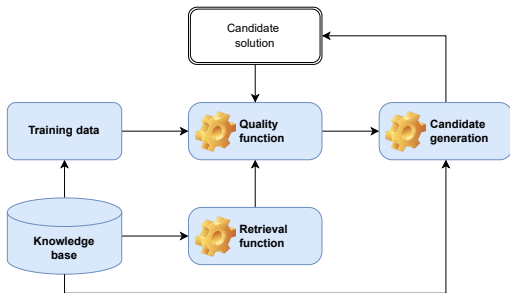
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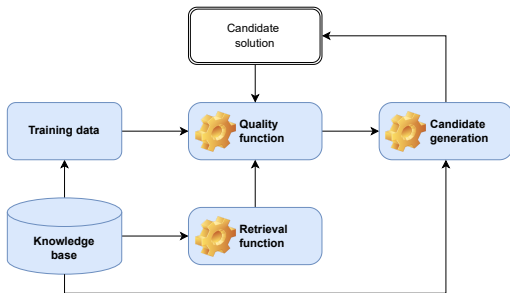


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- ▶ **Search space** is large  $\Rightarrow$  Prune by length

## Section 3

# Representing Concepts as SPARQL

## From *ALC* to SPARQL

- ▶ Assume closed world and **fully materialized** knowledge graph
- ▶ Retrieval in *ALC* can be realized by representing **concepts as SPARQL queries** [?]

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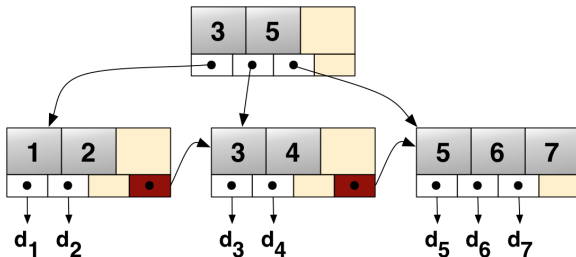
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| $\forall r.C$                 | <code>{ ?var r ?s0.</code><br><code>{ SELECT ?var (count(?s1) AS ?cnt1)</code><br><code>WHERE { ?var r ?s1. <math>\tau(C, ?s1)</math>}</code><br><code>GROUP BY ?var }</code><br><code>{ SELECT ?var (count(?s2) AS ?cnt2)</code><br><code>WHERE { ?var r ?s2 .}</code><br><code>GROUP BY ?var }</code><br><code>FILTER ( ?cnt1 = ?cnt2 ) }</code> |

# Representing Concepts as SPARQL

## Storage Solutions

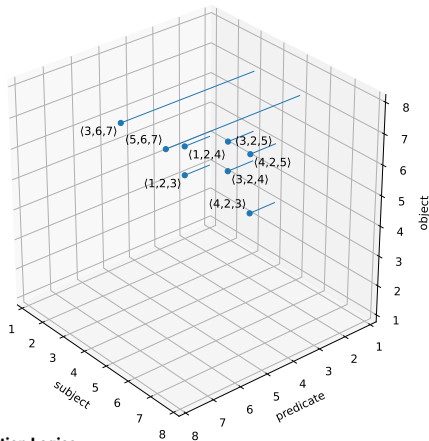
- ▶ Important difference are indexing data structures
- ▶ Typical indexes include
  - ▶ **Resource index**, e.g., a hash table
  - ▶ **Triple index**, e.g., a B<sup>+</sup> tree



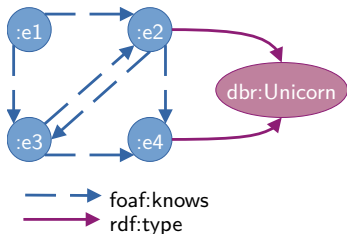
## TENTRIS: Idea

### Idea [?]

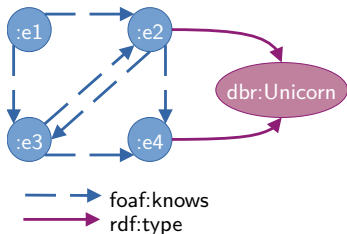
- ▶ Exploit tensor representation to accelerate querying
- ▶ Devise data structure to accommodate rapid querying



## From RDF to Tensors

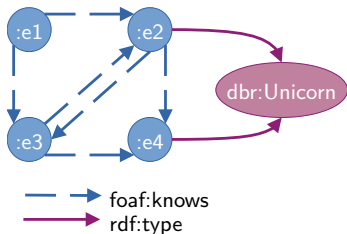


## From RDF to Tensors



| term           | id(term) |
|----------------|----------|
| :e1            | 1        |
| foaf:knows     | 2        |
| :e2            | 3        |
| :e3            | 4        |
| :e4            | 5        |
| rdf:type       | 6        |
| dbr:Unicorn    | 7        |
| <i>unbound</i> | 8        |

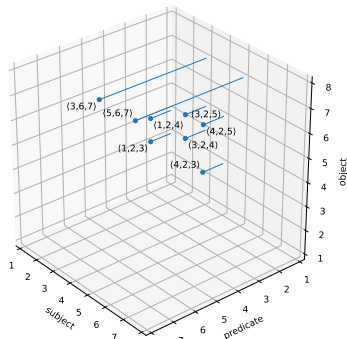
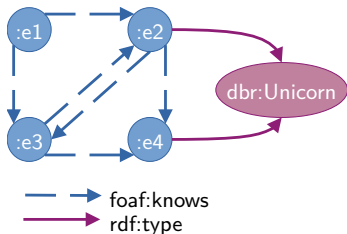
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| <i>id(s)</i> | <i>id(p)</i> | <i>id(o)</i> |
|--------------|--------------|--------------|
| 1            | 2            | 3            |
| 1            | 2            | 4            |
| 3            | 2            | 4            |
| 3            | 2            | 5            |
| 4            | 2            | 3            |
| 4            | 2            | 5            |
| 3            | 6            | 7            |
| 5            | 6            | 7            |

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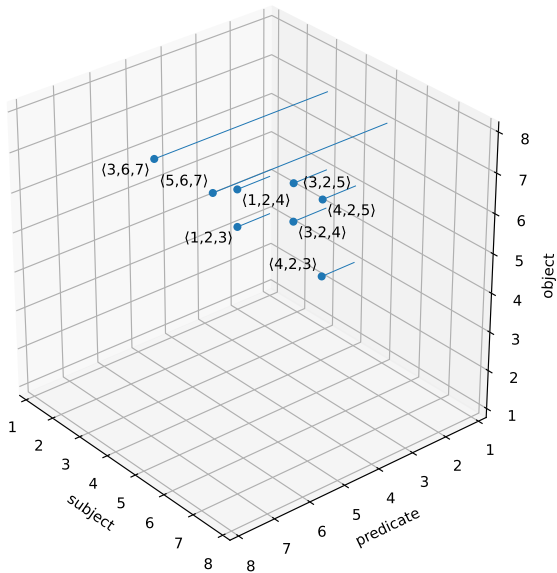
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  - ▶  $\mathbb{B}$  or  $\mathbb{N}$  as co-domain

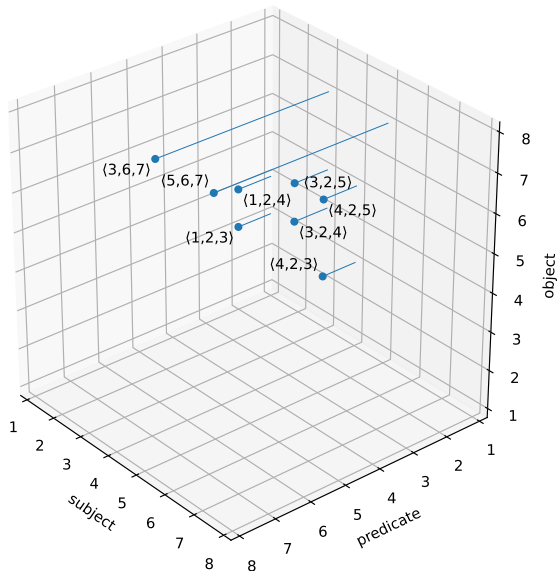
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  - ▶  $\mathbf{K}_1 = \dots = \mathbf{K}_n \subset \mathbb{N}$
  - ▶  $\mathbb{B}$  or  $\mathbb{N}$  as co-domain
- ▶  $\mathbf{k} \in \mathbf{K}$  is a **key** with key parts  $\langle \mathbf{k}_1, \dots, \mathbf{k}_n \rangle$
- ▶ Values  $v$  in a tensor are accessed in array style, e.g.,  $T[\mathbf{k}] = v$

