Deep Deductive Reasoning over Knowledge Graphs and Ontologies

Pascal Hitzler
Data Semantics Laboratory (DaSe Lab)
Kansas State University

http://www.daselab.org

Neural

- Refers to computational abstractions of (natural) neural network systems.
- Prominently includes Artificial Neural Networks and Deep Learning as machine learning paradigms.
- More generally sometimes referred to as *connectionist systems*.

- Prominent applications come from the machine learning world.

- And of course, there is the current deep learning hype.

Symbolic

- Refers to (computational) symbol manipulations of all kind.

- Graphs and trees, traversal, data structure operations.
- Knowledge representation in explicit symbolic form (data base, ontology, knowledge graph)
- Inductive and statistical inference.
- Formal logical (deductive or abductive) reasoning.

- Prominent applications all over computer science, including expert systems (and their modern versions), information systems, data management, added value of data annotation, etc.

- Semantic Web data is inherently symbolic.

Neuro-Symbolic

Computer Science perspective:

- Connectionist machine learning systems are
  - very powerful for some machine learning problems
  - robust to data noise
  - very hard to understand or explain
  - really poor at symbol manipulation
  - unclear how to effectively use background (domain) knowledge
- Symbolic systems are
  - Usually rather poor regarding machine learning problems
  - Intolerant to data noise
  - Relatively easy to analyse and understand
  - Really good at symbol manipulation
  - Designed to work with other (background) knowledge

Neuro-Symbolic

Computer Science perspective:

- **Let’s try to get the best of both worlds:**
  - **very powerful machine learning paradigm**
  - **robust to data noise**
  - **easy to understand and assess by humans**
  - **good at symbol manipulation**
  - **work seamlessly with background (domain) knowledge**

- **How to do that?**
  - **Endow connectionist systems with symbolic components?**
  - **Add connectionist learning to symbolic reasoners?**

Neuro-Symbolic

Note:

- Deep Learning systems are a far cry from how natural neural networks work.
- There are things that our brain can do, and things that symbolic approaches can do, where we do not have the faintest idea how to solve them through deep learning (or any other connectionist learning approach).

- The argument that we “just don’t have enough training data” speaks (understandably) to the current hype, but is a hope that is unfounded: While this may be the case in some cases, there is no rationale to overgeneralize.
  [Note: if we had “enough computational power,” we could also solve all reasonable-size NP-complete problems in an instant.]

Neuro-symbolic AI

Publications on neuro-symbolic AI in major conferences (research papers only):

conference	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	total
ICML	0	0	0	0	0	1	3	2	5	6	17
NeurIPS	0	0	0	0	0	0	0	4	2	4	10
AAAI	0	0	0	0	0	1	0	1	1	1	4
IJCAI	1	0	0	0	0	0	2	2	0	2	7
ICLR	N/A	N/A	0	0	0	0	1	1	1	3	6
total	1	0	0	0	0	2	6	10	9	16	44

See

Md Kamruzzaman Sarker, Lu Zhou, Aaron Eberhart, Pascal Hitzler

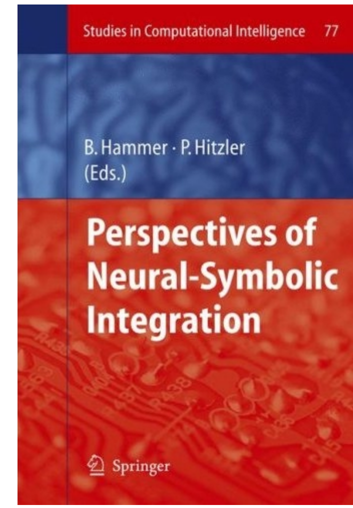
Neuro-Symbolic Artificial Integration: Current Trends

AI Communications, to appear; https://arxiv.org/abs/2105.05330 for more analysis.

Some Background

Workshop Series on Neural-Symbolic Learning and Reasoning, since 2005. Joint with Artur d'Avila Garcez.
http://neural-symbolic.org/

Barbara Hammer and Pascal Hitzler (eds), Perspectives of Neural-Symbolic Integration, Springer, 2007

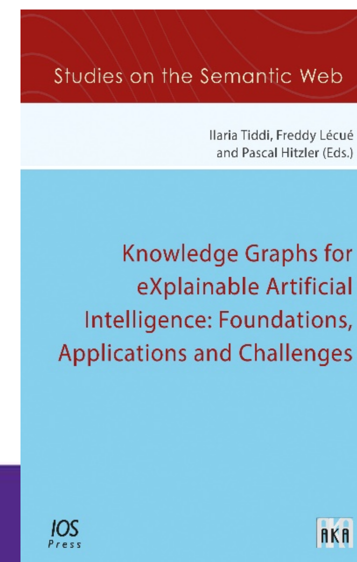


Neural-Symbolic Learning and Reasoning: A Survey and Interpretation

Tarek R. Besold, Artur d'Avila Garcez, Sebastian Bader,
Howard Bowman, Pedro Domingos, Pascal Hitzler,
Kai-Uwe Kuehnberger, Luis C. Lamb, Daniel Lowd,
Priscila Machado Vieira Lima, Leo de Penning, Gadi Pinkas,
Hoifung Poon, Gerson Zaverucha

https://arxiv.org/abs/1711.03902 (2017)

Ilaria Tiddi, Freddy Lecue, Pascal Hitzler (eds.), Knowledge Graphs for eXplainable Artificial Intelligence: Foundations, Applications and Challenges. Studies on the Semantic Web Vol. 47, IOS Press, 2020.



Deep Deductive Reasoners

Monireh Ebrahimi, Aaron Eberhart, Federico Bianchi, Pascal Hitzler,
Towards Bridging the Neuro-Symbolic Gap: Deep Deductive Reasoners.
Applied Intelligence 51 (9), 6326-6348, 2021.

Pascal Hitzler, Frank van Harmelen
A reasonable Semantic Web.
Semantic Web 1 (1-2), 39-44, 2010.

Deep Deductive Reasoners

- We trained deep learning systems to do deductive reasoning.

- Why is this interesting?
  - For dealing with noisy data (where symbolic reasoners do very poorly).
  - For speed, as symbolic algorithms are of very high complexity.
  - Out of principle because we want to learn about the capabilities of deep learning for complicated cognitive tasks.
  - To perhaps begin to understand how our (neural) brains can learn to do highly symbolic tasks like formal logical reasoning, or in more generality, mathematics.
    A fundamental quest in Cognitive Science.

Reasoning as Classification

- Given a set of logical formulas (a theory).

- Any formula expressible over the same language is either
  - a logical consequence or
  - not a logical consequence.

- This can be understood as a classification problem for machine learning.

- It turns out to be a really hard machine learning problem.

Knowledge Materialization

- **Given a set of logical formulas (a theory).**

- **Produce all logical consequences under certain constraints.**

- **Without the qualifier this is in general not possible as the set of all logical consequences is infinite.**

- **So we have to constrain to consequences of, e.g., a certain syntactic form. For relatively simple logics, this is often reasonably possible.**

Published deep deductive reasoning work

paper	logic	transfer	generative	scale	performance
[12]	RDFS	yes	no	moderate	high
[25]	RDFS	no	yes	low	high
[10]	$\mathcal{EL}^+$	yes	yes	moderate	low
[20]	OWL RL	no*	no	low	high
[6]	FOL	no	yes	very low	high
(new)	RDFS	yes	yes	moderate	high
(new)	EL+	yes	yes	moderate	high

[12]: Ebrahimi, Sarker, Bianchi, Xie, Eberhart, Doran, Kim, Hitzler, AAAI-MAKE 2021

[25]: Makni, Hendler, SWJ 2019

[10]: Eberhart, Ebrahimi, Zhou, Shimizu, Hitzler, AAAI-MAKE 2020

[20]: Hohenecker, Lukasiewicz, JAIR 2020

[6]: Bianchi, Hitzler, AAAI-MAKE 2019

(new): Ebrahimi, Eberhart, Hitzler, June 2021

Knowledge Graphs and Ontologies

Pascal Hitzler, Semantic Web: A Review of the Field.
Communications of the ACM 64 (2), 76-82, 2021.

Knowledge Graphs and Ontologies (Schemas)

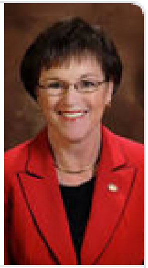
Knowledge Graphs (and their schemas) are made to enable easier

- **data sharing**
- **data discovery**
- **data integration**
- **data reuse**

Google Knowledge Graph

Laura Kelly

Governor of Kansas



Laura Kelly is an American politician serving as the 48th governor of Kansas since 2019. A member of the Democratic Party, she represented the 18th district in the Kansas Senate from 2005 to 2019. Kelly ran for governor in the 2018 election and defeated the Republican nominee, Kansas Secretary of State Kris Kobach. Wikipedia

Born: January 24, 1950 (age 69 years), New York, NY

Spouse: Ted Daughety

Party: Democratic Party

Office: Governor of Kansas since 2019

Education: Indiana University, Bradley University, Indiana University Bloomington

Children: Kathleen Daughety, Molly Daughety

hasEducation →

Indiana University

iu.edu

Indiana University is a multi-campus public university system in the state of Indiana, United States. Indiana University has a combined student body of more than 110,000 students, which includes approximately 46,000 students enrolled at the Indiana University Bloomington campus. Wikipedia

Mascot: Referred to as "The Hoosiers"

Endowment: 1.986 billion USD

Students: 110,436 university-wide

President: Michael McRobbie

Academic staff: 8,733 university-wide

Subsidiaries: Indiana University Bloomington, MORE

hasPresident →

Michael McRobbie

President of Indiana University

president.iu.edu

Michael Alexander McRobbie AO is an Australian-American computer scientist, educator and academic administrator. He became the eighteenth president of Indiana University on July 1, 2007. Wikipedia

