

Scaling Machine Learning on Knowledge Graphs

Keynote at EGC 2023

Axel Ngonga



January 18, 2023

Introduction

Disclaimer



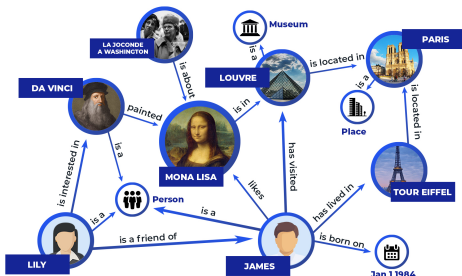
- ▶ Very incomplete
- ▶ Assumes familiarity with description logics

Section 1

Motivation

Motivation

Example

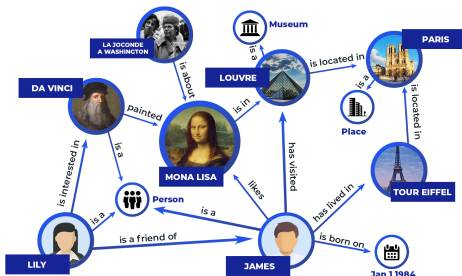


1

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- ▶ $E^- = \{\text{Lily}, \text{James}\}$

Motivation

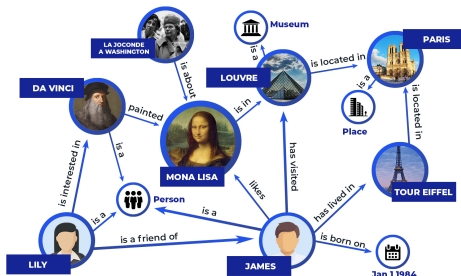
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- ▶ $E^+ = \{\text{Louvre}, \text{TourEiffel}\}$
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- ▶ $\mathcal{H} = \{\exists \text{ isLocatedIn.Place}, \exists \text{ isLocatedIn.}\{\text{Paris}\}\}$

Example



- $E^+ = \{Louvre, TourEiffel\}$
- $E^- = \{Lily, James\}$
- $\mathcal{H} = \{\exists isLocatedIn.Place, \exists isLocatedIn.\{Paris\}\}$

Pros and Cons

- ▶ **Pro**: explainable, exploits background knowledge
- ▶ **Contra**: slow :-)

Motivation

Let's play!



^a<https://www.flickr.com/photos/willwm/2065975725>

Motivation

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► What is $3+3$?



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- ▶ What is $3+3$?
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- ▶ What's the capital of France?



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Motivation

Let's play!

- ▶ What is $3+3$?
- ▶ Square root of 4?
- ▶ What's the capital of France?
- ▶ Close your eyes.

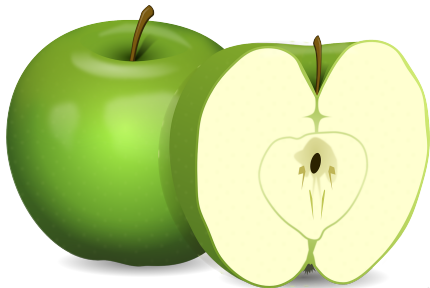


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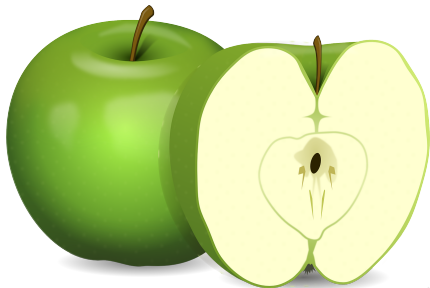
How does the brain form thoughts?

- ▶ System 1 [Kahneman, 2011]
 - ▶ Intuitive responses
 - ▶ Time-efficient
 - ▶ Unconscious



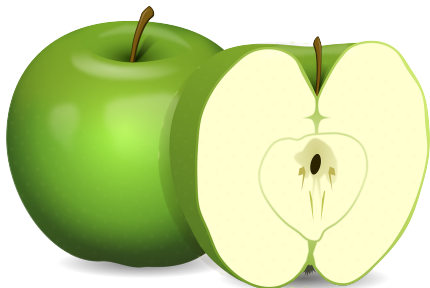
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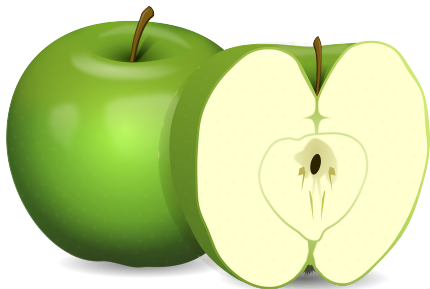
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How does the brain form thoughts?

In a nutshell

- ▶ Multiple representations seem to be beneficial for **rapid cognition**
 - ▶ Can they help **improve the runtime** of class expression learning?
-
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Section 2

Class Expression Learning

Class Expression Learning

Formal definition

- ▶ **Supervised learning** with background knowledge (adapted from [Lehmann and Hitzler, 2010])
- ▶ **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 $E^+ \subseteq N_I$
 - ▶ Set of negative examples $E^- \subseteq N_I$

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- ▶ **Goal:** Find at least one hypothesis $H \in \mathcal{H}$ with
 1. H is a class expression in \mathcal{L} , and (ideally)
 2. $\forall e^+ \in E^+ : \mathcal{K} \models H(e^+)$
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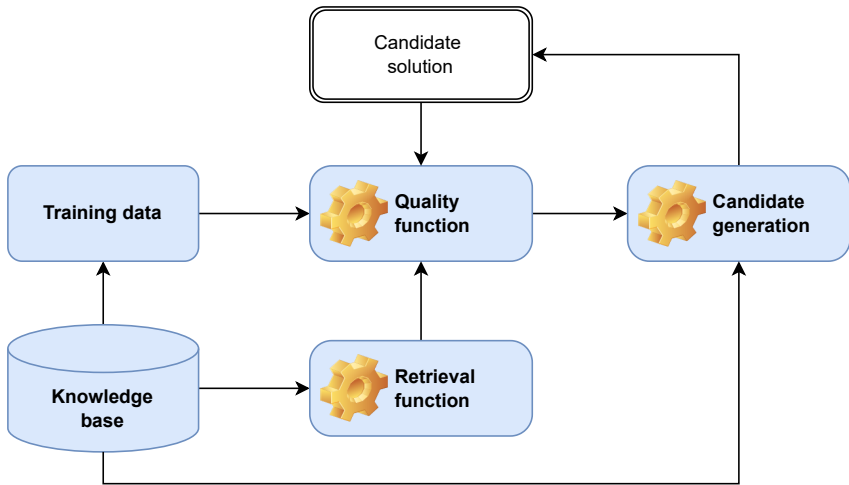
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- ▶ Practically, aim to find $H \in \underset{C \in \mathcal{L}}{\operatorname{argmax}} Q(C)$ [Heindorf et al., 2022]

Class Expression Learning

Common Approach



Example: $\mathcal{L} = \mathcal{ALC}$

- ▶ Let C and D be \mathcal{ALC} concepts
- ▶ Let $r \in N_R$ be a role
- ▶ Then, the following are \mathcal{ALC} concepts
[Schmidt-Schauß and Smolka, 1991]

Syntax	Semantics
\top	$\Delta^{\mathcal{I}}$
\perp	\emptyset
$C \in N_C$	$C^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$
$\neg C$	$\Delta^{\mathcal{I}} \setminus C^{\mathcal{I}}$
$C \sqcap D$	$C^{\mathcal{I}} \cap D^{\mathcal{I}}$
$C \sqcup D$	$C^{\mathcal{I}} \cup D^{\mathcal{I}}$
$\exists r.C$	$\{x \in \Delta^{\mathcal{I}} : \exists y \in C^{\mathcal{I}} \text{ with } (x, y) \in r^{\mathcal{I}}\}$
$\forall r.C$	$\{x \in \Delta^{\mathcal{I}} : (x, y) \in r^{\mathcal{I}} \rightarrow y \in C^{\mathcal{I}}\}$