## TENTRIS: Data Model



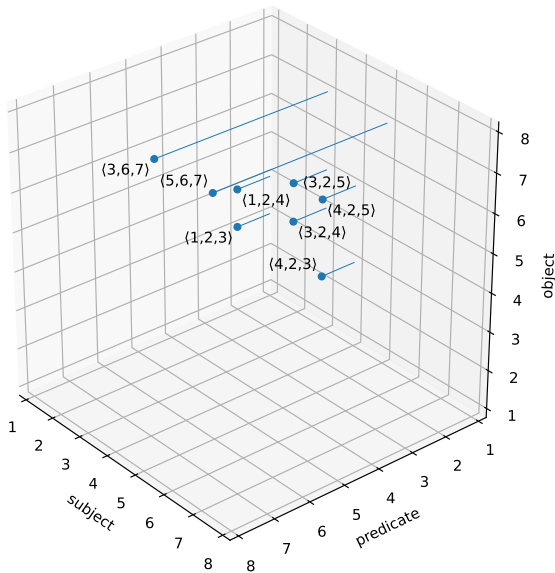
## TENTRIS: Data Model



►  $\mathbf{K} = \mathbb{N}^3$

►  $\mathbf{V} = \mathbb{B}$

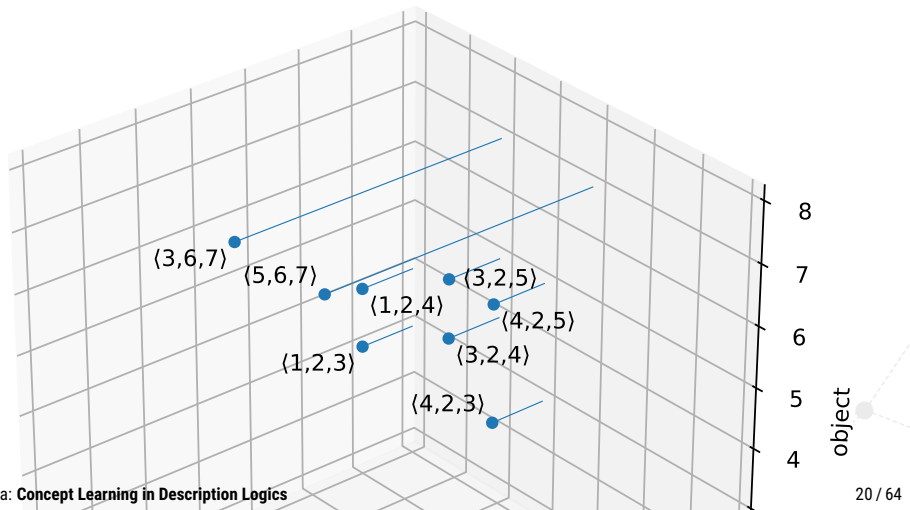
## TENTRIS: Data Model



- ▶  $\mathbf{K} = \mathbb{N}^3$
- ▶  $\mathbf{V} = \mathbb{B}$
- ▶  $T[\langle 3, 6, 7 \rangle] = 1$
- ▶  $T[\langle 3, 6, 3 \rangle] = 0$

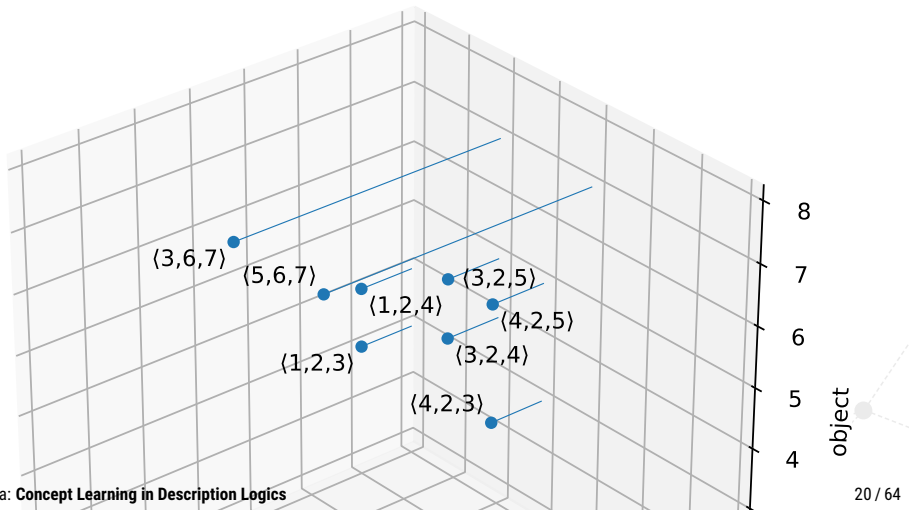
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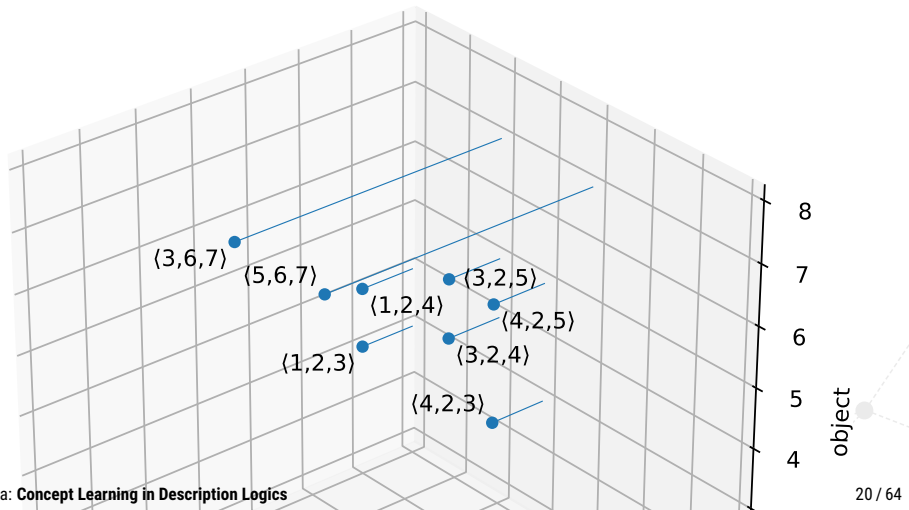
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- ▶ For our example,  $T[1, 2, :] = [0, 0, 1, 1, 0, 0, 0, 0]$
- ▶ Slices can be **joined** via Einstein summation [?]



## TENTRIS–Einstein Summation

```
1 SELECT ?f WHERE {  
2   :e1 foaf:knows ?f .  
3   ?f foaf:knows ?u .  
4   ?u rdf:type dbr:Unicorn  
5 }
```

## TENTRIS-Einstein Summation

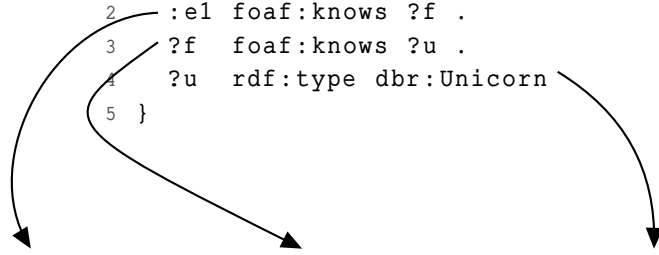
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3   ?f foaf:knows ?u .
4   ?u rdf:type dbr:Unicorn
5 }
  
```

$T[1, 2, :]$

$T[:, 2, :]$

$T[:, 6, 7]$



## TENTRIS-Einstein Summation

```

1 SELECT ?f WHERE {
2   :e1 foaf:knows ?f .
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 $T[1, 2, :]$ 
 $T[:, 2, :]$ 
 $T[:, 6, 7]$ 

$$R_f \leftarrow T[1, 2, :]_f \times T[:, 2, :]_{f,u} \times T[:, 6, 7]_u$$

## TENTRIS: Querying

- ▶ **Triple pattern** is mapped to

$$\mathbf{k}_i^{(Q)} := \begin{cases} :, & \text{if } Q_i \in U, \\ id(Q_i), & \text{otherwise.} \end{cases}$$

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$$T'_{\langle I \in U \rangle} \leftarrow \bigtimes_i T[\mathbf{k}^{B^{(i)}}]_{\langle I \in B^{(i)} \mid I \in U \rangle}$$

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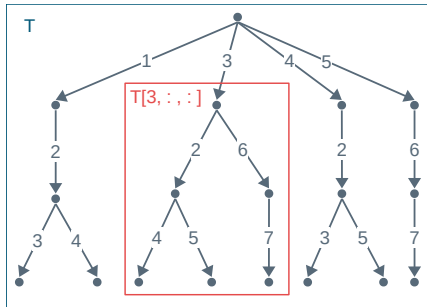
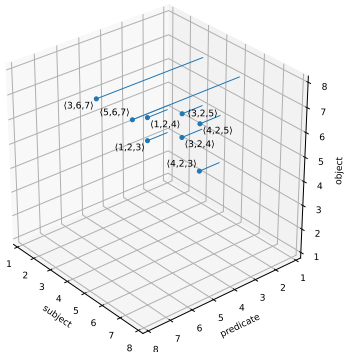
$$T'_{\langle I \in U \rangle} \leftarrow \bigtimes_i T[\mathbf{k}^{B^{(i)}}]_{\langle I \in B^{(i)} \mid I \in U \rangle}$$