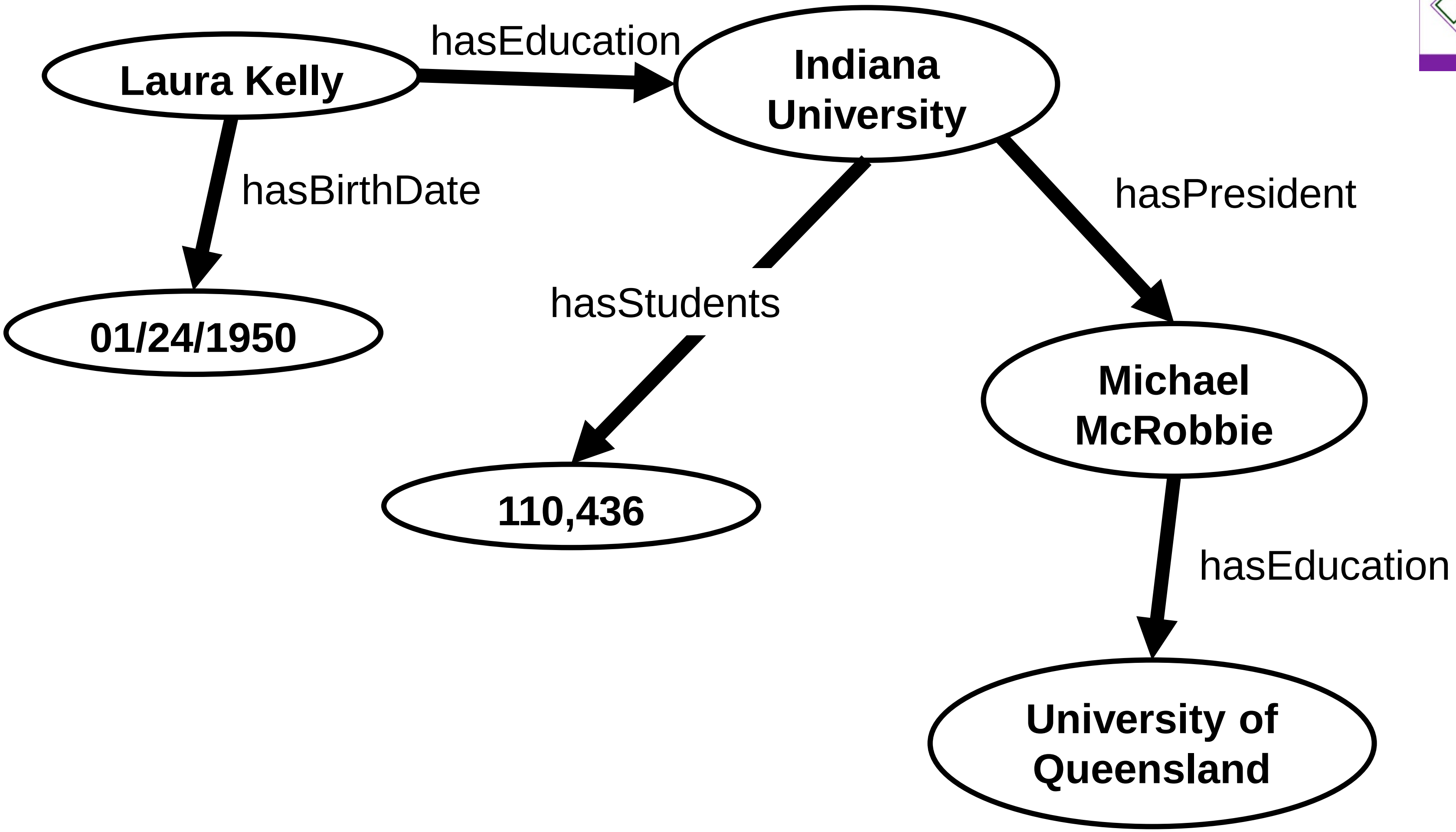
Born: October 11, 1950 (age 69 years), Melbourne, Australia

Spouse: Laurie Burns (m. 2005)

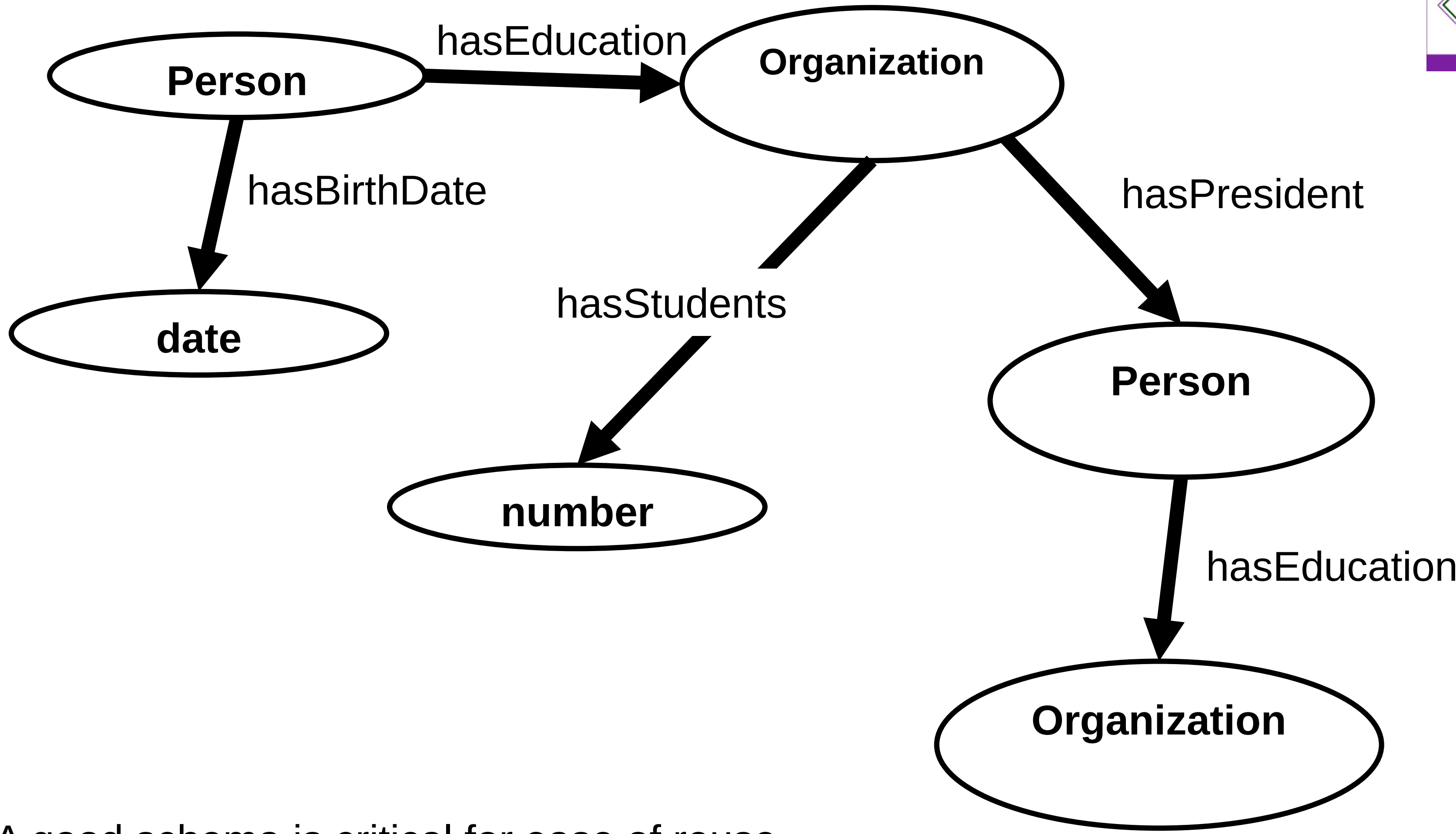
Education: The Australian National University, The University of Queensland

Books: Automated Theorem-proving in Non-classical Logics, Automated Deduction - Cade-13