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 $\rho(x) \sqsubseteq x$ [Lehmann and Hitzler, 2010]

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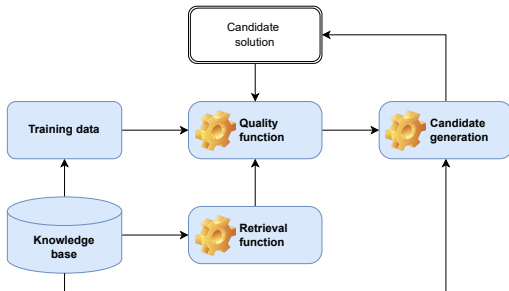
Example

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

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

Learning problem

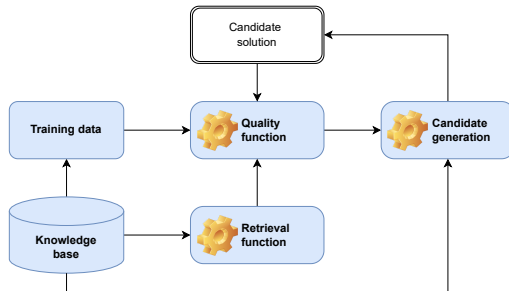
Challenges



- **Retrieval** is expensive

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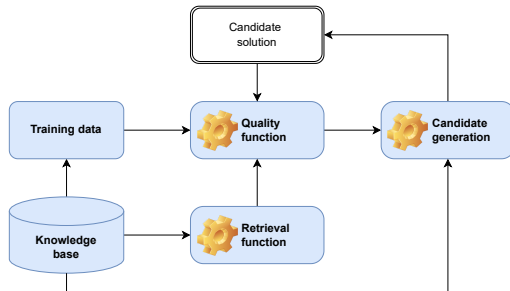
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- ▶ **Retrieval** is expensive \Rightarrow Exploit SPARQL
- ▶ **Quality functions** are often myopic

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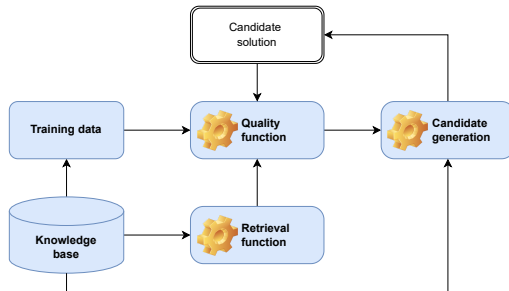
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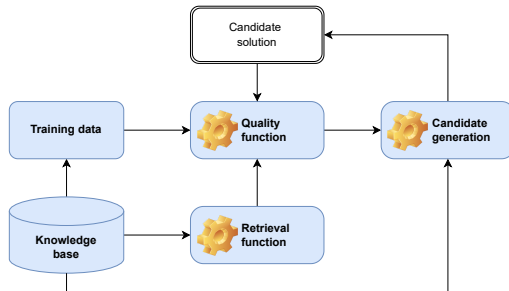
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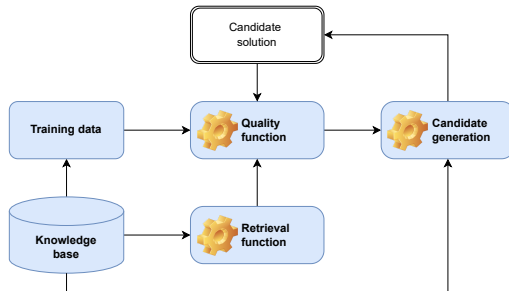
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Section 3

Representing Concepts as SPARQL

From \mathcal{ALC} to SPARQL

- ▶ Assume closed world and **fully materialized** knowledge graph
- ▶ Retrieval in \mathcal{ALC} can be realized by representing **concepts as SPARQL queries** [Bin et al., 2016]

From \mathcal{ALC} to SPARQL

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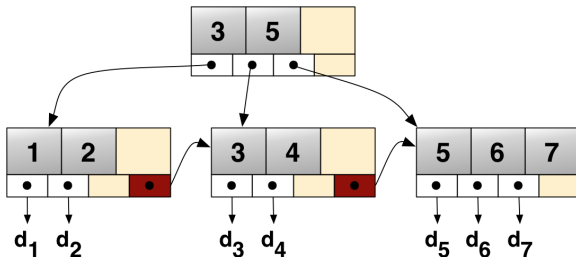
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$\forall r.C$	<code>{ ?var r ?s0.</code> <code> { SELECT ?var (count(?s1) AS ?cnt1)</code> <code> WHERE { ?var r ?s1. $\tau(C, ?s1)$}</code> <code> GROUP BY ?var }</code> <code> { SELECT ?var (count(?s2) AS ?cnt2)</code> <code> WHERE { ?var r ?s2 .}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

Representing Concepts as SPARQL

Storage Solutions

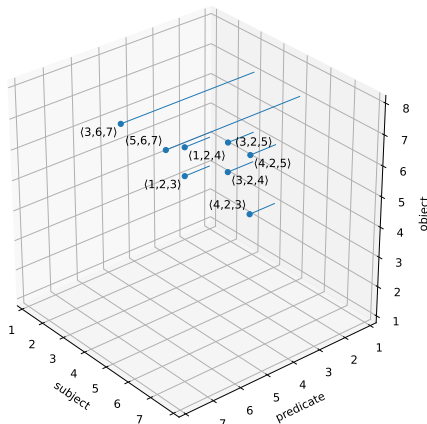
- ▶ Important difference are indexing data structures
- ▶ Typical indexes include
 - ▶ **Resource index**, e.g., a hash table
 - ▶ **Triple index**, e.g., a B⁺ tree



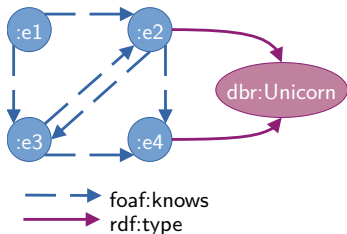
TENTRIS: Idea

Idea [Bigerl et al., 2020]

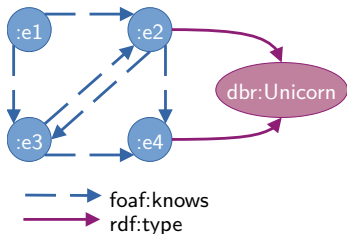
- Exploit tensor representation to accelerate querying
- Devise data structure to accommodate rapid querying



From RDF to Tensors

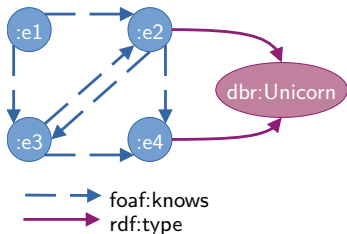


From RDF to Tensors



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

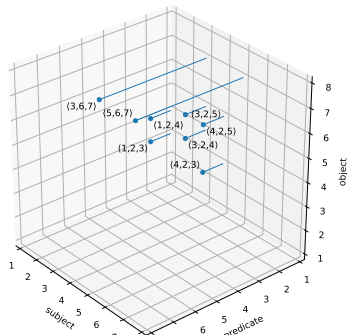
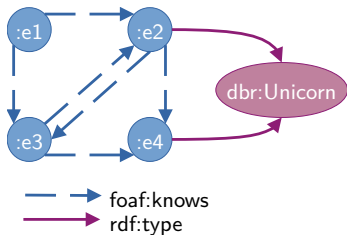
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TENTRIS: Data Model

- Consider order- n tensors $T : \mathbf{K} = \mathbf{K}_1 \times \dots \times \mathbf{K}_n \rightarrow V$