- ▶ The **projection**  $\Pi_{U'}(B(g))$  with  $U' \subseteq U$  is given by

$$T''_{\langle I \in U' \rangle} \leftarrow \bigtimes_i T[\mathbf{k}^{B^{(i)}}]_{\langle I \in B^{(i)} \mid I \in U \rangle}$$

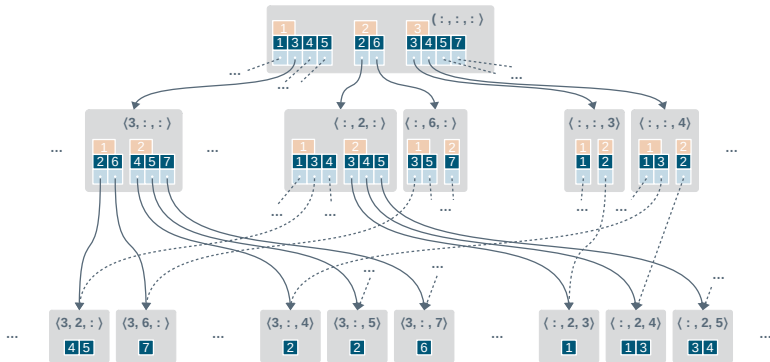
## TENTRIS: Hypertrie

- ▶ Query for any tensor slice efficiently
- ▶ Allow for efficient querying



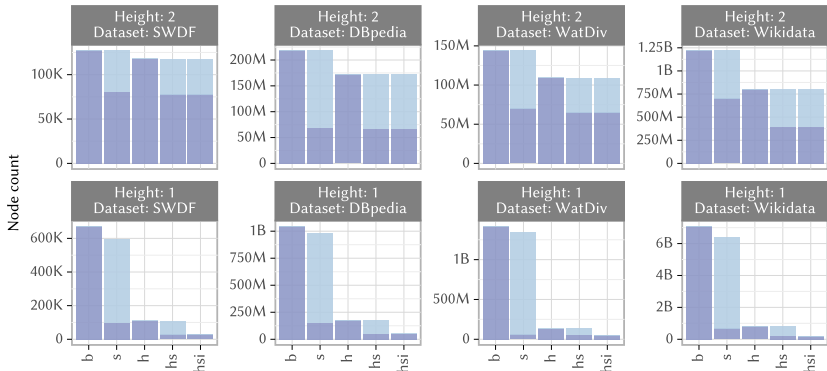


## TENTRIS: Hypertrie



- ▶ Query for any tensor slice efficiently
- ▶ Storage bound is reduced from  $\mathcal{O}(d! \cdot d \cdot z(h))$  for all collation orders to  $\mathcal{O}(2^{d-1} \cdot d \cdot z(h))$

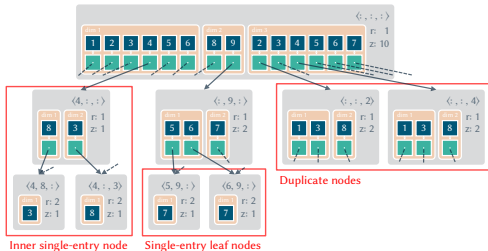
## TENTRIS: Hypertrie



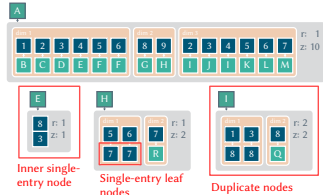
- ▶ Hypertrie topology seems sparse
- ▶ Compression to improve space, loading and query times [?]

## TENTRIS: Compressed Hypertrie

Baseline hypertrie



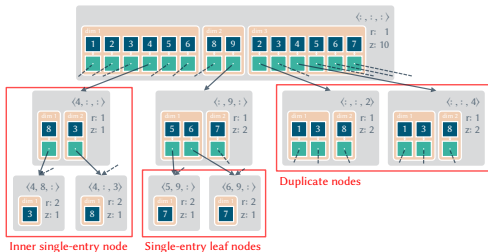
Optimized hypertrie



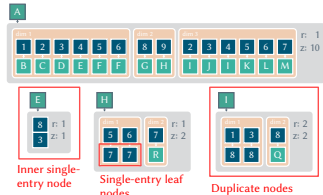
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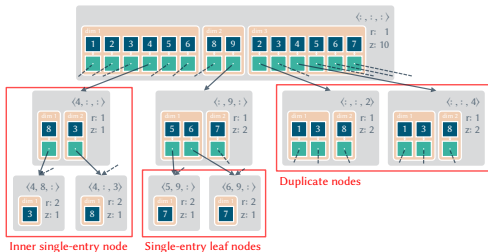
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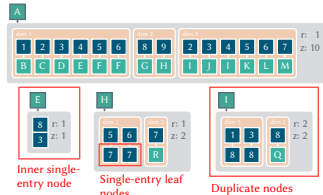
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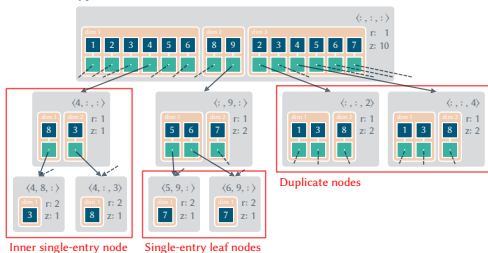
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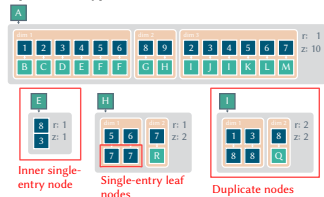
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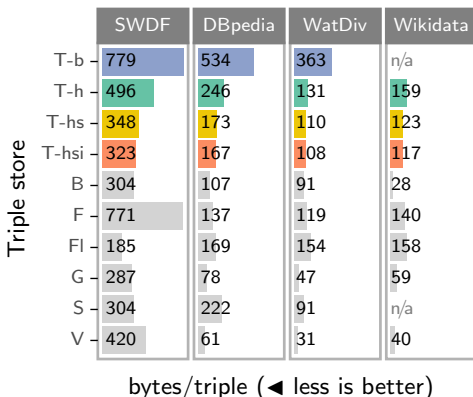
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  3. Single-entry leaf nodes are eliminated via in-place storage (local)

## TENTRIS: Compressed Hypertrie

- ▶ Comparison with state-of-the-art approaches
- ▶ **Hardware**: AMD EPYC 7742, 1 TB RAM and  $2 \times 3$  TB NVMe SSDs
- ▶ **Datasets**: Between 372K (SWDF) and 5.5B triples (WikiData)

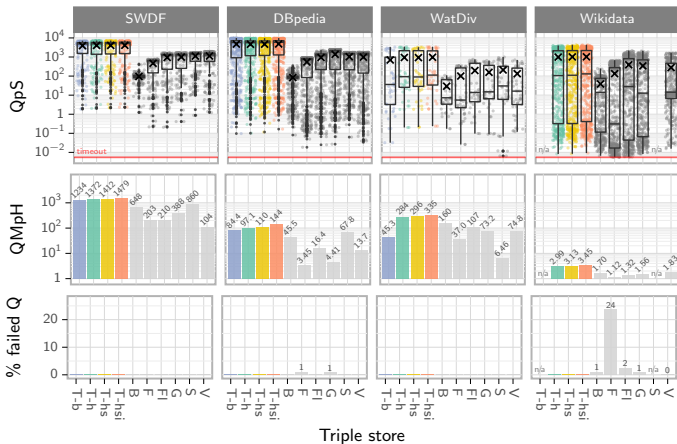
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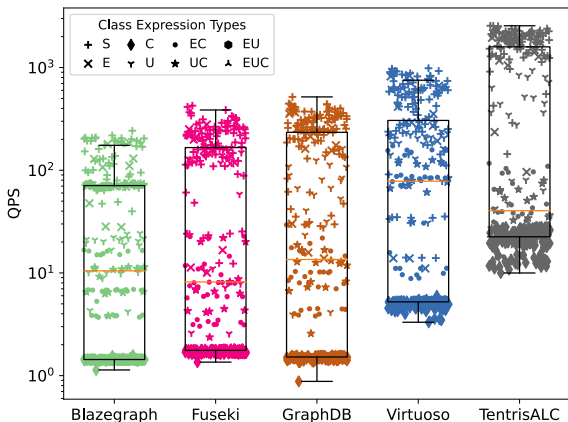


## TENTRIS: Compressed Hypertrie



- ▶ Better runtimes on all datasets
- ▶ Can operate on very large datasets (no time-outs)

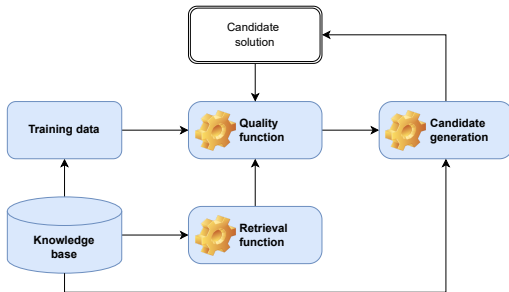
## TENTRIS: Carcinogenesis



- ▶ Comparison on supervised machine learning tasks in  $ACC$
- ▶ Better runtimes on all datasets considered