Knowledge Graphs

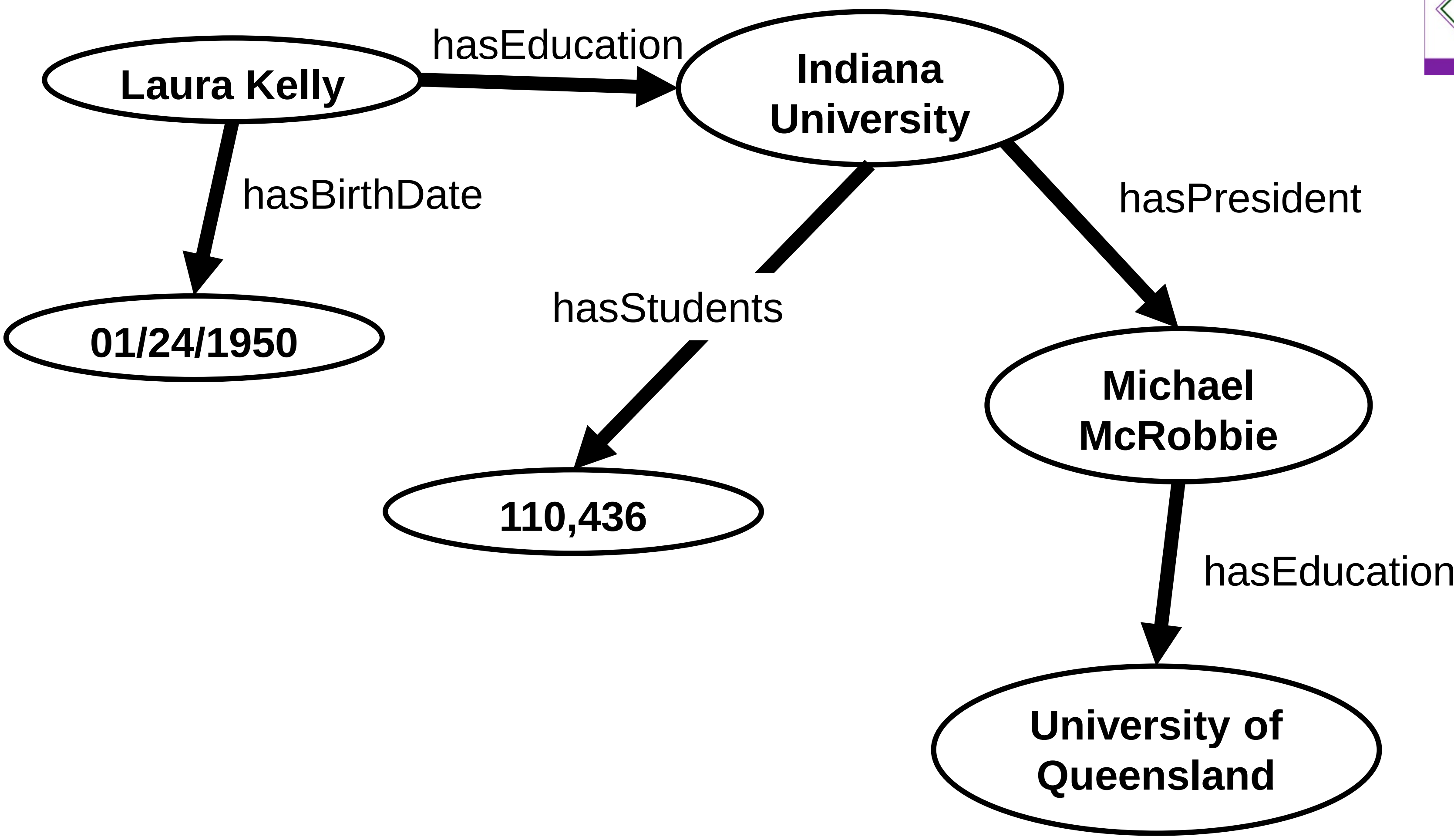


Schema (as diagram)



A good schema is critical for ease of reuse

This is not a good Knowledge Graph!



W3C Standards

W3C Recommendation

RDF 1.1 Concepts and Abstract Syntax

W3C Recommendation 25 February 2014

This version:
http://www.w3.org/TR/2014/REC-rdf11-concepts-20140225/
Latest published version:
http://www.w3.org/TR/rdf11-concepts/
Previous version:
http://www.w3.org/TR/2014/PR-rdf11-concepts-20140109/
Previous Recommendation:
http://www.w3.org/TR/rdf-concepts
Editors:
Richard Cyganiak, DERI, NUI Galway
David Wood, 3 Round Stones
Markus Lanthaler, Graz University of Technology

Both established 2004
as versions 1.0.

W3C Recommendation

OWL 2 Web Ontology Language Primer (Second Edition)

W3C Recommendation 11 December 2012

This version:
http://www.w3.org/TR/2012/REC-owl2-primer-20121211/
Latest version (series 2):
http://www.w3.org/TR/owl2-primer/
Latest Recommendation:
http://www.w3.org/TR/owl-primer
Previous version:
http://www.w3.org/TR/2012/PER-owl2-primer-20121018/
Editors:
Pascal Hitzler, Wright State University
Markus Krötzsch, University of Oxford
Bijan Parsia, University of Manchester
Peter F. Patel-Schneider, Nuance Communications
Sebastian Rudolph, FZI Research Center for Information

PRACTICE

Industry-Scale Knowledge Graphs: Lessons and Challenges

By Natasha Noy, Yuqing Gao, Anshu Jain, Anant Narayanan, Alan Patterson, Jamie Taylor

Communications of the ACM, August 2019, Vol. 62 No. 8, Pages 36-43
10.1145/3331166

Comments

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Credit: Adempercem / Stutterstock

Knowledge graphs are critical to many enterprises today: They provide the structured data and factual knowledge that drive many products and make them more intelligent and "magical."

In general, a knowledge graph describes objects of interest and connections between them. For example, a knowledge graph may have nodes for a movie, the actors in this movie, the director, and so on. Each node may have properties such as an actor's name and age. There may be nodes for multiple movies involving a particular actor. The user can then traverse the knowledge graph to collect information on all the movies in which the actor appeared or, if applicable, directed.

Many practical implementations impose constraints on the links in knowledge graphs by defining a *schema* or *ontology*. For example, a link from a movie to its director must connect an object of type Movie to an object of type Person. In some cases the links themselves might have their own properties: a link connecting an actor and a movie might have the name of the specific role the actor

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Back to:

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AAAI-MAKE 2021

[25]: Makni, Hendler, SWJ 2019

[10]: Eberhart, Ebrahimi, Zhou, Shimizu, Hitzler, AAAI-MAKE 2020

[20]: Hohenecker, Lukasiewicz, JAIR 2020

[6]: Bianchi, Hitzler, AAAI-MAKE 2019

(new): Ebrahimi, Eberhart, Hitzler, June 2021

Deep Reasoners Overview

1. RDFS via Memory Networks (classification) [12].
2. RDFS via Pointer Networks (generative) (new).
3. EL+ via LSTMs (generative) [10].
4. EL+ via Pointer networks (new).
5. LTNs for first-order predicate logic [6].

- Monireh Ebrahimi, Aaron Eberhart, Federico Bianchi, Pascal Hitzler, Towards Bridging the Neuro-Symbolic Gap: Deep Deductive Reasoners. Applied Intelligence 51 (9), 6326-6348, 2021.
  [covers 6,10,12]

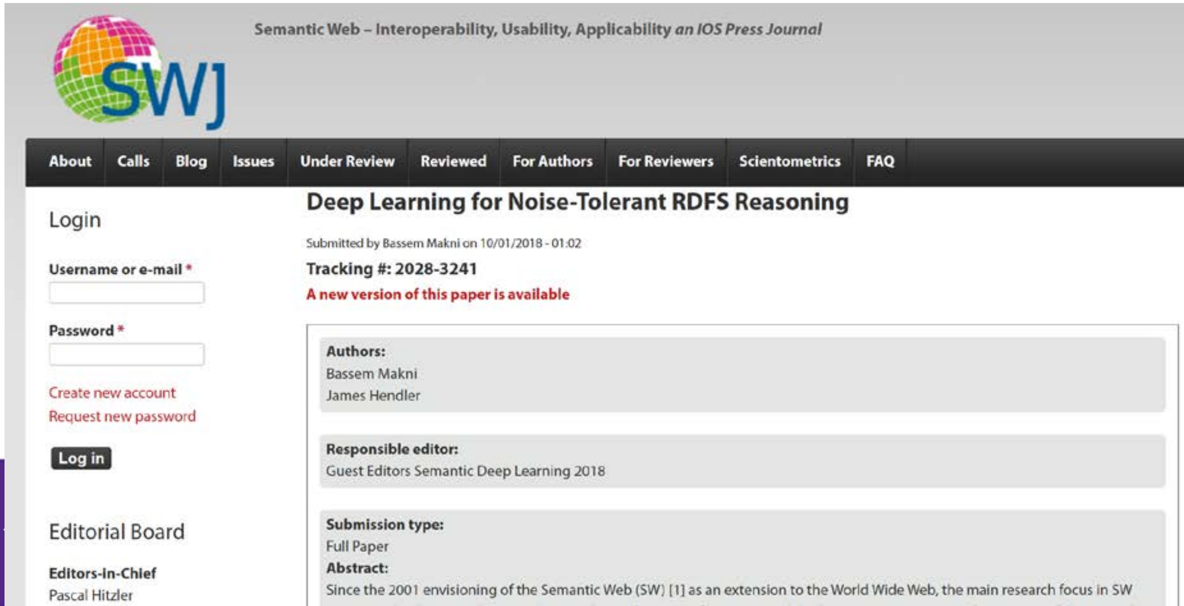
RDFS Reasoning using Memory Networks

Monireh Ebrahimi, Md Kamruzzaman Sarker, Federico Bianchi, Ning Xie,
Aaron Eberhart, Derek Doran, Hyeongsik Kim, Pascal Hitzler,
Neuro-Symbolic Deductive Reasoning for Cross-Knowledge Graph Entailment.
In: Proc. AAAI-MAKE 2021.

additional analysis by Sulogna Chowdhury, Aaron Eberhart
and Brayden Pankaskie

RDF reasoning

- Essentially, RDF reasoning is Datalog reasoning restricted to:
  - Unary and binary predicates only.
  - A fixed set of rules that are not facts.
- You can try the following:
  - Use a vector embedding for one RDF graph.
  - Create all logical consequences.
  - Throw n% of them away.
  - Use the rest to train a DL system.
  - Check how many of those you threw away can be recovered this way.



RDF reasoning

- The problem with the approach just described:
  – It works only with that graph.

- What you'd really like to do is:
  – Train a deep learning system so that you can present a new, unseen graph to it, and it can correctly derive the deductively inferred triples.

- Note:
  – You don't know the IRIs in the graph up front. The only overlap may or may not be the IRIs in the rdf/s namespace.
  – You don't know up front how "deep" the reasoning needs to be.
  – There is no lack of training data, it can be auto-generated.

RDF reasoning

- [Note: RDF is one of the simplest useful knowledge representation languages that is not propositional.]

- Think knowledge graph.
- Think node-edge-node triples such as

BarackObama	rdf:type	President
BarackObama	husbandOf	MichelleObama
President	rdfs:subClassOf	Human
husbandOf	rdfs:subPropertyOf	spouseOf

- Then there is a (fixed, small) set of inference rules, such as

  rdf:type(x,y) AND rdfs:subClassOf(y,z)THEN rdf:type(x,z)

Representation

- Goal is to be able to reason over unseen knowledge graphs. I.e. the out-of-vocabulary problem needs addressing.