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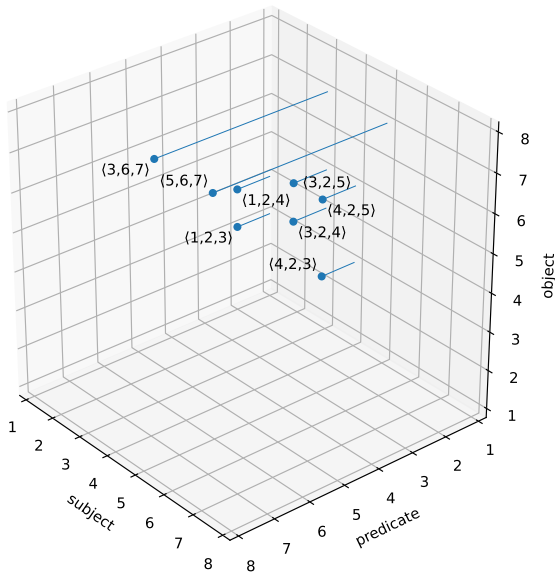
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 - ▶ \mathbb{B} or \mathbb{N} as co-domain

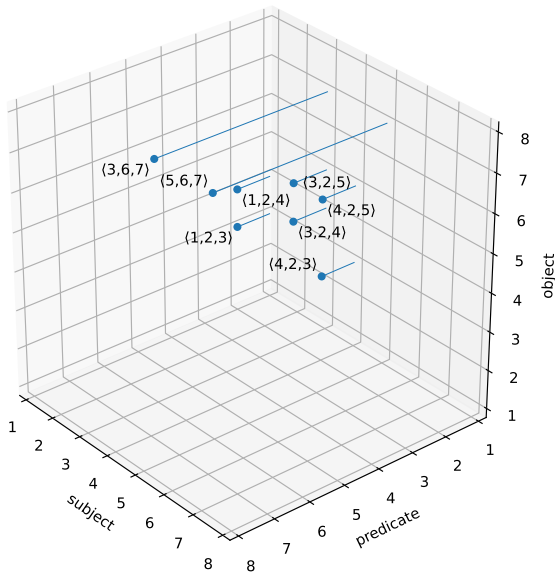
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 - ▶ \mathbb{B} or \mathbb{N} as co-domain
- ▶ $\mathbf{k} \in \mathbf{K}$ is a **key** with key parts $\langle \mathbf{k}_1, \dots, \mathbf{k}_n \rangle$
- ▶ Values v in a tensor are accessed in array style, e.g., $T[\mathbf{k}] = v$

TENTRIS: Data Model



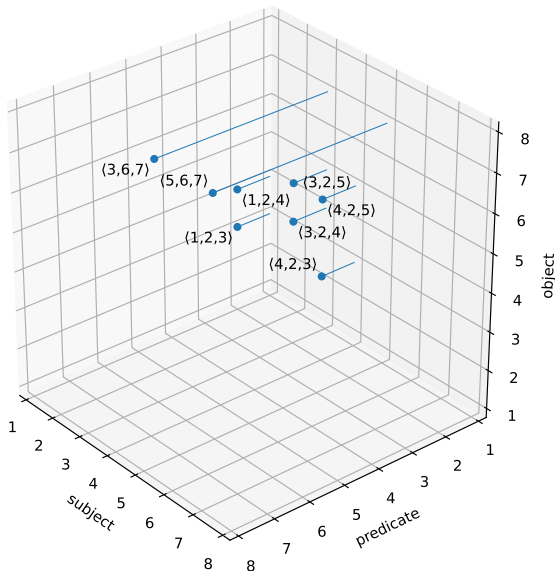
TENTRIS: Data Model



► $\mathbf{K} = \mathbb{N}^3$

► $\mathbf{V} = \mathbb{B}$

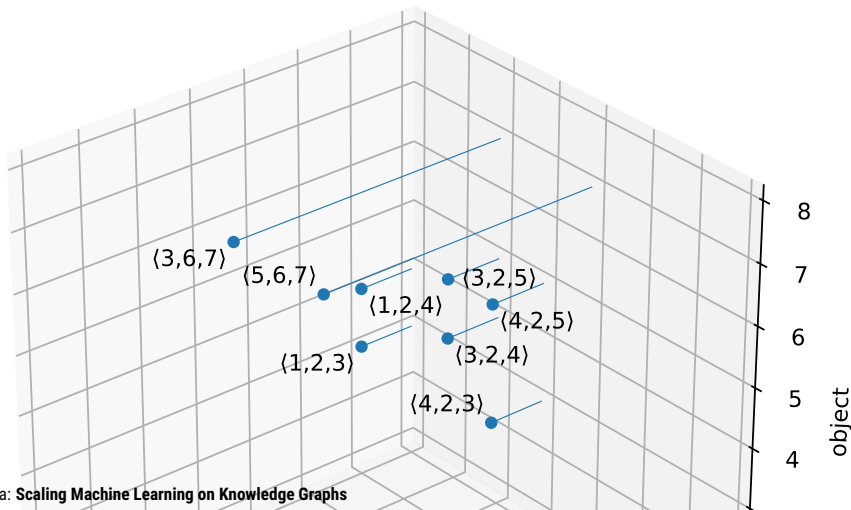
TENTRIS: Data Model



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

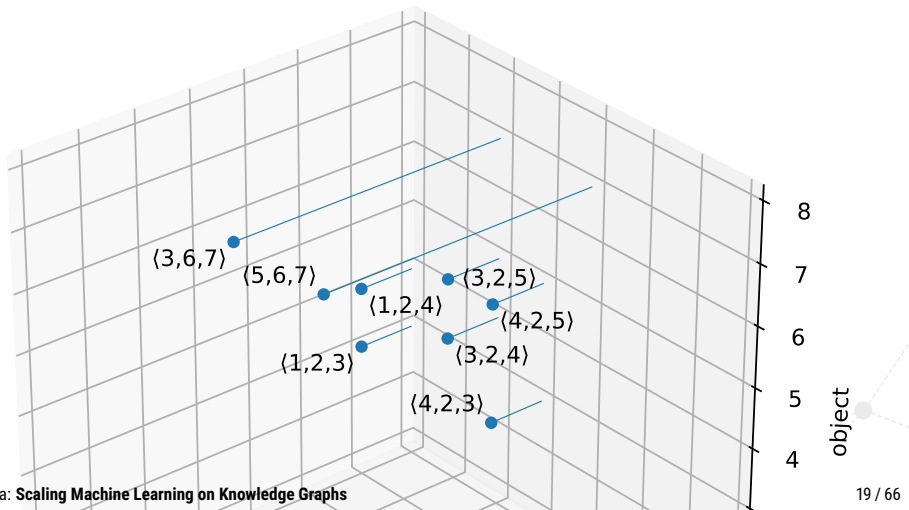
TENTRIS: Data Model

- **Slicing** selects portion of T , e.g., $T^{(1)} := T[1, 2, :]$ is order-1 tensor



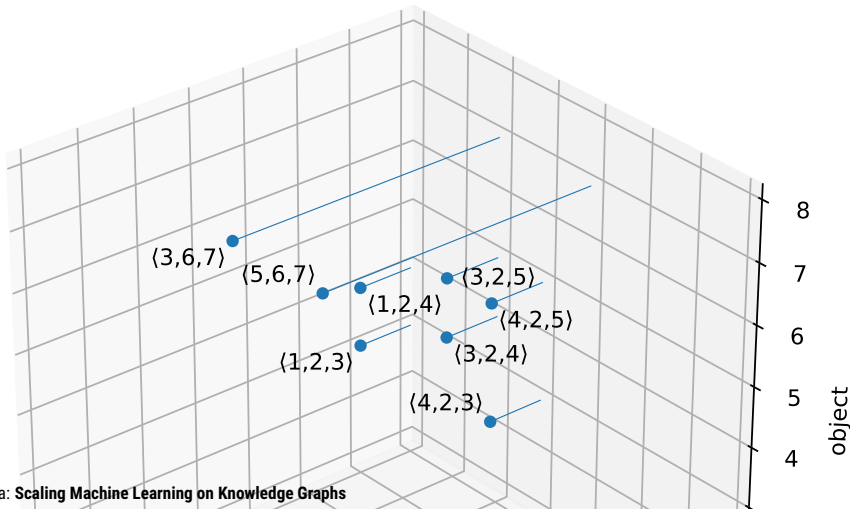
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- Slices can be **joined** via Einstein summation [Barr, 1989]