# Learning problem

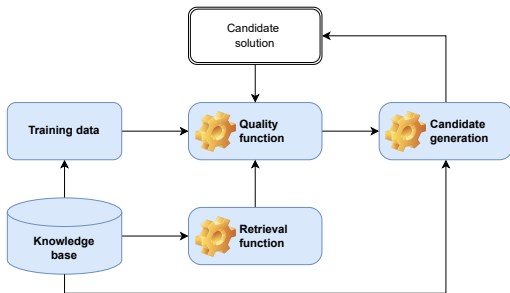
## Challenges



- ✓ Retrieval is expensive  $\Rightarrow$  Exploit SPARQL
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# Learning problem

## Challenges



- ✓ **Retrieval** is expensive  $\Rightarrow$  Exploit SPARQL
- ▶ **Quality functions** are often myopic  $\Rightarrow$  Exploit embeddings
- ▶ **Candidate generation** is expensive  $\Rightarrow$  Exploit priming
- ▶ **Search space** is large  $\Rightarrow$  Prune by length

## Section 4

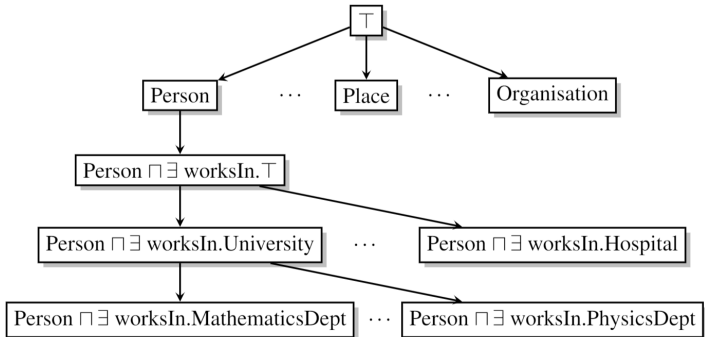
# Improving Quality Functions

## Refinement Operators

- ▶ Implement **informed search** in space  $\mathcal{S}$  of all concepts with partial ordering  $\sqsubseteq$
- ▶ Refinement operator  $\rho : \mathcal{S} \rightarrow 2^{\mathcal{S}}$  with
  - ▶  $\forall x \in \rho(s) : x \sqsubseteq s$  (**downward**)
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- ▶ The **score** is given by

$$\text{score}(C) = \text{acc}(C) + \alpha \cdot \text{acc\_gain}(C) - \beta \cdot |C| \quad (\alpha, \beta \geq 0),$$

where  $\alpha = 0.5$  and  $\beta = 0.02$  are typical default values.

## Quality Functions – CELOE

- Accuracy metric  $\text{acc}_c$  for CELOE:

$$\text{acc}_c(C, t) = \frac{1}{t+1} \cdot \left( t \cdot \frac{|E^+ \cap R(C)|}{|E^+|} + \sqrt{\frac{|E^+ \cap R(C)|}{|R(C)|}} \right)$$

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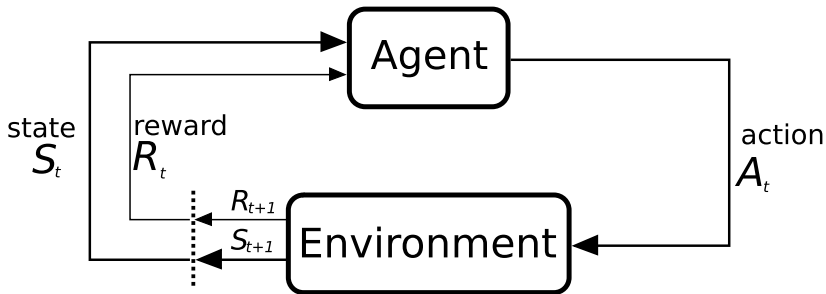
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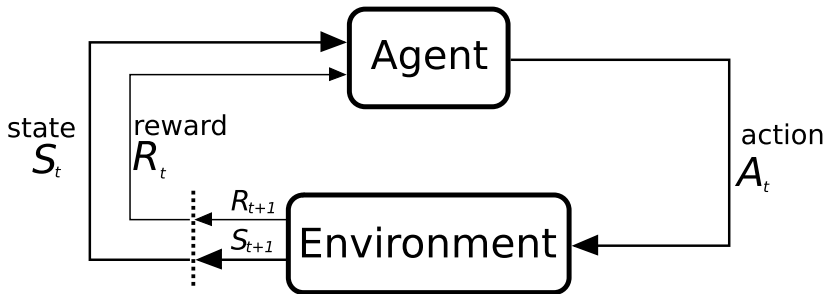
### Problem: Myopia

- ▶ Current metrics do not consider future accuracy of concepts
- ▶ Optimize for **cumulative discounted future rewards** [?]

## Reinforcement Learning



## Reinforcement Learning



- ▶  $S_t = \text{Concept } C$
- ▶  $R_t = \begin{cases} 1 & \text{if } \text{acc}(C) = 1 \\ 0 & \text{else} \end{cases}$
- ▶  $A_t = \text{Transition from concept } C \text{ to some concept } D$



# Improving Quality Functions

## Reinforcement Learning – Q Function

- ▶ Maximize

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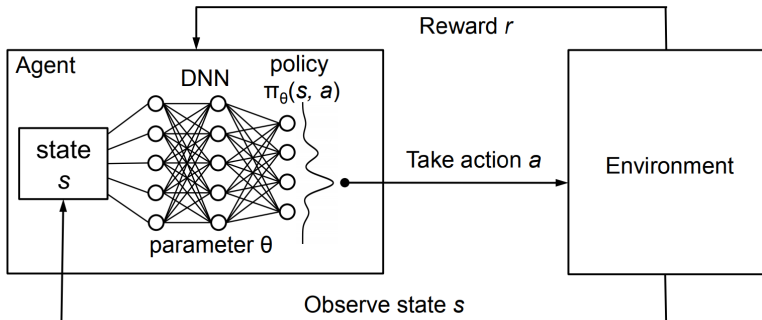
- ▶ **Observation:** Infinite number of states as search space is infinite
- ▶ Apply deep Q learning with target network [?]

$$\mathcal{L}(\Theta_i) = \mathbb{E}_{(s,a,R,s') \sim U(\mathcal{D})} \left[ \left( R + \gamma \max_{a' \in A(s')} Q(s', a'; \Theta_i^-) - Q(s, a; \Theta_i) \right)^2 \right]$$

## Reinforcement Learning – DRILL

- Convolutional deep Q-Network with  $\Theta = [\omega, \mathbf{W}, \mathbf{H}]$

$$\varphi([s, s', \mathbf{e}_+, \mathbf{e}_-]; \Theta) = \text{ReLU}\left(\text{vec}\left(\text{ReLU}\left[\Psi([s, s', \mathbf{e}_+, \mathbf{e}_-]) * \omega\right]\right) \cdot \mathbf{W}\right) \cdot \mathbf{H}$$



Source: [?]

## TransE

### ► Assumptions

- Resources and properties are vectors
- If  $(s, p, o) \in E$ , then  $\vec{s} + \vec{p} = \vec{o}$

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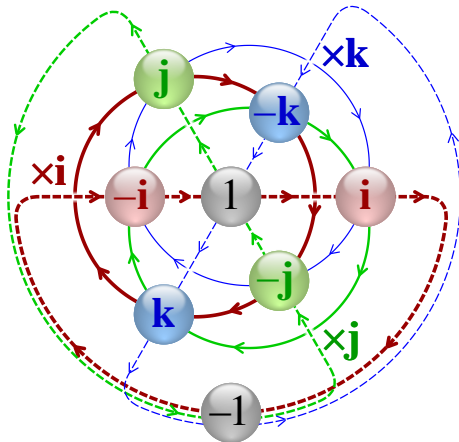
- ▶ **Problem:** Loss function converges to trivial solution
- ▶ **Solution:** Add **negative information** and **margin**  $\gamma \in \mathbb{R}^+$
- ▶ Loss is now

$$L = \sum_{(s,p,o) \in E} \sum_{(s',p,o') \in S'(s,p,o)} [\gamma + d(\vec{s} + \vec{p}, \vec{o}) - d(\vec{s}' + \vec{p}, \vec{o}')]_+$$

where

- ▶  $S'(s, p, o) = \text{sample}(\{(s', p, o) | s' \in V\} \cup \{(s, p, o') | o' \in V\}, 1)$
- ▶  $S'(s, p, o) \cap E = \emptyset$
- ▶  $[x]_+ = \max\{0, x\}$