- Normalization of vocabulary (i.e., it becomes shared vocabulary across all input knowledge graphs.
- One vocabulary item becomes a one-hot vector (dimension d, number of normalized vocabulary terms)
- One triple becomes a 3 x d matrix.
- The knowledge graph becomes an n x 3 x d tensor (n is the number of knowledge graph triples)

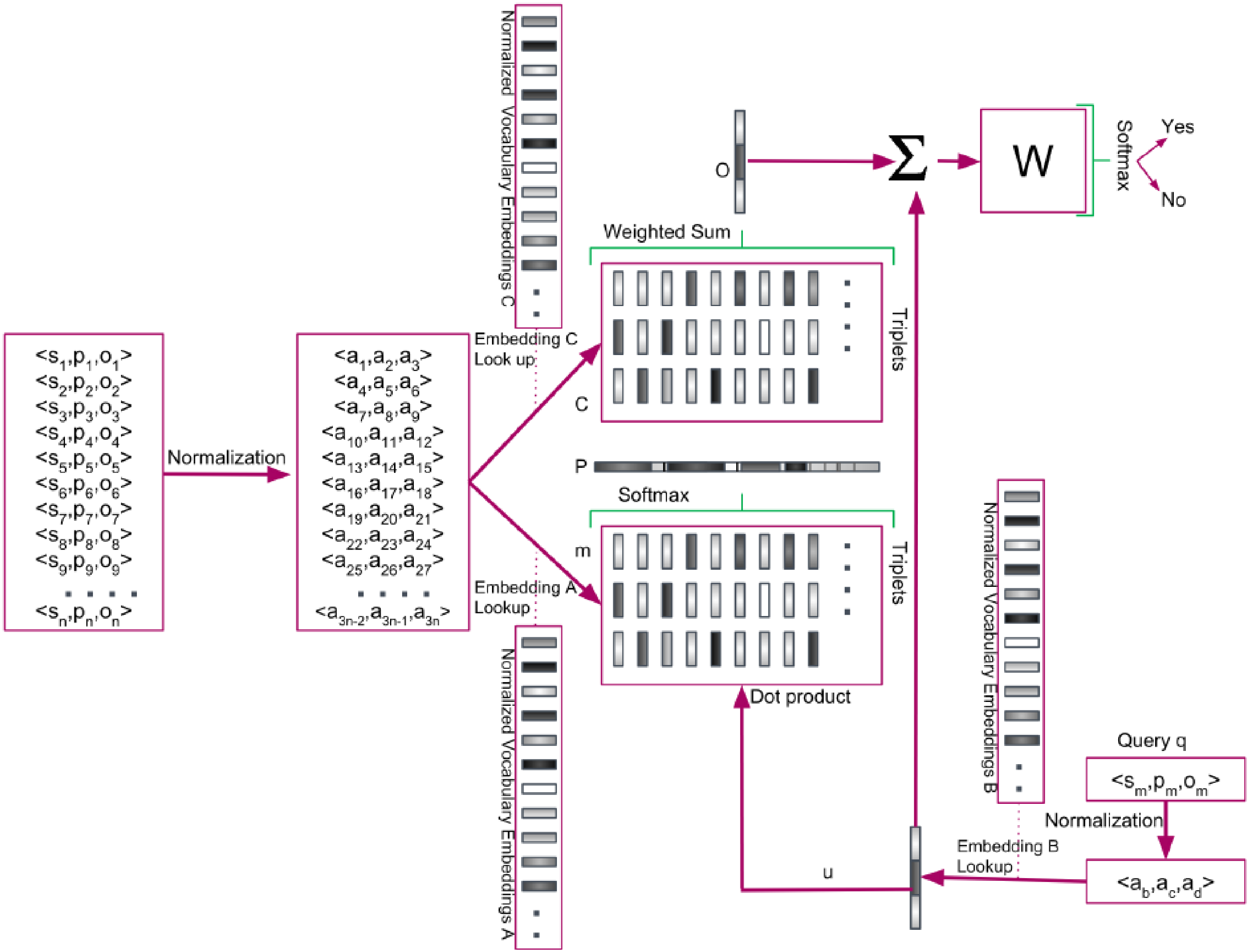
- Knowledge graph is stored in “memory”

Mechanics

- **An attention mechanism retrieves memory slots useful for finding the correct answer to a query.**
- **These are combined with the query and run through a (learned) matrix to retrieve a new (processed) query.**

- **This is repeated (in our experiment with 10 “hops”).**
- **The final out put is a yes/no answer to the query.**

Memory Network based on MemN2N



Experiments: Performance

Test Dataset	#KG	Base						Inferred						Invalid
		#Facts	#Ent.	%Class	%Indv	%R.	%Axiom.	#Facts	#Ent.	%Class	%Indv	%R.	%Axiom.	#Facts
OWL-Centric	2464	996	832	14	19	3	0	494	832	14	0.01	1	20	462
Linked Data	20527	999	787	3	22	5	0	124	787	3	0.006	1	85	124
OWL-Centric Test Set	21	622	400	36	41	3	0	837	400	36	3	1	12	476
Synthetic Data	2	752	506	52	0	1	0	126356	506	52	0	1	0.07	700

Table 2: Statistics of various datasets used in experiments

Baseline: non-normalized embeddings, same architecture

Training Dataset	Test Dataset	Valid Triples Class			Invalid Triples Class			Accuracy
		Precision	Recall /Sensitivity	F-measure	Precision	Recall /Specificity	F-measure	
OWL-Centric Dataset	Linked Data	93	98	96	98	93	95	**96**
OWL-Centric Dataset (90%)	OWL-Centric Dataset (10%)	88	91	89	90	88	89	**90**
OWL-Centric Dataset	OWL-Centric Test Set [b]	79	62	68	70	84	76	**69**
OWL-Centric Dataset	Synthetic Data	65	49	40	52	54	42	**52**
OWL-Centric Dataset	Linked Data [a]	54	98	70	91	16	27	86
OWL-Centric Dataset [a]	Linked Data [a]	62	72	67	67	56	61	91
OWL-Centric Dataset(90%) [a]	OWL-Centric Dataset(10%) [a]	79	72	75	74	81	77	80
OWL-Centric Dataset	OWL-Centric Test Set [ab]	58	68	62	62	50	54	58
OWL-Centric Dataset [a]	OWL-Centric Test Set [ab]	77	57	65	66	82	73	73
OWL-Centric Dataset	Synthetic Data [a]	70	51	40	47	52	38	51
OWL-Centric Dataset [a]	Synthetic Data [a]	67	23	25	52	80	62	50
Baseline								
OWL-Centric Dataset	Linked Data	73	98	83	94	46	61	43
OWL-Centric Dataset (90%)	OWL-Centric Dataset (10%)	84	83	84	84	84	84	82
OWL-Centric Dataset	OWL-Centric Test Set [b]	62	84	70	80	40	48	61
OWL-Centric Dataset	Synthetic Data	35	41	32	48	55	45	48

[a] More Tricky Nos & Balanced Dataset
[b] Completely Different Domain.

Table 3: Experimental results of proposed model

Experiments: Reasoning Depth

Test Dataset	Hop 0			Hop 1			Hop 2			Hop 3			Hop 4			Hop 5			Hop 6			Hop 7			Hop 8			Hop 9			Hop 10		
	P	R	F	P	R	F	P	R	F	P	R	F	P	R	F	P	R	F	P	R	F	P	R	F	P	R	F	P	R	F	P	R	F
Linked Data[a]	0	0	0	80	99	88	89	97	93	77	98	86	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Linked Data[b]	2	0	0	82	91	86	89	98	93	79	100	88	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
OWL-Centric[c]	19	5	9	31	75	42	78	80	78	48	47	44	4	34	6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Synthetic	32	46	33	31	87	38	66	55	44	25	45	32	29	46	33	26	46	33	25	46	33	25	46	33	24	43	31	25	43	31	22	36	28

[a] LemonUby Ontology
[b] Agrovoc Ontology
[c] Completely Different Domain

Table 4: Experimental results over each reasoning hop

Dataset	Hop 1	Hop 2	Hop 3	Hop 4	Hop 5	Hop 6	Hop 7	Hop 8	Hop 9	Hop 10
OWL-Centric[a]	8%	67%	24%	0.01%	0%	0%	0%	0%	0%	0%
Linked Data[b]	31%	50%	19%	0%	0%	0%	0%	0%	0%	0%
Linked Data[c]	34%	46%	20%	0%	0%	0%	0%	0%	0%	0%
OWL-Centric[d]	5%	64%	30%	1%	0%	0%	0%	0%	0%	0%
Synthetic Data	0.03%	1.42%	1%	1.56%	3.09%	6.03%	11.46%	20.48%	31.25%	23.65%

[a] *Training Set*
[b] LemonUby Ontology
[c] Agrovoc Ontology
[d] Completely Different Domain

Table 5: Data distribution per knowledge graph over each reasoning hop

Training time: just over a full day

Generative RDFS Reasoning using Pointer Networks

Monireh Ebrahimi, Aaron Eberhart, Pascal Hitzler
On the Capabilities of Pointer Networks for Deep Deductive Reasoning
https://arxiv.org/abs/2106.09225

Pointer Networks

DaSe Lab

- **Pointer Networks 'point' to input elements!**

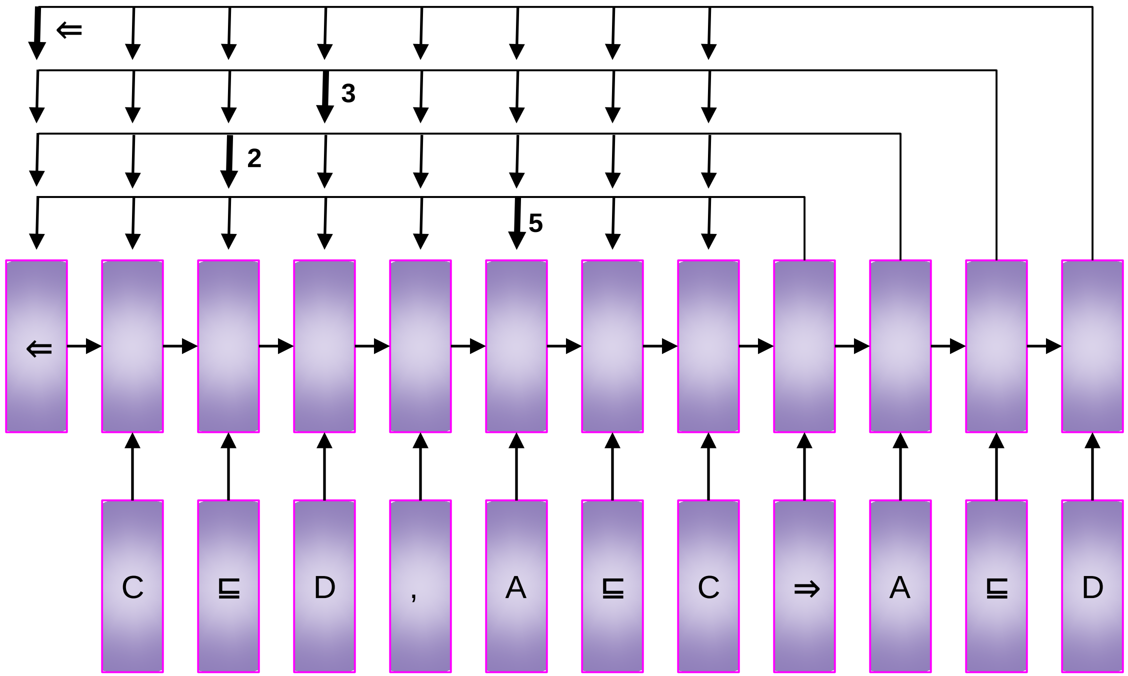
- **Ptr-Net approach specifically targets problems whose outputs are discrete and correspond to positions in the input.**