TENTRIS-Einstein Summation

```
1 SELECT ?f WHERE {  
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3   ?f foaf:knows ?u .  
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$T[:, 2, :]$

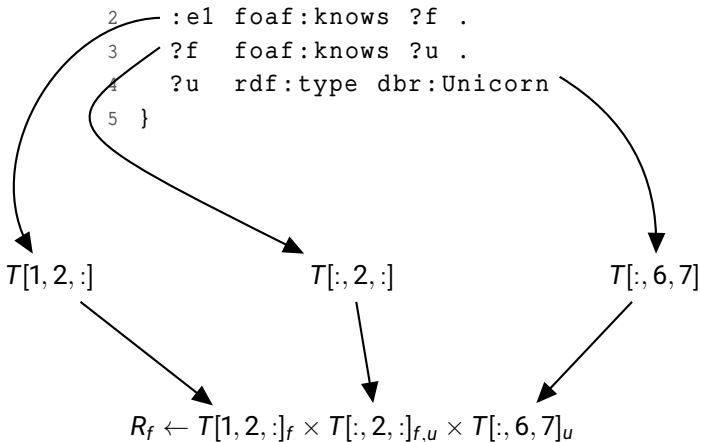
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TENTRIS: Querying

- ▶ **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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- ▶ **BGP** $B = \{B^{(1)}, \dots, B^{(r)}\}$ 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: Querying

- ▶ **Triple pattern** is mapped to

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

- ▶ **BGP** $B = \{B^{(1)}, \dots, B^{(r)}\}$ is given by

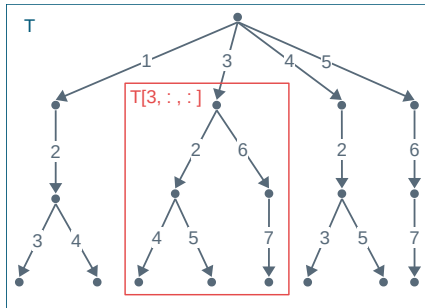
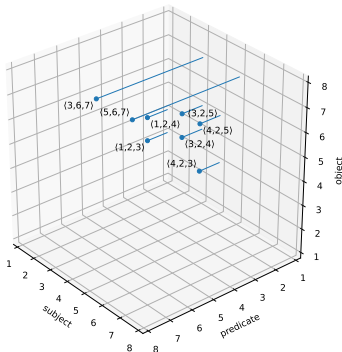
$$T'_{\langle I \in U \rangle} \leftarrow \bigtimes_i T[\mathbf{k}^{B^{(i)}}]_{\langle I \in B^{(i)} | I \in U \rangle}$$

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

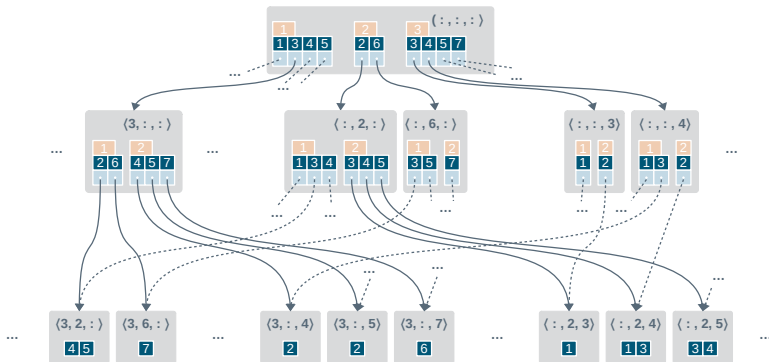
$$T''_{\langle I \in U' \rangle} \leftarrow \bigtimes_i T[\mathbf{k}^{B^{(i)}}]_{\langle I \in B^{(i)} | I \in U \rangle}$$

TENTRIS: Hypertrie

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

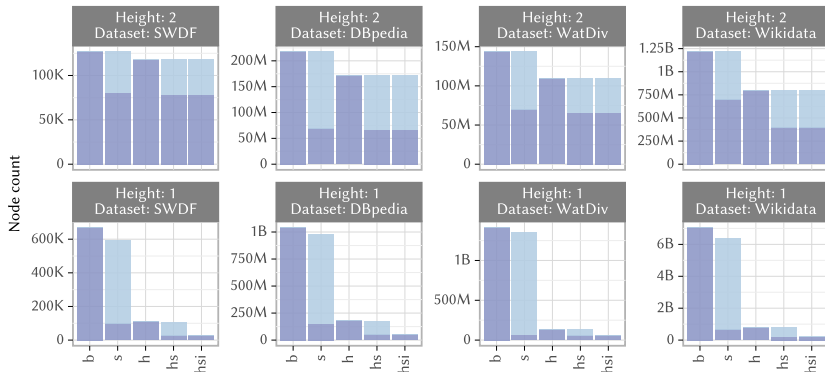


TENTRIS: Hypertrie



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

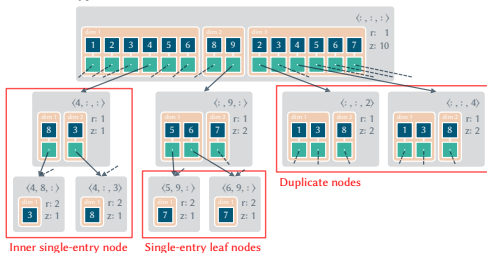
TENTRIS: Hypertrie



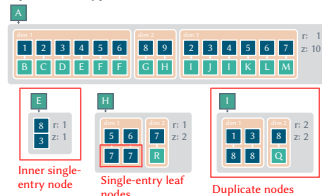
- Hypertrie topology seems sparse
- Compression to improve space, loading and query times [Bigerl et al., 2022]

TENTRIS: Compressed Hypertrie

Baseline hypertrie



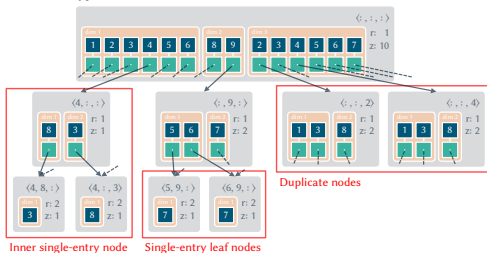
Optimized hypertrie



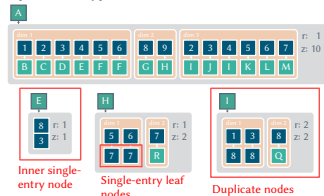
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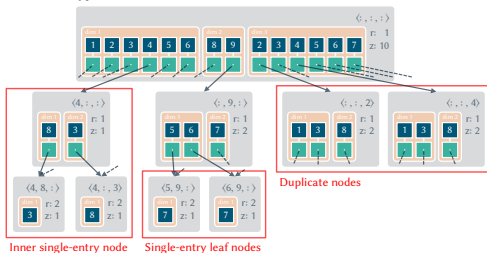
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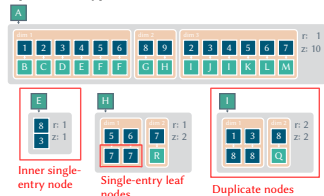
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 1. Remove duplicates via hashing (global)

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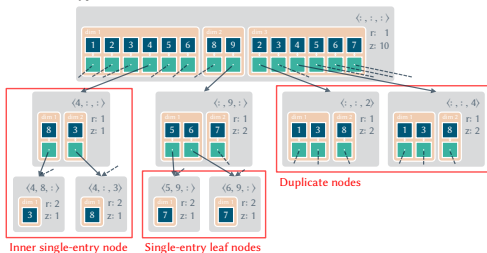
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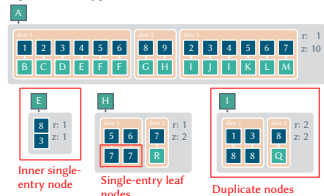
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 2. Single-entry inner nodes (local) store **sub-hypertries** directly