## Quaternions: $\mathbb{H}$



5

<sup>5</sup>[https://en.wikipedia.org/wiki/Quaternion#/media/File:Cayley\\_Q8\\_quaternion\\_multiplication\\_graph.svg](https://en.wikipedia.org/wiki/Quaternion#/media/File:Cayley_Q8_quaternion_multiplication_graph.svg)

## Quaternions: $\mathbb{H}$

- ▶ Can define embeddings in this space: QMult [?]
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- ▶ Similar construction for **octonions**

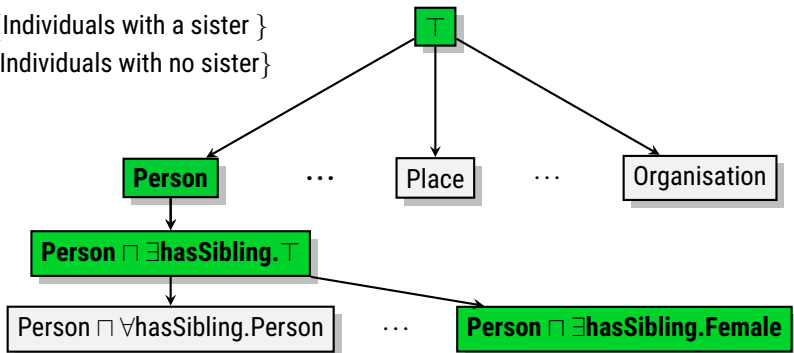
# Improving Quality Functions

## Unsupervised Learning – Training Data

- ▶ Follow refinement path at random
- ▶ Select concept  $C$
- ▶ Set  $E^+ \subseteq R(C)$  and  $E^- \cap R(C) = \emptyset$

$E^+ = \{\text{Individuals with a sister}\}$

$E^- = \{\text{Individuals with no sister}\}$



# Improving Quality Functions

## Evaluation

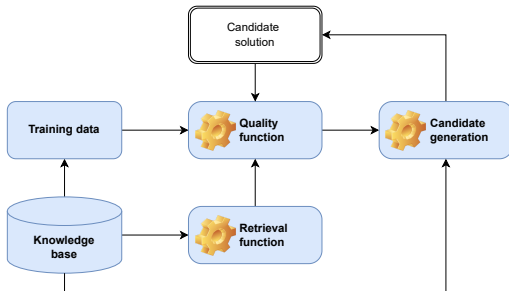
- ▶ Used Family und BioPax datasets
- ▶ Evaluation on 114 learning problems

| Approaches | F1              | Acc             | Runtime        | # Exp.              |
|------------|-----------------|-----------------|----------------|---------------------|
| CELOE      | $.995 \pm 0.03$ | $.993 \pm 0.04$ | $7.5 \pm 1.1$  | $33.5 \pm 129.3$    |
| OCEL       | *               | $1.00 \pm 0.00$ | $11.0 \pm 1.4$ | $2271.6 \pm 1269.2$ |
| ELTL       | $.990 \pm 0.06$ | $.984 \pm 0.09$ | $8.1 \pm 1.6$  | *                   |
| DRILL      | $1.00 \pm 0.00$ | $1.00 \pm 0.00$ | $1.1 \pm 0.5$  | $9.88 \pm 38.5$     |



# Learning problem

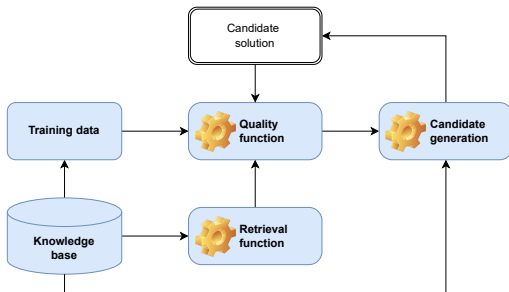
## Challenges



✓ Retrieval is expensive

# Learning problem

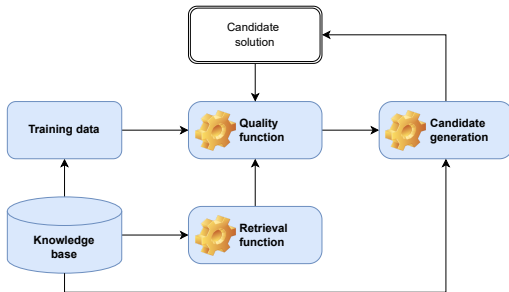
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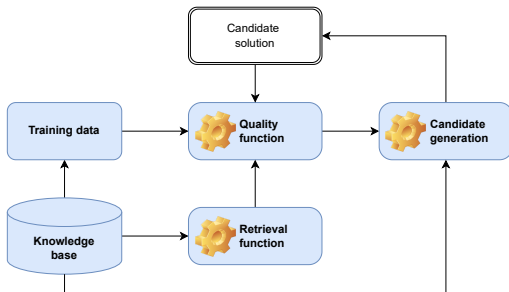
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- ✓ Retrieval is expensive  $\Rightarrow$  Exploit SPARQL
- ✓ Quality functions are often myopic  $\Rightarrow$  Exploit embeddings
- ▶ Candidate generation is expensive

# Learning problem

## Challenges



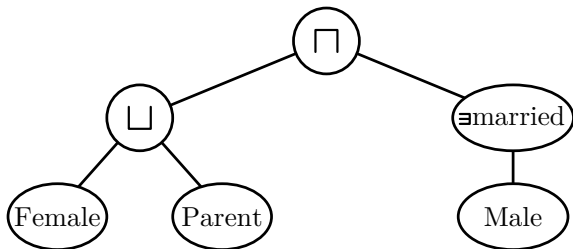
- ✓ **Retrieval** is expensive  $\Rightarrow$  Exploit SPARQL
- ✓ **Quality functions** are often myopic  $\Rightarrow$  Exploit embeddings
- ▶ **Candidate generation** is expensive  $\Rightarrow$  Exploit priming
- ▶ **Search space** is large  $\Rightarrow$  Prune by length

## Section 5

# Learning with Priming

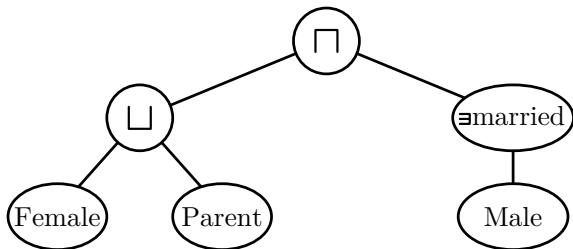
## EVOLARNER – Idea

- Represent concepts as trees, e.g.,  
 $(\text{Female} \sqcup \text{Parent}) \sqcap \exists \text{married.Male}$



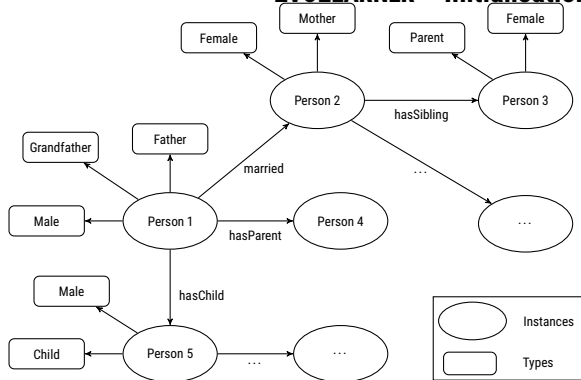
## EVOLARNER – Idea

- ▶ Represent concepts as trees, e.g.,  
 $(\text{Female} \sqcup \text{Parent}) \sqcap \exists \text{married.Male}$
- ▶ Learn in evolutionary fashion using genetic programming
- ▶ Exploit **priming effect** (remember the green apple)
- ▶ **Intuition**: An individual is an overlap several concepts [?]