- **At each time step, the distribution of the attention is the answer!**

- **Application:**
  - **NP-hard Travelling Salesman Problem (TSP)**
  - **Delaunay Triangulation**
  - **Convex Hull**
  - **Text Summarization**
  - **Code completion**
  - **Dependency Parsing**

Pointer Networks for Reasoning

- **To mimic human reasoning behaviour where one can learn to choose a set of symbols in different locations and copy these symbols to suitable locations to generate new logical consequences based on a set of predefined logical entailment rules**



$$C \sqsubseteq D, A \sqsubseteq C \mapsto A \sqsubseteq D$$

Results without transfer

Logic	KG Size	Pointer Networks		Transformer			LSTM
		SubWordText	Tokenizer	Normalized	Not-Normalized		
					SubWordText	Tokenizer	
RDF	3 - 735	87%	99%	5%	25%	4%	0.17%

- On RDF, slightly outperforms [Hendler Makni SWJ 2019] approach.
- Our approach is a more straightforward application.
- Evaluation is on the same dataset.

Results with transfer

DaSe Lab

Table 6 Exact Match Accuracy Results for Transfer Learning/Representation: SubWord-Text Tokenization Encoding

Train \ Test	LUBM	Awards	University
LUBM	*	75%	78%
Awards	79%	*	77%
University	81%	82%	*

Table 7 Exact Match Accuracy Results for Transfer Learning/ Representation: Whitespace Tokenization Encoding

Train \ Test	LUBM	Awards	University
LUBM	*	61%	47%
Awards	96%	*	84%
University	82%	88%	*

Completion Reasoning Emulation for the Description Logic EL+

Aaron Eberhart, Monireh Ebrahimi, Lu Zhou, Cogan Shimizu, Pascal Hitzler, Completion Reasoning Emulation for the Description Logic EL+.
In: Andreas Martin, Knut Hinkelmann, Hans-Georg Fill, Aurona Gerber, Doug Lenat, Reinhard Stolle, Frank van Harmelen (eds.), Proceedings of the AAAI 2020 Spring Symposium on Combining Machine Learning and Knowledge Engineering in Practice, AAAI-MAKE 2020, Palo Alto, CA, USA, March 23-25, 2020, Volume I.

EL+ is essentially OWL 2 EL

$CX \sqsubseteq CY$
$CX \sqcap CY \sqsubseteq CZ$
$CX \sqsubseteq \exists RY.CZ$
$\exists RX.CY \sqsubseteq CZ$
$RX \sqsubseteq RY$
$RX \circ RY \sqsubseteq RZ$

Table 2: $\mathcal{EL}^+$ Completion Rules

(1)	$A \sqsubseteq C$	$C \sqsubseteq D$		$\models A \sqsubseteq D$
(2)	$A \sqsubseteq C_1$	$A \sqsubseteq C_2$	$C_1 \sqcap C_2 \sqsubseteq D$	$\models A \sqsubseteq D$
(3)	$A \sqsubseteq C$	$C \sqsubseteq \exists R.D$		$\models A \sqsubseteq \exists R.D$
(4)	$A \sqsubseteq \exists R.B$	$B \sqsubseteq C$	$\exists R.C \sqsubseteq D$	$\models A \sqsubseteq D$
(5)	$A \sqsubseteq \exists S.D$	$S \sqsubseteq R$		$\models A \sqsubseteq \exists R.D$
(6)	$A \sqsubseteq \exists R_1.C$	$C \sqsubseteq \exists R_2.D$	$R_1 \circ R_2 \sqsubseteq R$	$\models A \sqsubseteq \exists R.D$

Table 1: $\mathcal{EL}^+$ Semantics

Description	Expression	Semantics
Individual	a	$a \in \Delta^{\mathcal{I}}$
Top	$\top$	$\Delta^{\mathcal{I}}$
Bottom	$\bot$	$\emptyset$
Concept	C	$C^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$
Role	R	$R^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$
Conjunction	$C \sqcap D$	$C^{\mathcal{I}} \cap D^{\mathcal{I}}$
Existential Restriction	$\exists R.C$	$\{ a \mid \text{there is } b \in \Delta^{\mathcal{I}} \text{ such that } (a,b) \in R^{\mathcal{I}} \text{ and } b \in C^{\mathcal{I}} \}$
Concept Subsumption	$C \sqsubseteq D$	$C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$
Role Subsumption	$R \sqsubseteq S$	$R^{\mathcal{I}} \subseteq S^{\mathcal{I}}$
Role Chain	$R_1 \circ \cdots \circ R_n \sqsubseteq R$	$R_1^{\mathcal{I}} \circ \cdots \circ R_n^{\mathcal{I}} \subseteq R^{\mathcal{I}}$

with $\circ$ signifying standard binary composition

Support

	New Fact	Rule	Support
Step 1	$C1 \sqsubseteq C3$	(1)	$C1 \sqsubseteq C2, C2 \sqsubseteq C3$
	$C1 \sqsubseteq C4$	(4)	$C1 \sqsubseteq C2, C1 \sqsubseteq \exists R1.C1, \exists R1.C2 \sqsubseteq C4$
	$C1 \sqsubseteq \exists R1.C3$	(3)	$C1 \sqsubseteq C2, C2 \sqsubseteq \exists R1.C3$
	$C1 \sqsubseteq \exists R2.C1$	(5)	$C1 \sqsubseteq \exists R1.C1, R1 \sqsubseteq R2$
	$C1 \sqsubseteq \exists R4.C4$	(6)	$C1 \sqsubseteq \exists R1.C1, R1 \circ R3 \sqsubseteq R4, C1 \sqsubseteq \exists R3.C4$
Step 2	$C1 \sqsubseteq C5$	(2)	$C3 \sqcap C4 \sqsubseteq C5, C1 \sqsubseteq C2, C2 \sqsubseteq C3, C1 \sqsubseteq C2, C1 \sqsubseteq \exists R1.C1, \exists R1.C2 \sqsubseteq C4$