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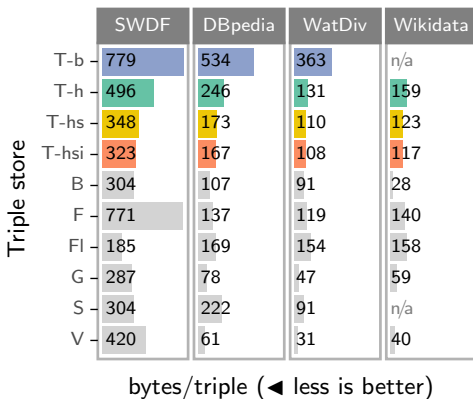
- Compress data based on local and global node topology
- 3 compression approaches
 1. Remove duplicates via **hashing** (global)
 2. Single-entry inner nodes (local) store **sub-hypertries** directly
 3. Single-entry leaf nodes are eliminated via **in-place storage** (local)

TENTRIS: Compressed Hypertrie

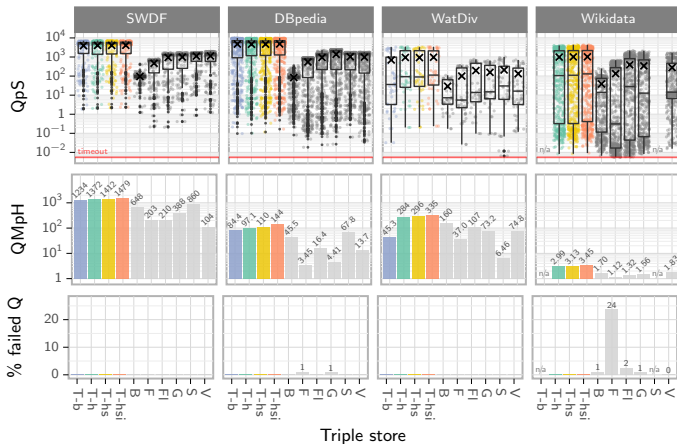
- ▶ Comparison with state-of-the-art approaches
- ▶ **Hardware**: AMD EPYC 7742, 1 TB RAM and 2×3 TB NVMe SSDs
- ▶ **Datasets**: Between 372K (SWDF) and 5.5B triples (WikiData)

TENTRIS: Compressed Hypertrie

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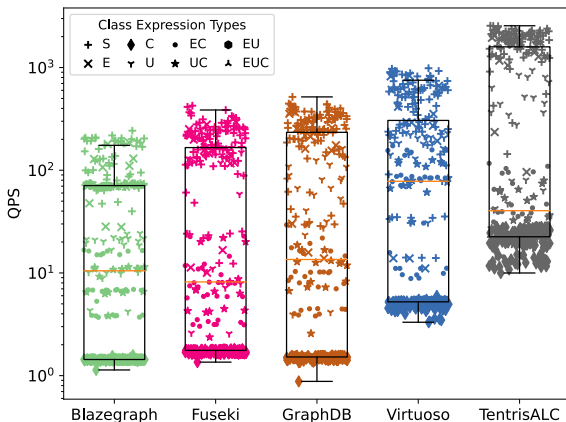


TENTRIS: Compressed Hypertrie



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

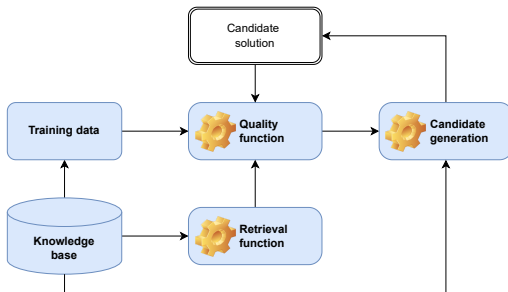
TENTRIS: Carcinogenesis



- Comparison on supervised machine learning tasks in \mathcal{ACC}
- Better runtimes on all datasets considered

Learning problem

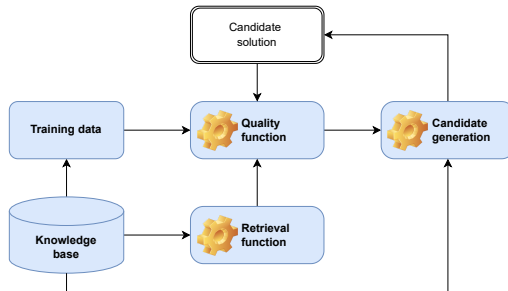
Challenges



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

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

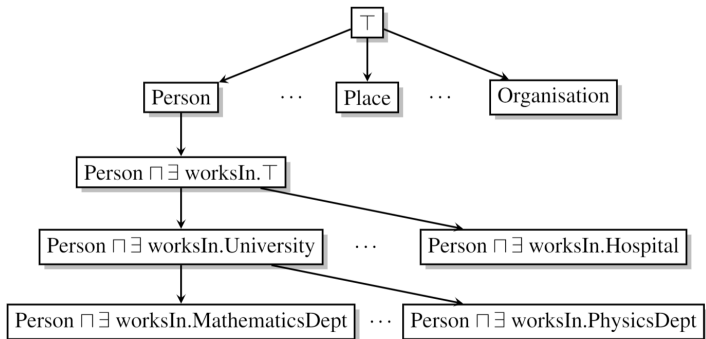
Improving Quality Functions

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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Quality Functions – OCEL

- ▶ Let $R(C)$ be the set of instances of C
- ▶ Let C' be the parent concept of C in the search tree

Improving Quality Functions

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$$\text{acc}(C) = 1 - \frac{|E^+ \setminus R(C)| + |R(C) \cap E^-|}{|E|}$$

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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 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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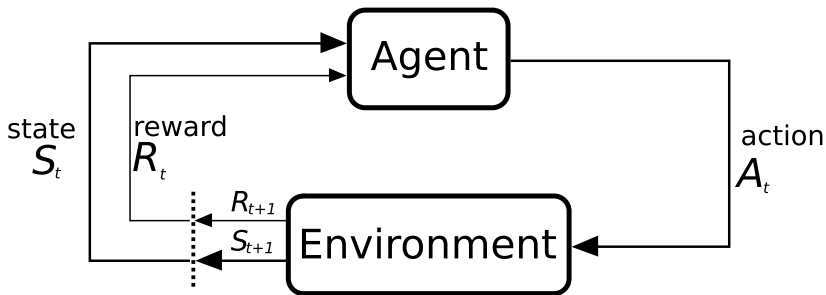
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Problem: Myopia

- Current metrics do not consider future accuracy of concepts
- Optimize for **cumulative discounted future rewards**
[Demir and Ngonga Ngomo, 2021]

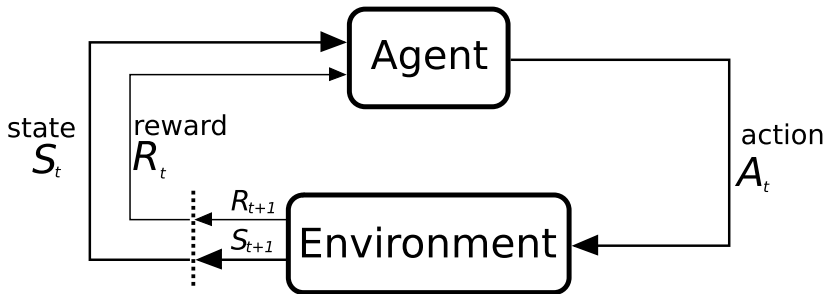
Improving Quality Functions

Reinforcement Learning



Improving Quality Functions

Reinforcement Learning



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