# Learning with Priming

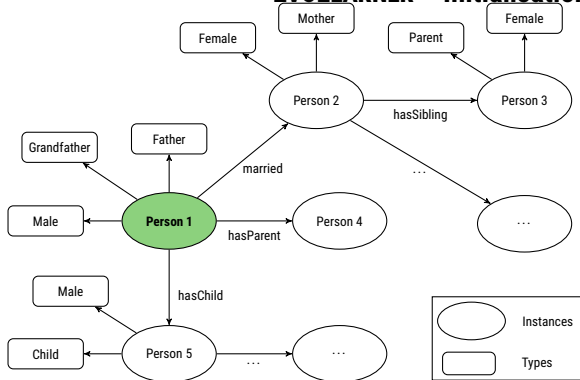
## EVOLARNER - Initialisation





# Learning with Priming

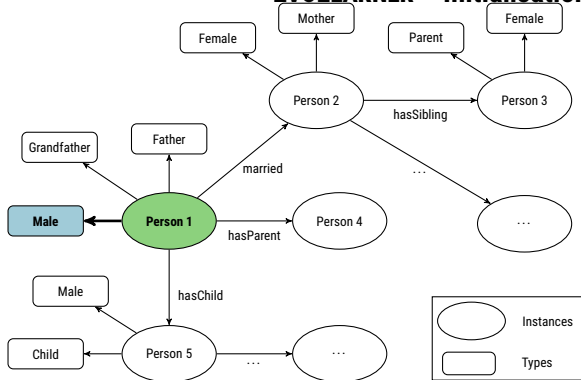
## EVOLARNER - Initialisation



1. Select a **positive example  $e^+$**  and one of its types:

# Learning with Priming

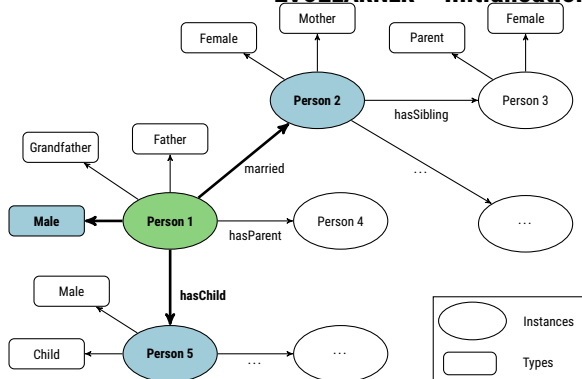
## EVOLARNER - Initialisation



1. Select a positive example  $e^+$  and one of its types: **Male**

# Learning with Priming

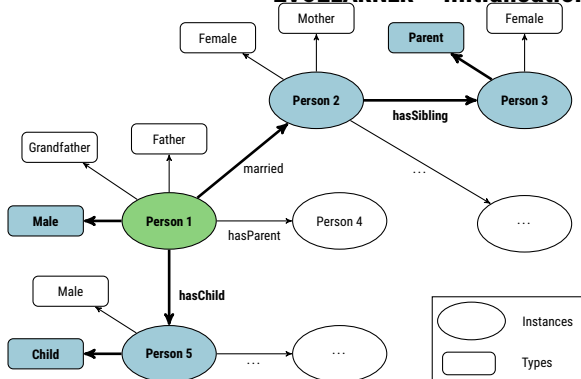
## EVOLARNER – Initialisation



1. Select a **positive example  $e^+$**  and one of its types: **Male**
2. Randomly select up to  $maxT$  outgoing triples of  **$e^+$** :  
 $Male \sqcap (\exists married \dots \sqcap \exists hasChild \dots)$

# Learning with Priming

## EVOLARNER – Initialisation



1. Select a **positive example  $e^+$**  and one of its types: **Male**

2. Randomly select up to  $maxT$  outgoing triples of  **$e^+$** :

**Male**  $\sqcap$  ( **$\exists$ married** ...  $\sqcap$   **$\exists$ hasChild** ...)

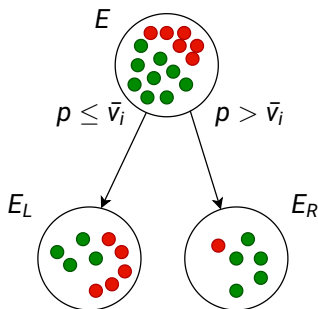
3. Complete incomplete subconcepts:

**Male**  $\sqcap$  (( **$\exists$ married.**  **$\exists$ hasSibling.Parent**)  $\sqcap$  ( **$\exists$ hasChild.Child**))

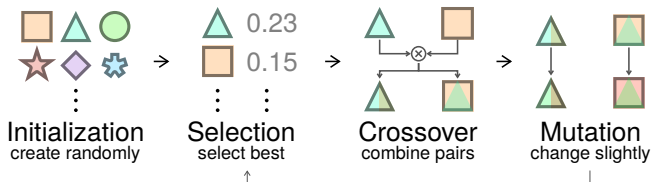
## EVOLARNER – Data Properties

- ▶ Given a data property  $d$  from the knowledge base  $\mathcal{K}$  and a set  $E$  of positive and negative examples
- ▶ We precompute up to  $k$  splits of the form  $d \leq \bar{v}_i$  per data property
- ▶ Splits are computed to maximize information gain:

$$IG(E, \bar{v}_i) = H(E) - H(E|\bar{v}_i) = H(E) - \left( \frac{|E_L|}{|E|} H(E_L) + \frac{|E_R|}{|E|} H(E_R) \right)$$



## EVOLARNER – Training



## EvoLEARNER – Evaluation

| Learn. Problem | EvoLearner<br>(ours)              | DL-Learner<br>(CELOE)             | DL-Learner<br>(OCEL)              | Aleph           | SPaCEL                            |
|----------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------|-----------------------------------|
| Carcinogenesis | $0.70 \pm 0.12$                   | <b><math>0.71 \pm 0.01</math></b> | <i>no results</i>                 | $0.46 \pm 0.12$ | $0.60 \pm 0.08$                   |
| Family         | $1.00 \pm 0.01$                   | $0.98 \pm 0.05$                   | <b><math>1.00 \pm 0.00</math></b> | –               | $0.97 \pm 0.11$                   |
| Hepatitis      | <b><math>0.79 \pm 0.08</math></b> | $0.61 \pm 0.03$                   | <i>no results</i>                 | $0.38 \pm 0.12$ | <i>no results</i>                 |
| Lymphography   | $0.84 \pm 0.09$                   | $0.78 \pm 0.10$                   | <b><math>0.85 \pm 0.10</math></b> | $0.84 \pm 0.09$ | $0.75 \pm 0.13$                   |
| Mammographic   | <b><math>0.81 \pm 0.06</math></b> | $0.64 \pm 0.01$                   | $0.78 \pm 0.08$                   | $0.48 \pm 0.08$ | $0.64 \pm 0.06$                   |
| Mutagenesis    | <b><math>1.00 \pm 0.00</math></b> | $0.93 \pm 0.14$                   | <i>timeout</i>                    | $0.43 \pm 0.47$ | <b><math>1.00 \pm 0.00</math></b> |
| NCTRRER        | <b><math>1.00 \pm 0.00</math></b> | $0.74 \pm 0.01$                   | $0.94 \pm 0.06$                   | $0.71 \pm 0.18$ | <b><math>1.00 \pm 0.00</math></b> |
| Premier League | <b><math>1.00 \pm 0.00</math></b> | $0.99 \pm 0.04$                   | $0.81 \pm 0.13$                   | $0.94 \pm 0.11$ | $0.98 \pm 0.04$                   |
| Pyrimidine     | <b><math>0.91 \pm 0.14</math></b> | $0.84 \pm 0.15$                   | $0.84 \pm 0.22$                   | $0.90 \pm 0.32$ | $0.86 \pm 0.29$                   |

# Learning with Priming

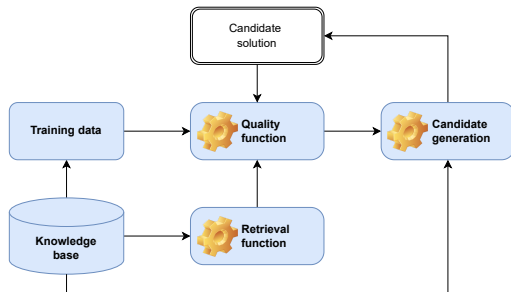
## EvoLEARNER – Ablation Study

| Learning Problem | EvoLearner<br>(ours) | Without<br>Rand. Walk Init. | Without<br>Data Properties | Without<br>Both |
|------------------|----------------------|-----------------------------|----------------------------|-----------------|
| Carcinogenesis   | $0.70 \pm 0.12$      | $0.60 \pm 0.21$             | $0.63 \pm 0.13$            | $0.62 \pm 0.13$ |
| Family           | $1.00 \pm 0.01$      | $0.87 \pm 0.13$             | –                          | $0.86 \pm 0.14$ |
| Hepatitis        | $0.79 \pm 0.08$      | $0.67 \pm 0.15$             | $0.46 \pm 0.14$            | $0.47 \pm 0.13$ |
| Lymphography     | $0.84 \pm 0.09$      | $0.83 \pm 0.11$             | –                          | $0.83 \pm 0.09$ |
| Mammographic     | $0.81 \pm 0.06$      | $0.78 \pm 0.08$             | $0.77 \pm 0.07$            | $0.75 \pm 0.06$ |
| Mutagenesis      | $1.00 \pm 0.00$      | $1.00 \pm 0.00$             | $0.44 \pm 0.48$            | $0.50 \pm 0.51$ |
| NCTRER           | $1.00 \pm 0.00$      | $1.00 \pm 0.00$             | $0.74 \pm 0.05$            | $0.75 \pm 0.05$ |
| Premier League   | $1.00 \pm 0.00$      | $0.98 \pm 0.04$             | $0.50 \pm 0.23$            | $0.50 \pm 0.22$ |
| Pyrimidine       | $0.91 \pm 0.14$      | $0.83 \pm 0.22$             | $0.67 \pm 0.00$            | $0.67 \pm 0.00$ |