Architecture

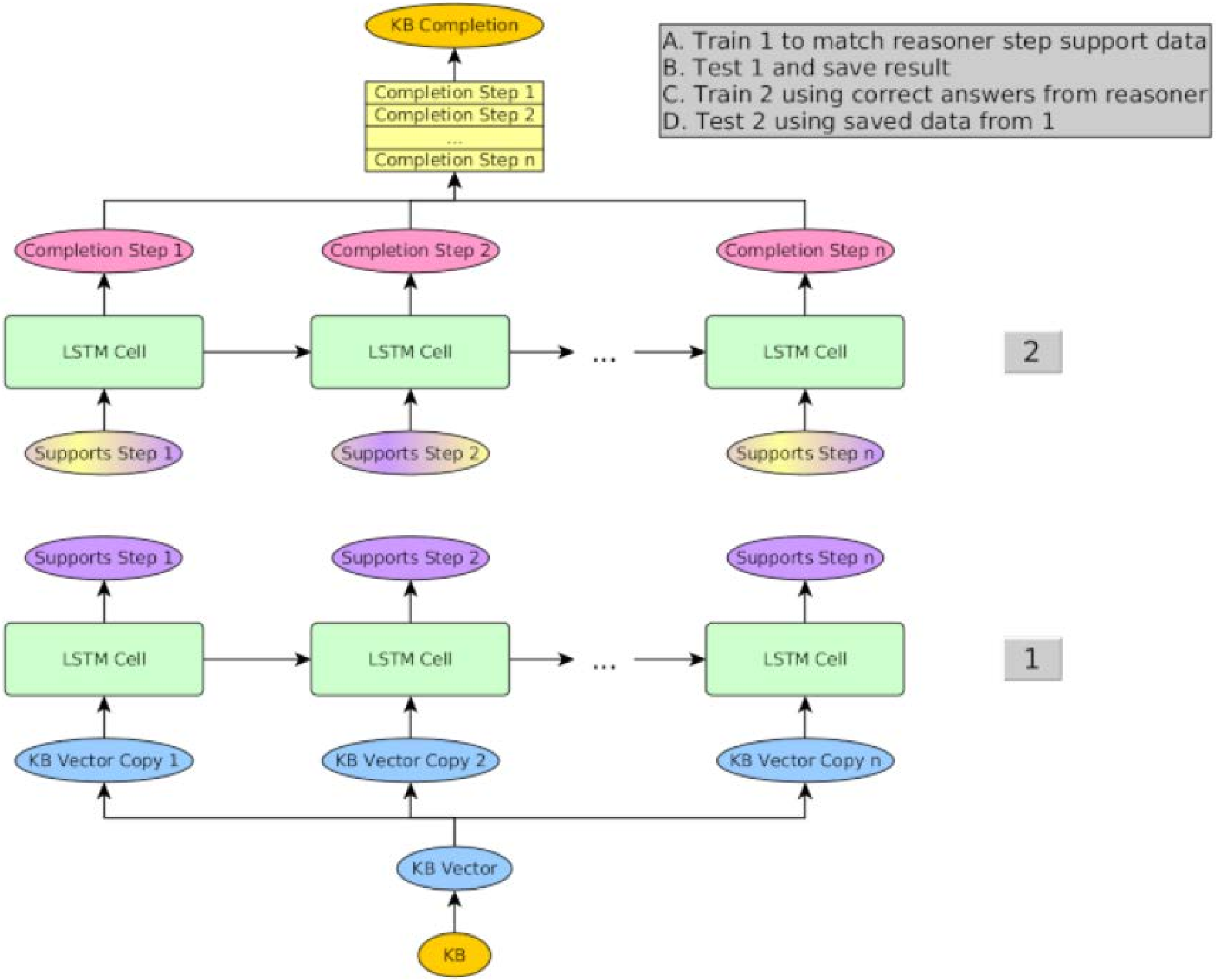


Figure 2: Piecewise Architecture

Architecture

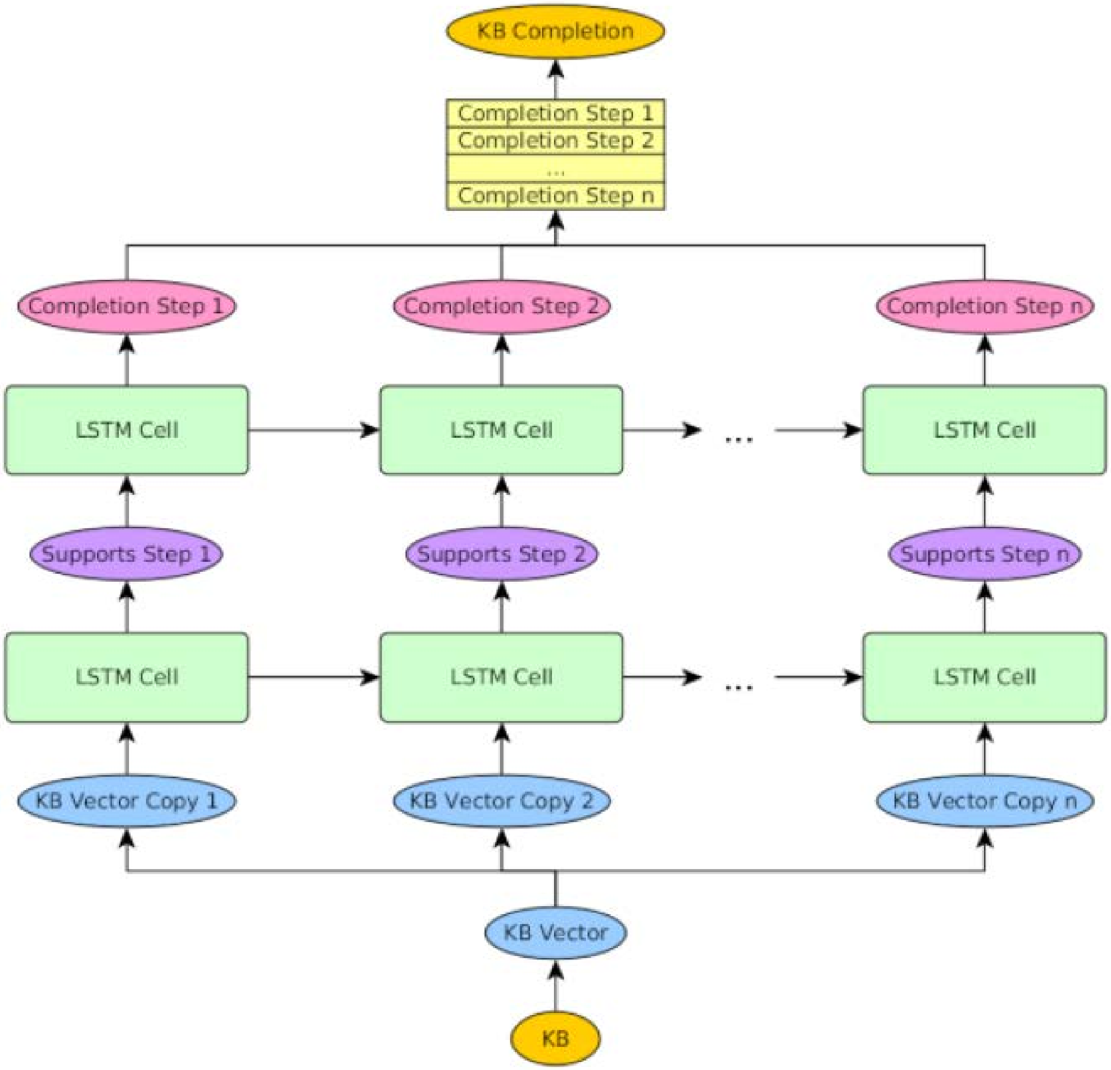


Figure 3: Deep Architecture

Architecture

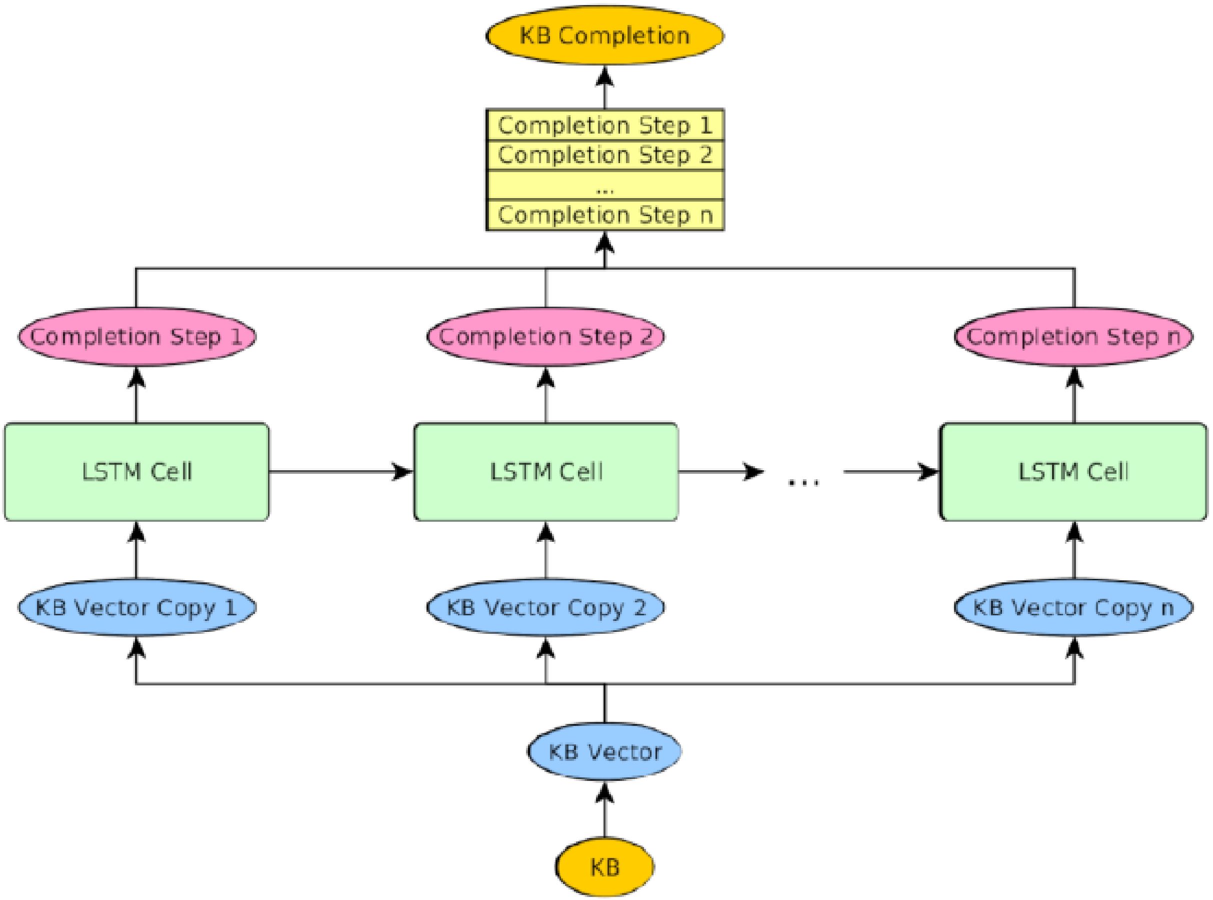


Figure 4: Flat Architecture

Encoding

KB statement		Vectorization
$CX \sqsubseteq CY$	$\rightarrow$	$[0.0, \frac{X}{c}, \frac{Y}{c}, 0.0]$
$CX \sqcap CY \sqsubseteq CZ$	$\rightarrow$	$[\frac{X}{c}, \frac{Y}{c}, \frac{Z}{c}, 0.0]$
$CX \sqsubseteq \exists RY.CZ$	$\rightarrow$	$[0.0, \frac{X}{c}, \frac{-Y}{r}, \frac{Z}{c}]$
$\exists RX.CY \sqsubseteq CZ$	$\rightarrow$	$[\frac{-X}{r}, \frac{Y}{c}, \frac{Z}{c}, 0.0]$
$RX \sqsubseteq RY$	$\rightarrow$	$[0.0, \frac{-X}{r}, \frac{-Y}{r}, 0.0]$
$RX \circ RY \sqsubseteq RZ$	$\rightarrow$	$[\frac{-X}{r}, \frac{-Y}{r}, \frac{-Z}{r}, 0.0]$