Improving Quality Functions

Reinforcement Learning – Q Function

- Maximize

$$G_t = \sum_{i=0}^n \gamma^i R_{t+i}$$

Improving Quality Functions

Reinforcement Learning – Q Function

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- Optimize **state-action value function** $Q_\pi : S \times A \rightarrow \mathbb{R}$ with

$$Q_\pi(\mathbf{s}, \mathbf{a}) = \mathbb{E}_\pi [G_t \mid S_t = \mathbf{s}, A_t = \mathbf{a}]$$

Improving Quality Functions

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Improving Quality Functions

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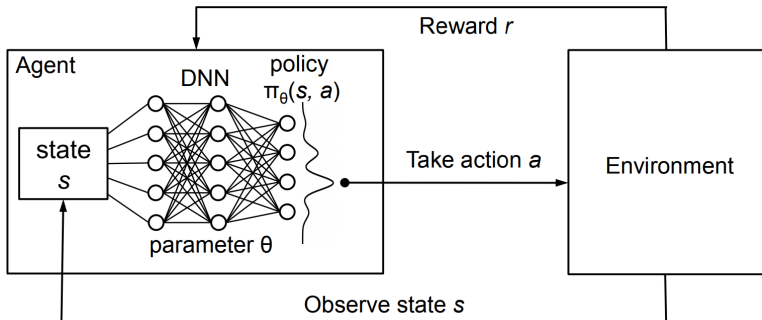
- **Observation:** Infinite number of states as search space is infinite
- Apply deep Q learning with target network [Mnih et al., 2015]

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

Reinforcement Learning – DRILL

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

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



Source: [Mao et al., 2016]

TransE

► Assumptions

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

TransE

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

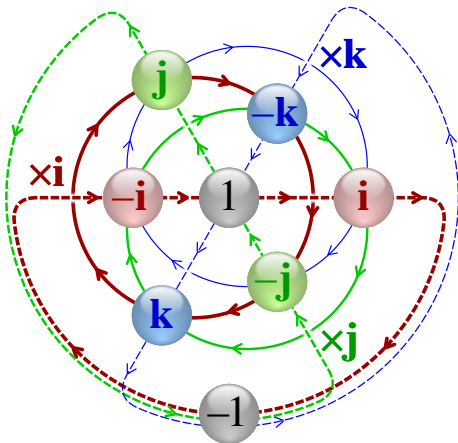
$$L = \sum_{(s,p,o) \in E} \sum_{(s',p,o') \in S'(s,p,o)} [\gamma + d(\vec{s} + \vec{p}, \vec{o}) - d(\vec{s}' + \vec{p}, \vec{o}')]_+$$

where

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

Improving Quality Functions

Quaternions: \mathbb{H}



2

²https://en.wikipedia.org/wiki/Quaternion#/media/File:Cayley_Q8_quaternion_multiplication_graph.svg

Quaternions: \mathbb{H}

- ▶ Can define embeddings in this space: QMult [Demir et al., 2021]
 - ▶ $\vec{s}, \vec{p}, \vec{o} \in \mathbb{H}^k$
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- ▶ Similar construction for **octonions**

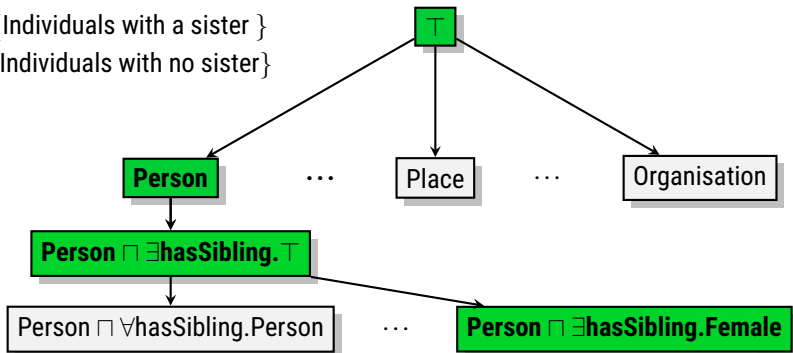
Improving Quality Functions

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

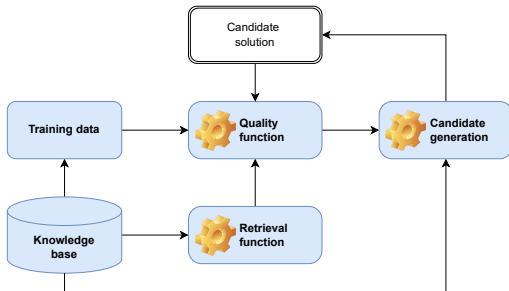
Evaluation

- 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 ± 1.1	33.5 ± 129.3
OCEL	*	1.00 ± 0.00	11.0 ± 1.4	2271.6 ± 1269.2
ELTL	$.990 \pm 0.06$	$.984 \pm 0.09$	8.1 ± 1.6	*
DRILL	1.00 ± 0.00	1.00 ± 0.00	1.1 ± 0.5	9.88 ± 38.5

Learning problem

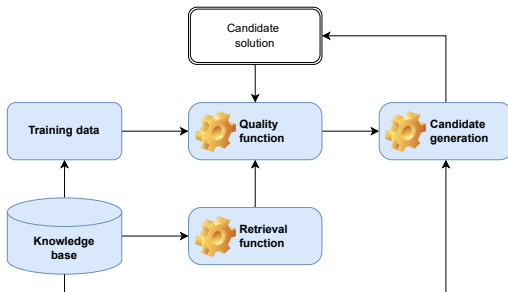
Challenges



✓ Retrieval is expensive

Learning problem

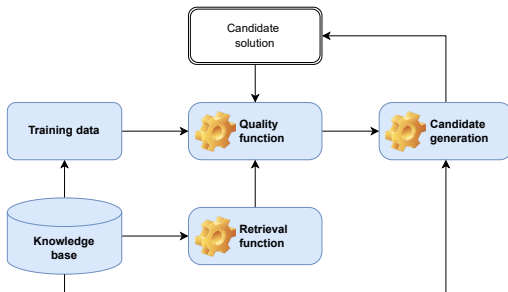