# Learning problem

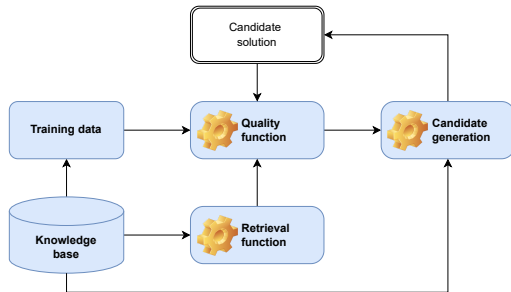
## Challenges



- ✓ **Retrieval** is expensive  $\Rightarrow$  Exploit SPARQL
- ✓ **Quality functions** are often myopic

# Learning problem

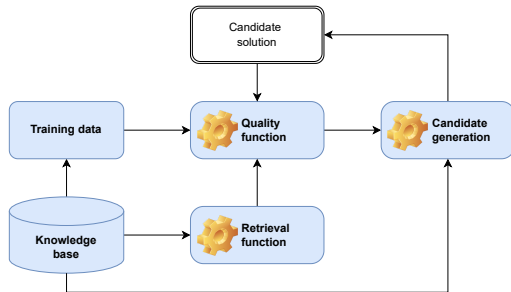
## Challenges



- ✓ **Retrieval** is expensive  $\Rightarrow$  Exploit SPARQL
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- ✓ **Candidate generation** is expensive

# Learning problem

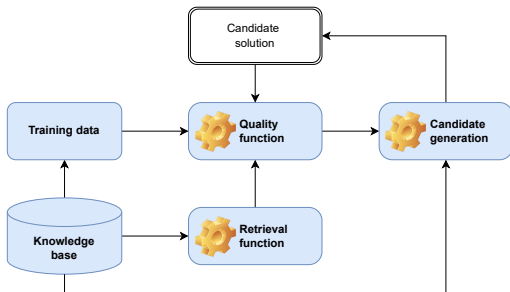
## Challenges



- ✓ **Retrieval** is expensive  $\Rightarrow$  Exploit SPARQL
- ✓ **Quality functions** are often myopic  $\Rightarrow$  Exploit embeddings
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# Learning problem

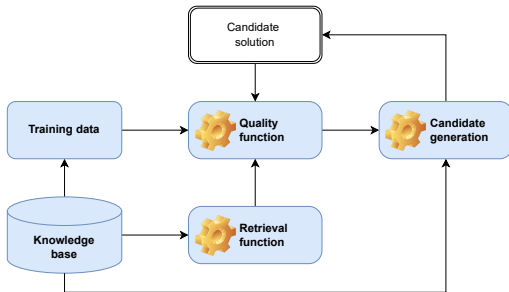
## Challenges



- ✓ **Retrieval** is expensive  $\Rightarrow$  Exploit SPARQL
- ✓ **Quality functions** are often myopic  $\Rightarrow$  Exploit embeddings
- ✓ **Candidate generation** is expensive  $\Rightarrow$  Exploit priming
- ▶ **Search space** is large

# Learning problem

## Challenges



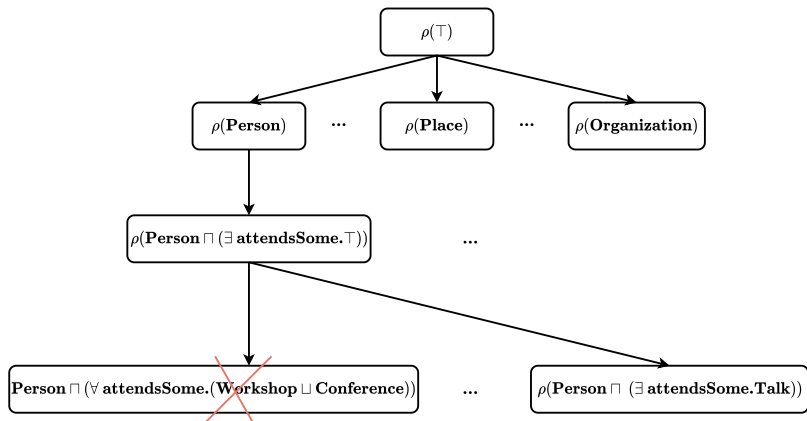
- ✓ **Retrieval** is expensive  $\Rightarrow$  Exploit SPARQL
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- ✓ **Candidate generation** is expensive  $\Rightarrow$  Exploit priming
- ▶ **Search space** is large  $\Rightarrow$  Prune by length

## Section 6

# CLIP

## Approach

- ▶ **Idea:** Prune horizontally by
- ▶ predicting target concept length and
- ▶ discarding longer refinements



# CLIP

## Concept Lengths

- ▶  $length(A) = length(\top) = length(\perp) = 1$  (if  $A$  is an atomic concept)



# CLIP

## Concept Lengths

- ▶  $length(A) = length(\top) = length(\perp) = 1$  (if  $A$  is an atomic concept)
- ▶  $length(\neg C) = 1 + length(C)$ , for all concepts  $C$

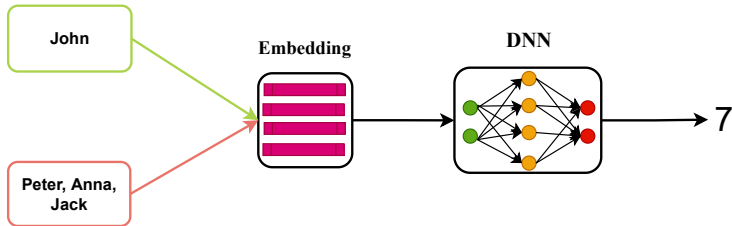
## Concept Lengths

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## Concept Lengths

- ▶  $length(A) = length(\top) = length(\perp) = 1$  (if  $A$  is an atomic concept)
- ▶  $length(\neg C) = 1 + length(C)$ , for all concepts  $C$
- ▶  $length(\exists r.C) = length(\forall r.C) = 2 + length(C)$ , for all concepts  $C$
- ▶  $length(C \sqcup D) = length(C \sqcap D) = 1 + length(C) + length(D)$ , for all concepts  $C$  and  $D$ .

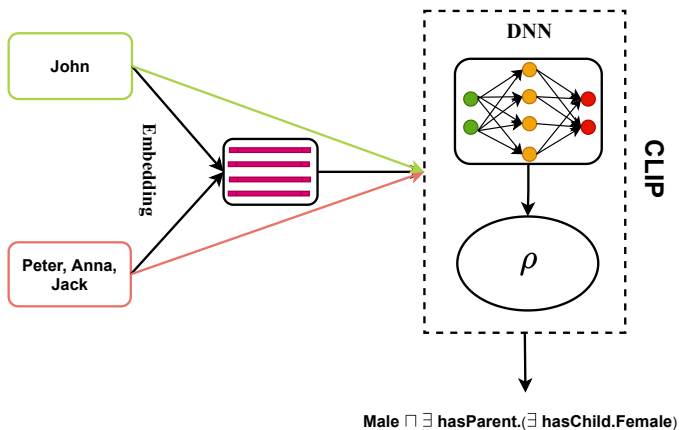
## Concept Length Prediction



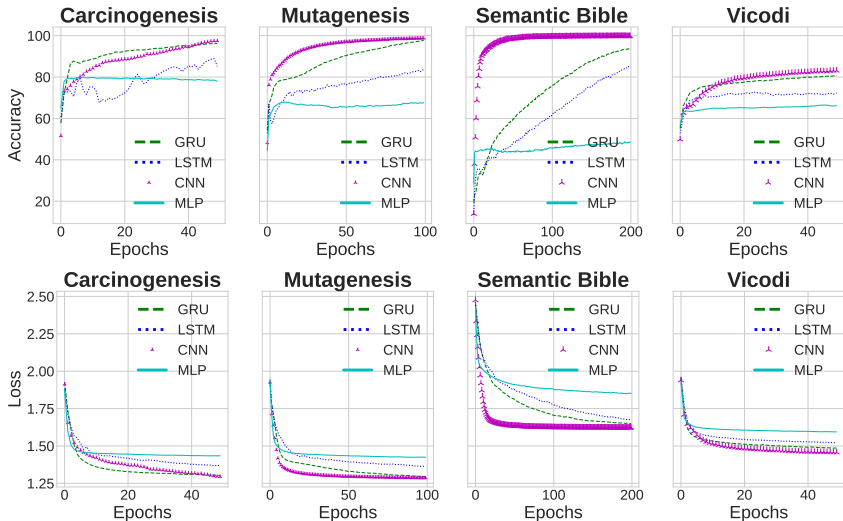
- ▶ Input: positive and negative examples
- ▶ Output: length of the target concept