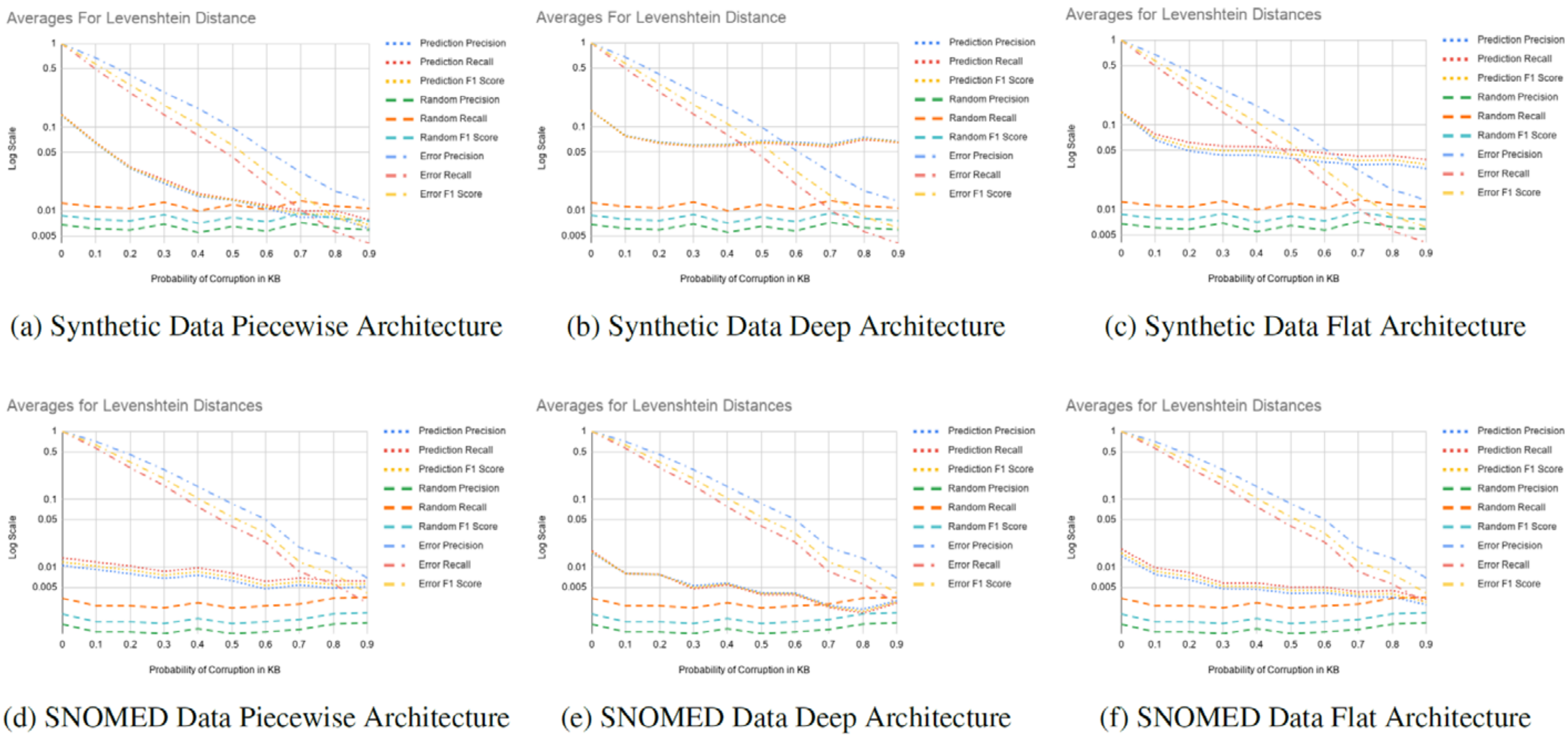
c = Number of Possible Concept Names
r = Number of Possible Role Names

Results

Table 7: Average Precision Recall and F1-score For each Distance Evaluation

	Atomic Levenshtein Distance			Character Levenshtein Distance			Predicate Distance		
	Precision	Recall	F1-score	Precision	Recall	F1-score	Precision	Recall	F1-score
	Synthetic Data								
Piecewise Prediction	0.138663	0.142208	0.140412	0.138663	0.142208	0.140412	0.138646	0.141923	0.140264
Deep Prediction	**0.154398**	**0.156056**	**0.155222**	**0.154398**	**0.156056**	**0.155222**	**0.154258**	**0.155736**	**0.154993**
Flat Prediction	0.140410	0.142976	0.141681	0.140410	0.142976	0.141681	0.140375	0.142687	0.141521
Random Prediction	0.010951	0.0200518	0.014166	0.006833	0.012401	0.008811	0.004352	0.007908	0.007908
	SNOMED Data								
Piecewise Prediction	0.010530	0.013554	0.011845	0.010530	0.013554	0.011845	0.010521	0.013554	0.011839
Deep Prediction	**0.015983**	0.0172811	**0.016595**	**0.015983**	0.017281	**0.016595**	**0.015614**	0.017281	**0.016396**
Flat Prediction	0.014414	**0.018300**	0.016112	0.0144140	**0.018300**	0.016112	0.013495	**0.018300**	0.015525
Random Prediction	0.002807	0.006803	0.003975	0.001433	0.003444	0.002023	0.001769	0.004281	0.002504

Noisy data

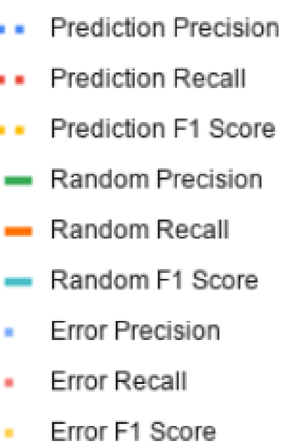


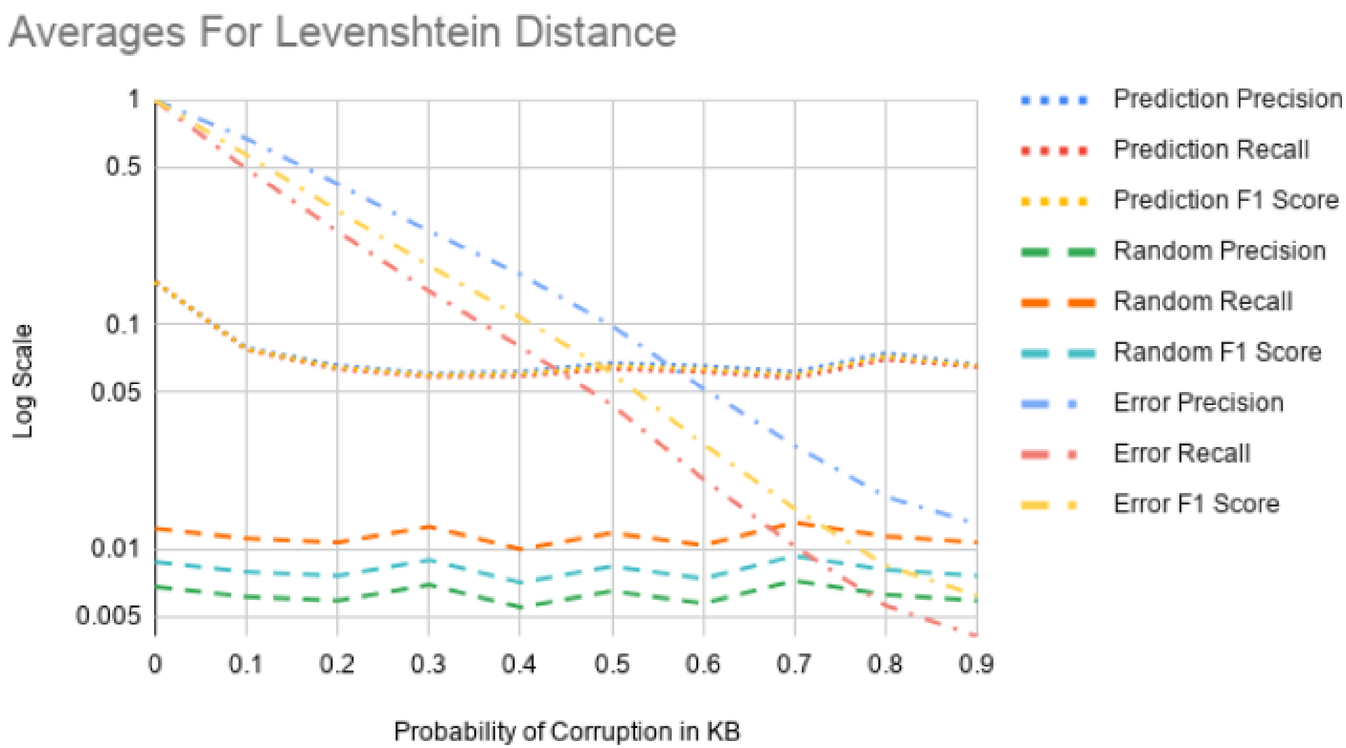
(a) Synthetic Data Piecewise Architecture (b) Synthetic Data Deep Architecture (c) Synthetic Data Flat Architecture

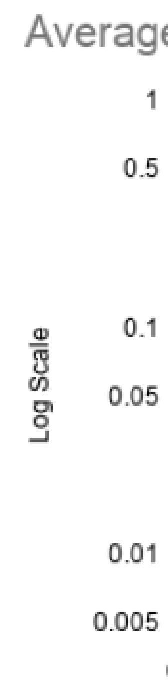
(d) SNOMED Data Piecewise Architecture (e) SNOMED Data Deep Architecture (f) SNOMED Data Flat Architecture