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Learning problem

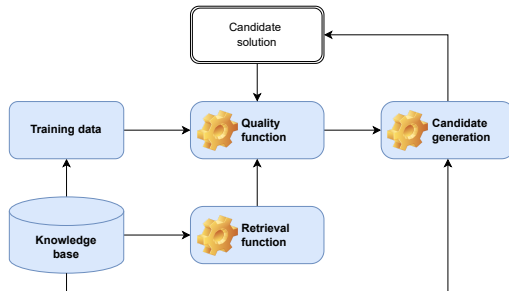
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Learning problem

Challenges



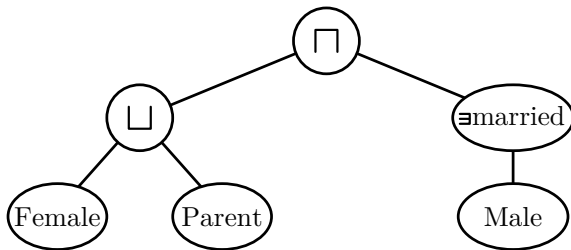
- ✓ Retrieval is expensive \Rightarrow Exploit SPARQL
- ✓ Quality functions are often myopic \Rightarrow Exploit embeddings
- ▶ Candidate generation is expensive \Rightarrow Exploit priming
- ▶ Search space is large \Rightarrow Prune by length

Section 5

Learning with Priming

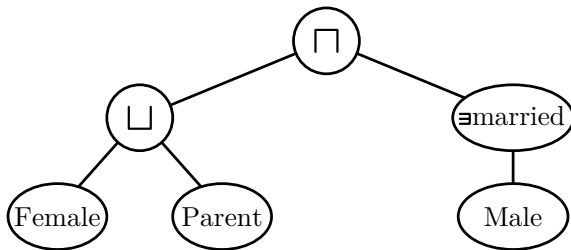
EVOLARNER – Idea

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



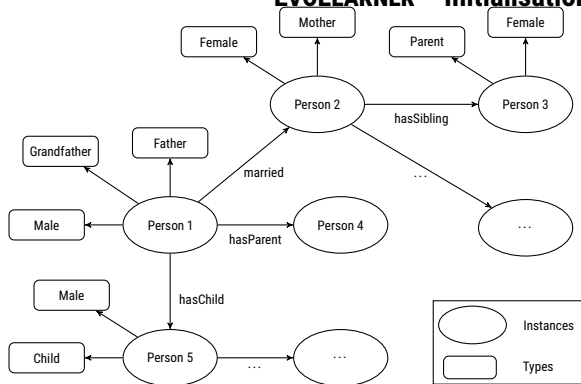
EOLEARNER – Idea

- Represent concepts as trees, e.g.,
(Female \sqcup Parent) \sqcap \exists married.Male
- Learn in evolutionary fashion using genetic programming
- Exploit **priming effect** (remember the green apple)
- **Intuition**: An individual is an overlap several concepts
[Heindorf et al., 2022]



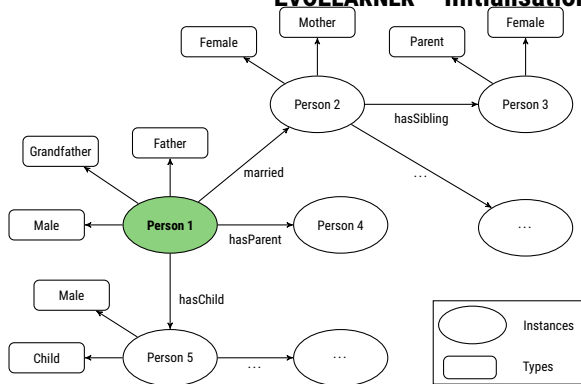
Learning with Priming

EVOLARNER – Initialisation



Learning with Priming

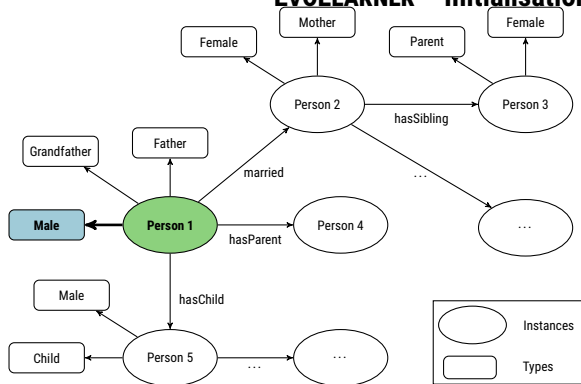
EVOLARNER – Initialisation



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

Learning with Priming

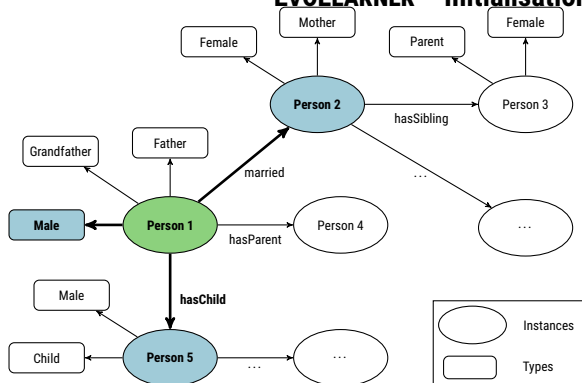
EVOLARNER – Initialisation



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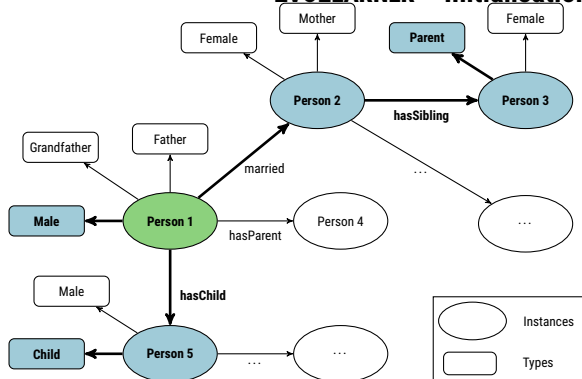
Learning with Priming

EVOLARNER – Initialisation



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

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:

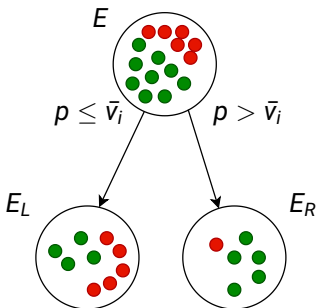
Male \sqcap ((**\exists married.** **\exists hasSibling.Parent**) \sqcap (**\exists hasChild.Child**))

Learning with Priming

EVOLARNER – Data Properties

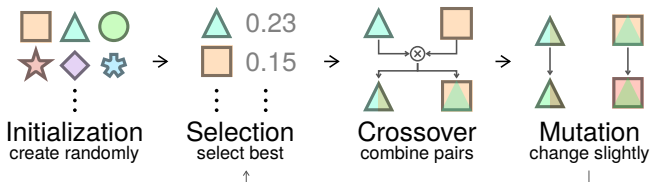
- ▶ Given a data property d from the knowledge base \mathcal{K} and a set E of positive and negative examples
- ▶ We precompute up to k splits of the form $d \leq \bar{v}_i$ per data property
- ▶ Splits are computed to maximize information gain:

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



Learning with Priming

EOLEARNER – Training



EOLEARNER – Evaluation

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

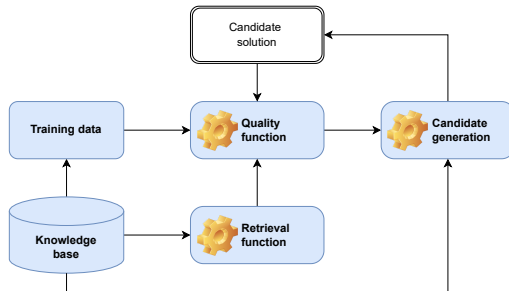
Learning with Priming