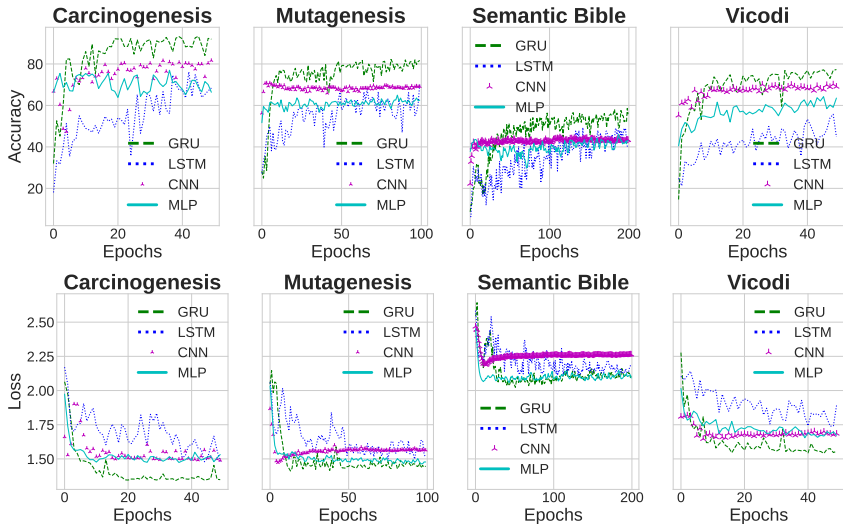
# CLIP

## Concept Learning



# CLIP Training





## Network Architecture

| Metric      | Carcinogenesis |             |      |      |      | Mutagenesis |             |      |      |      |
|-------------|----------------|-------------|------|------|------|-------------|-------------|------|------|------|
|             | LSTM           | GRU         | CNN  | MLP  | RM   | LSTM        | GRU         | CNN  | MLP  | RM   |
| Train. Acc. | 0.89           | 0.96        | 0.97 | 0.80 | 0.48 | 0.83        | 0.97        | 0.98 | 0.68 | 0.33 |
| Val. Acc.   | 0.76           | 0.93        | 0.82 | 0.77 | 0.48 | 0.70        | 0.82        | 0.71 | 0.65 | 0.35 |
| Test Acc.   | 0.92           | <b>0.95</b> | 0.84 | 0.80 | 0.49 | 0.78        | <b>0.85</b> | 0.70 | 0.68 | 0.33 |
| Test F1     | 0.88           | <b>0.92</b> | 0.71 | 0.59 | 0.33 | 0.76        | <b>0.85</b> | 0.70 | 0.67 | 0.32 |

| Metric      | Semantic Bible |             |      |      |      | Vicodi |             |      |      |      |
|-------------|----------------|-------------|------|------|------|--------|-------------|------|------|------|
|             | LSTM           | GRU         | CNN  | MLP  | RM   | LSTM   | GRU         | CNN  | MLP  | RM   |
| Train. Acc. | 0.85           | 0.93        | 0.99 | 0.68 | 0.33 | 0.73   | 0.81        | 0.83 | 0.66 | 0.28 |
| Val. Acc.   | 0.49           | 0.58        | 0.44 | 0.46 | 0.26 | 0.55   | 0.77        | 0.70 | 0.64 | 0.30 |
| Test Acc.   | 0.52           | <b>0.53</b> | 0.37 | 0.40 | 0.25 | 0.66   | <b>0.80</b> | 0.69 | 0.66 | 0.29 |
| Test F1     | 0.27           | <b>0.38</b> | 0.20 | 0.22 | 0.16 | 0.45   | <b>0.50</b> | 0.45 | 0.38 | 0.20 |



## Comparison with SOTA

| Carcinogenesis             |                        |                   |                  |                         |
|----------------------------|------------------------|-------------------|------------------|-------------------------|
| Metric                     | CELOE                  | OCEL              | ELTL             | CLIP                    |
| Acc. $\uparrow$            | 0.78 $\pm$ 0.27        | 0.89 $\pm$ 0.31   | 0.58 $\pm$ 0.46  | <b>0.99</b> $\pm$ 0.00  |
| F1 $\uparrow$              | 0.62 $\pm$ 0.46        | –                 | 0.51 $\pm$ 0.47  | <b>0.96*</b> $\pm$ 0.10 |
| Runtime (min) $\downarrow$ | 0.93 $\pm$ 0.94        | 3.01 $\pm$ 0.72   | 0.75 $\pm$ 0.07  | <b>0.10*</b> $\pm$ 0.09 |
| Length $\downarrow$        | <b>1.69</b> $\pm$ 0.89 | 7.81 $\pm$ 6.88   | 1.04 $\pm$ 0.39  | 2.00 $\pm$ 1.28         |
| Mutagenesis                |                        |                   |                  |                         |
| Metric                     | CELOE                  | OCEL              | ELTL             | CLIP                    |
| Acc. $\uparrow$            | 0.99 $\pm$ 0.00        | 0.71 $\pm$ 0.45   | 0.37 $\pm$ 0.43  | <b>0.99</b> $\pm$ 0.00  |
| F1 $\uparrow$              | 0.81 $\pm$ 0.35        | –                 | 0.29 $\pm$ 0.40  | <b>0.93*</b> $\pm$ 0.18 |
| Runtime (min) $\downarrow$ | 0.70 $\pm$ 0.77        | 2.39 $\pm$ 0.18   | 0.29 $\pm$ 0.16  | <b>0.07*</b> $\pm$ 0.05 |
| Length $\downarrow$        | 2.79 $\pm$ 1.17        | 12.63 $\pm$ 7.03  | 1.10 $\pm$ 0.81  | <b>2.20</b> $\pm$ 1.16  |
| Semantic Bible             |                        |                   |                  |                         |
| Metric                     | CELOE                  | OCEL              | ELTL             | CLIP                    |
| Acc. $\uparrow$            | 0.99 $\pm$ 0.02        | 0.66 $\pm$ 0.47   | 0.59 $\pm$ 0.37  | <b>0.99</b> $\pm$ 0.00  |
| F1 $\uparrow$              | 0.97 $\pm$ 0.10        | –                 | 0.57 $\pm$ 0.38  | <b>0.98</b> $\pm$ 0.05  |
| Runtime (min) $\downarrow$ | 0.47 $\pm$ 0.80        | 22.15 $\pm$ 96.55 | 0.09 $\pm$ 0.07  | <b>0.06*</b> $\pm$ 0.05 |
| Length $\downarrow$        | 3.85 $\pm$ 2.44        | 9.54 $\pm$ 5.73   | 1.38 $\pm$ 1.76  | <b>2.52*</b> $\pm$ 1.26 |
| Vicodi                     |                        |                   |                  |                         |
| Metric                     | CELOE                  | OCEL              | ELTL             | CLIP                    |
| Acc. $\uparrow$            | 0.29 $\pm$ 0.44        | 0.25 $\pm$ 0.43   | 0.28 $\pm$ 0.44  | <b>0.99*</b> $\pm$ 0.00 |
| F1 $\uparrow$              | 0.25 $\pm$ 0.44        | –                 | 0.25 $\pm$ 0.44  | <b>0.97*</b> $\pm$ 0.09 |
| Runtime (min) $\downarrow$ | 1.30 $\pm$ 0.71        | 4.78 $\pm$ 1.12   | 1.81 $\pm$ 0.46  | <b>0.16*</b> $\pm$ 0.12 |
| Length $\downarrow$        | 10.79 $\pm$ 6.30       | 11.54 $\pm$ 6.00  | 11.14 $\pm$ 6.11 | <b>1.68*</b> $\pm$ 0.98 |

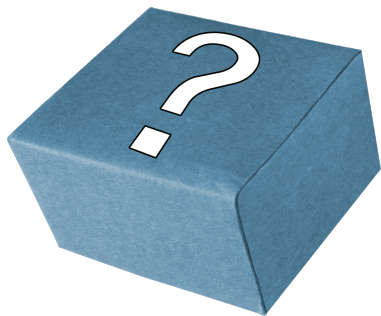
## Section 7

# Summary

# Summary

## Open Questions

- ▶ **Tensors**: Variable ordering?  
Compressed data structure?
- ▶ **RL**: Reduce training costs?  
Hyperparameters?  
Embeddings?
- ▶ **Evolutionary learning**: Myopia?  
Runtime? Continuous data?

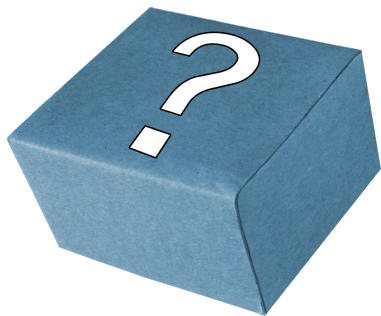


# Summary

## Open Questions

### Holy Grail

- ▶ Can the selection of representations be automated?
  - ▶ LEMUR and ENEXA
- 
- ▶ **Tensors**: Variable ordering?  
Compressed data structure?
  - ▶ **RL**: Reduce training costs?  
Hyperparameters?  
Embeddings?
  - ▶ **Evolutionary learning**: Myopia?  
Runtime? Continuous data?



## Thank You!

Joint works with Alexander Bigerl, Caglar Demir, Hamada Zahera, N'Dah Jean Kouagou, Nikoloas Karalis, Stefan Heindorf, Mohamed Sherif, Muhammed Saleem, and many more

Thank You!  
Questions?

- ▶ <https://dice-research.org>
- ▶ <https://twitter.com/DiceResearch>
- ▶ <https://twitter.com/NgongaAxel>