Figure 8: Character Levenshtein Distance Precision, Recall, and F1-score

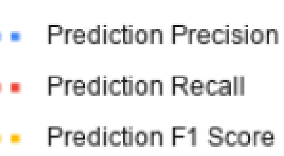
Noisy data

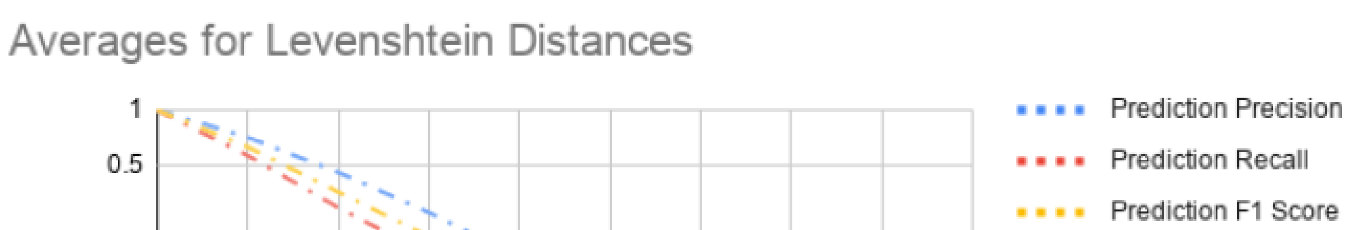


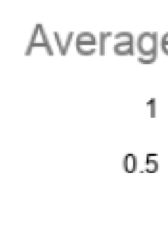




hitecture (b) Synthetic Data Deep Architecture (c







Generative EL Reasoning using Pointer Networks

Monireh Ebrahimi, Aaron Eberhart, Pascal Hitzler
On the Capabilities of Pointer Networks for Deep Deductive Reasoning
https://arxiv.org/abs/2106.09225

Results with transfer

Logic	KG Size	Pointer Networks		Transformer			LSTM
		SubWordText	Tokenizer	Normalized	Not-Normalized		
					SubWordText	Tokenizer	
[redacted]							
ER	40	73%	**73%**	8%	8%	0.4 %	0%
	50	68%	**68%**	11%	11%	0.3%	0%
	120	49%	**49%**	15%	NA	NA	0%

- **same architecture as before**

The Deductive Capability of Logic Tensor Networks

Federico Bianchi, Pascal Hitzler, On the Capabilities of Logic Tensor Networks for Deductive Reasoning. In: Andreas Martin et al. (eds.), Proceedings of the AAAI 2019 Spring Symposium on Combining Machine Learning with Knowledge Engineering (AAAI-MAKE 2019) Stanford University, Palo Alto, California, USA, March 25-27, 2019, Stanford University, Palo Alto, California, USA, March 25-27, 2019. CEUR Workshop Proceedings 2350, CEUR-WS.org 2019.

Logic Tensor Networks

Based on Neural Tensor Networks.

Logic Tensor Networks are due to Serafini and Garcez (2016). They have been used for image analysis under background knowledge.

Their capabilities for deductive reasoning have not been sufficiently explored.

Underlying logic: First-order predicate, fuzzyfied.

Every language primitive becomes a vector/matrix/tensor.

Terms/Atoms/Formulas are embedded as corresponding tensor/matrix/vector multiplications over the primitives.

Embeddings of primitives are learned s.t. the truth values of all formulas in the given theory are maximized.

A-priori Limitations

- Not clear how to adapt this such that you can transfer to unseen input theories.

- Scalability is an issue.

- While apparently designed for deductive reasoning, the inventors hardly report on this issue.

Transitive closure

- $\forall a,b,c \in A : (sub(a,b) \wedge sub(b,c)) \rightarrow sub(a,c)$
- $\forall a \in A : \neg sub(a,a)$
- $\forall a,b : sub(a,b) \rightarrow \neg sub(b,a)$

Satisfiability	MAE	Matthews	F1	Precision	Recall
0.99	**0.12** (0.12)	**0.58** (0.45)	**0.64** (0.51)	**0.60** (0.47)	0.68 (0.55)
0.56	0.51 (0.52)	0.09 (0.06)	0.27 (0.20)	0.20 (0.11)	**0.95** (0.93)
Random	0.50 (0.50)	0.00 (0.00)	0.22 (0.17)	0.14 (0.10)	0.50 (0.50)

parentheses: only newly entailed part of KB
MAE: mean absolute error;
Matthews: Matthews coefficient (for unbalanced classes)
top: top performing model, layer size and embeddings: 20, mean aggregator

Bottom: one of the worst performing models.

Multi-hop inferences difficult.

More take-aways from experiments

- **Error decreases with increasing satisfiability.**

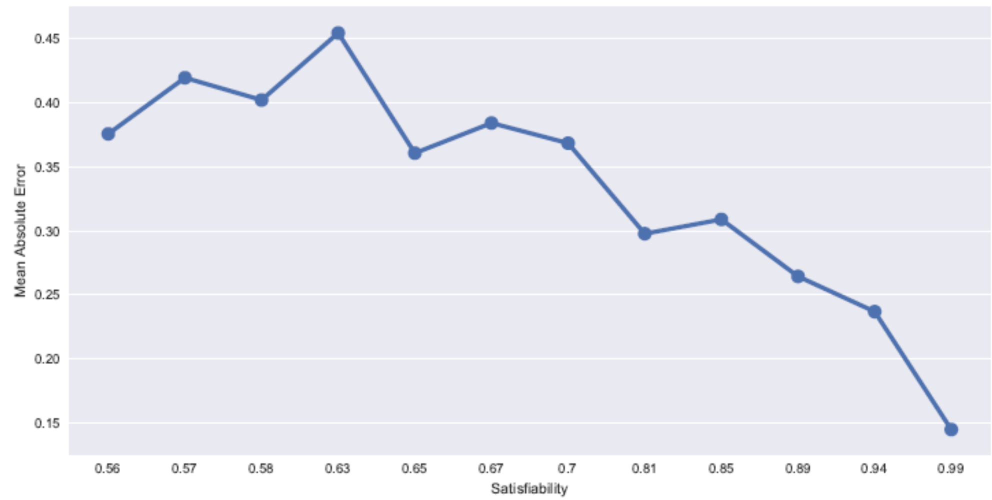


Figure 3: Average MAE for the ancestors tasks on rounded level of satisfiability. MAE decreases with the increase of satisfiability.

- **Adding redundant formulas to the input KB decreases error.**

Type	MAE	Matthews	F1	Precision	Recall
Six Axioms	0.16 (0.17)	0.73 (0.61)	0.77 (0.62)	0.64 (0.47)	**0.96** (0.92)
Eight Axioms	**0.14** (0.14)	**0.83** (0.69)	**0.85** (0.72)	**0.80** (0.66)	0.89 (0.79)

More take-aways from experiments

DaSe Lab

- **Higher arity of predicates significantly increases learning time.**

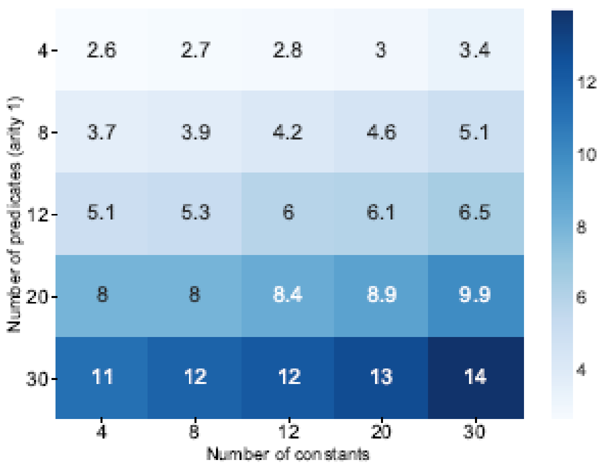


Figure 5: Computational times in seconds for predicates of arity one and constants

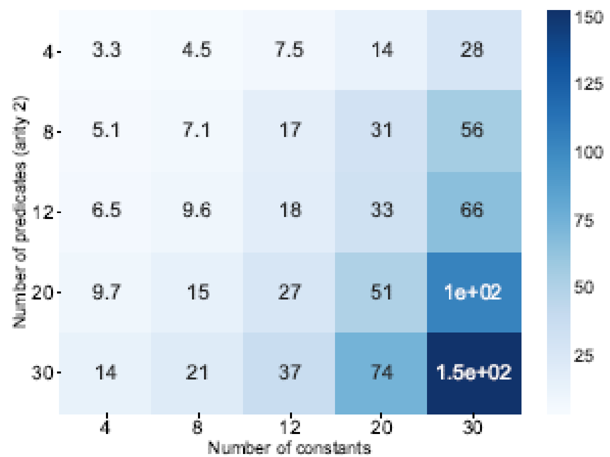


Figure 6: Computational times in seconds for predicates of arity two and constants

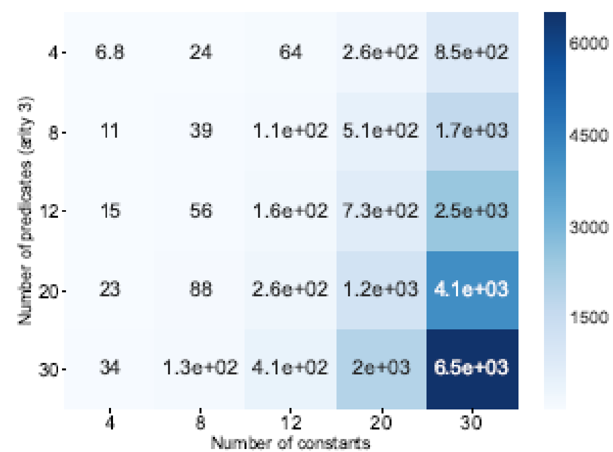


Figure 7: Computational times in seconds for predicates of arity three and constants

More take-aways from experiments

- Model seems to often end up in local minima. This may be addressable using known approaches.
- LTNs seem to predict many false positives, while they are better regarding true negatives. This may be just because of the test knowledge bases we used, but needs to be looked at.
- Overfitting is a problem, but it doesn't seem straightforward to address this for LTNs. [e.g. cross-validation may need completeness information, which may bias the network]
- Increasing layers and embedding size makes optimizing parameters much more difficult.

- Hence, there's a path for more investigations, we're only starting to understand this.

Conclusions

Conclusions

- **Bridging the neuro-symbolic gap is still a major quest.**
- **Research on Deep Deductive Reasoning is at the heart of neuro-symbolic Artificial Intelligence**
- **Research is needed to push the envelope with respect to core aspects such as**
  - **more complex logics**
  - **higher reasoning accuracy**
  - **better transfer**
  - **scalability**

Thanks!

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Thanks!