EvoLEARNER – Ablation Study

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

Learning problem

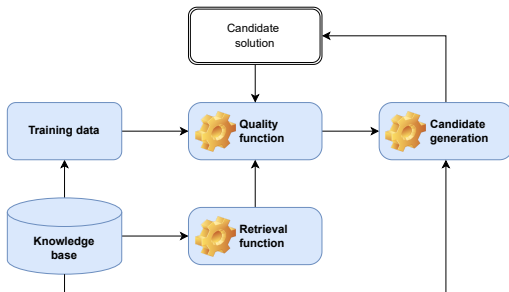
Challenges



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

Learning problem

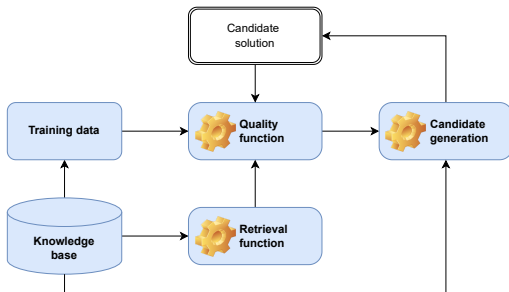
Challenges



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

Learning problem

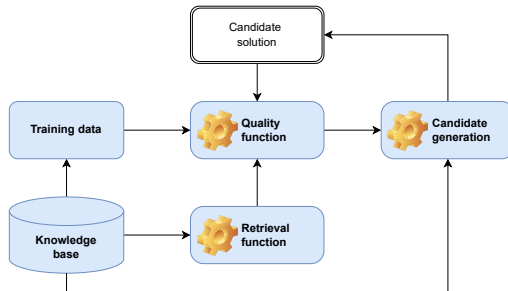
Challenges



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

Learning problem

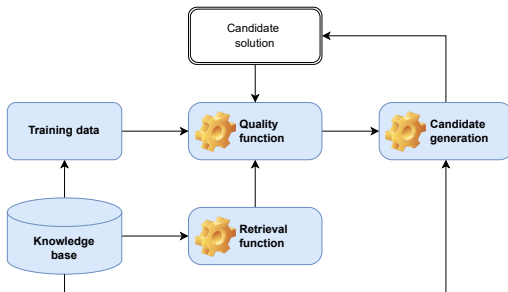
Challenges



- ✓ 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



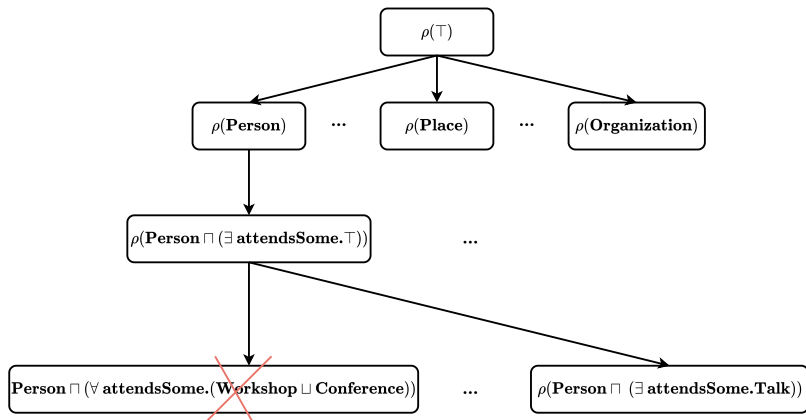
- ✓ Retrieval is expensive \Rightarrow Exploit SPARQL
- ✓ Quality functions are often myopic \Rightarrow Exploit embeddings
- ✓ Candidate generation is expensive \Rightarrow Exploit priming
- ▶ Search space is large \Rightarrow Prune by length

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)
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Concept Lengths

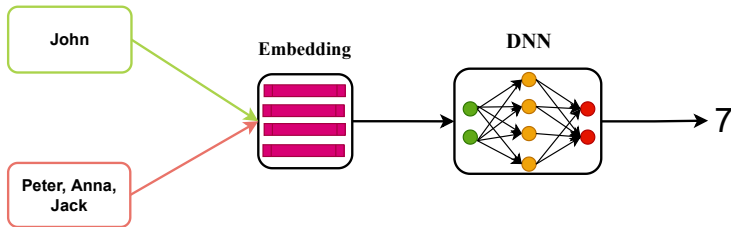
- ▶ $length(A) = length(\top) = length(\perp) = 1$ (if A is an atomic concept)
- ▶ $length(\neg C) = 1 + length(C)$, for all concepts C
- ▶ $length(\exists r.C) = length(\forall r.C) = 2 + length(C)$, for all concepts C

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 .

CLIP

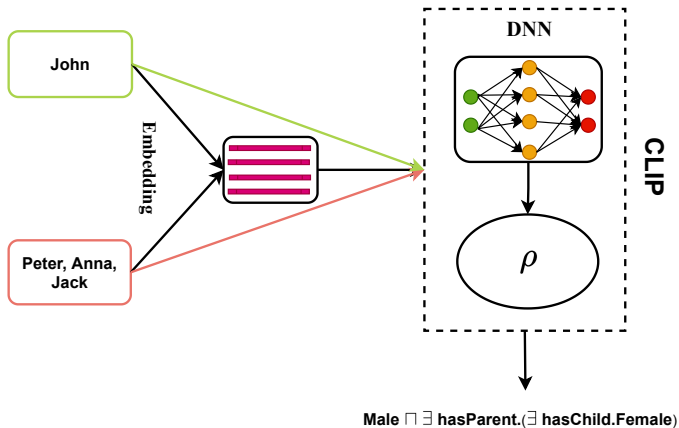
Concept Length Prediction



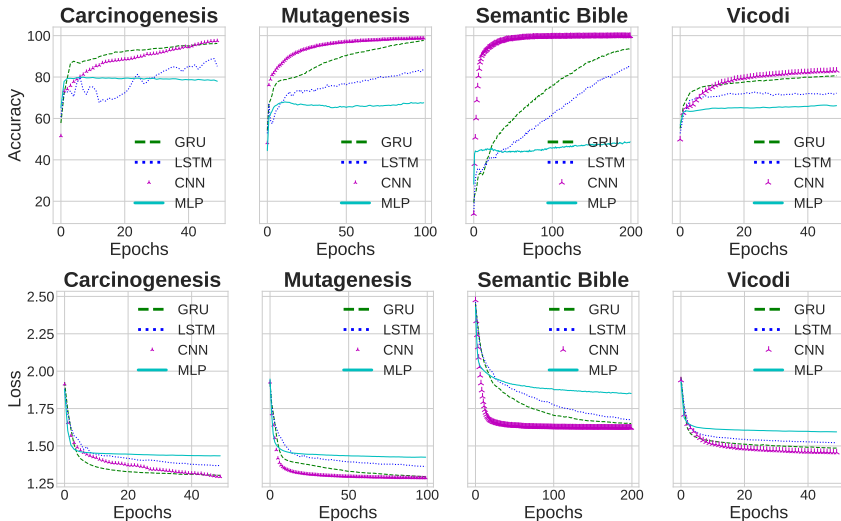
- Input: positive and negative examples
- Output: length of the target concept

CLIP

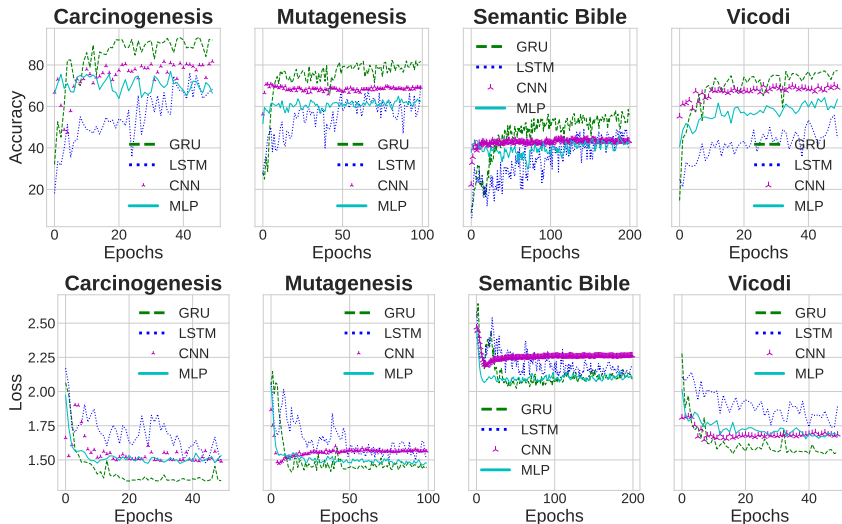
Concept Learning



CLIP Training



Validation



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	0.95	0.84	0.80	0.49	0.78	0.85	0.70	0.68	0.33
Test F1	0.88	0.92	0.71	0.59	0.33	0.76	0.85	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	0.53	0.37	0.40	0.25	0.66	0.80	0.69	0.66	0.29
Test F1	0.27	0.38	0.20	0.22	0.16	0.45	0.50	0.45	0.38	0.20

Comparison with SOTA

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

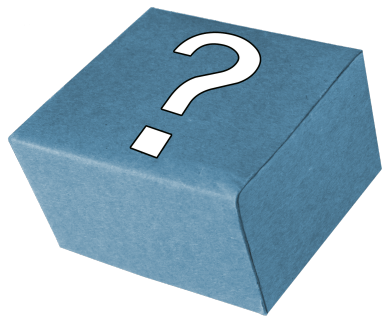
Section 7

Summary

Summary

Open Questions

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

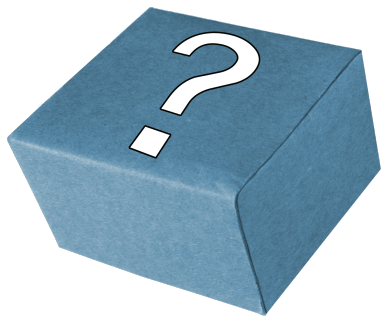


Summary

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>

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