

### **Knowledge Graphs in Neuro-Symbolic Al**



#### **Pascal Hitzler**

Data Semantics Laboratory (DaSe Lab) Kansas State University

http://www.daselab.org



### **Neuro-symbolic Al**

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; <u>https://arxiv.org/abs/2105.05330</u> for more analysis.



Explainable Graph-Based ML @ AKBC, October 2021

DaSe Lab

#### 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.





- 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.





KANSAS STATE

IVERSI



**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

KANSAS STATE

IVERS

- 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



**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?

KANSAS STATE

IVERS

- Endow connectionist systems with symbolic components?
- Add connectionist learning to symbolic reasoners?



### 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.





Knowledge Graphs for eXplainable Artificial Intelligence: Foundations, Applications and Challenges

### KANSAS STATE



## **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	$\log ic$	$\operatorname{transfer}$	generative	scale	performance	DaSe Lab
[12]	RDFS	yes	no	moderate	$\operatorname{high}$	×
[25]	RDFS	no	yes	low	$\operatorname{high}$	
[10]	$\mathcal{EL}^+$	yes	no	$\mathbf{moderate}$	low	
[20]	OWL RL	no*	no	low	$\operatorname{high}$	
[6]	FOL	no	yes	very low	$\operatorname{high}$	
(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

## KANSAS STATE



## **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



DaSe Lab

### Google Knowledge Graph

UNIVERSITY



### **Knowledge Graphs**





### Schema (as diagram)





#### W3C Standards

RDF 1.1 Concepts and Abstract S	Synta	X
W3C Recommendation 25 February 201	4	
This version: http://www.w3.org/TR/2014/REC-rdf11-concepts-20 Latest published version: http://www.w3.org/TR/rdf11-concepts/ Previous version: http://www.w3.org/TR/2014/PR-rdf11-concepts-201 Previous Recommendation: http://www.w3.org/TR/rdf10-concepts-201	0140225/ 140109/	<u>[</u>
Editors:	Ę	
David Wood, <u>3 Round Stones</u> Markus Lanthaler, <u>Graz University of Technology</u>	ndatio	Pri
Poth octablished 2004	Rec	This
as versions 1.0.	M3C	Lates
		Lates
		Prev
		Edito

#### KANSAS STATE UNIVERSITY

**Explainab** 

# DaSe Lab

#### VL 2 Web Ontology Language mer (Second Edition)

#### C Recommendation 11 December 2012

version:

http://www.w3.org/TR/2012/REC-owl2-primer-20121211/

st version (series 2):

http://www.w3.org/TR/owl2-primer/

st Recommendation:

http://www.w3.org/TR/owl-primer

ious version:

http://www.w3.org/TR/2012/PER-owl2-primer-20121018/ ors:

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



## 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

VIEW AS: 🚊 📋 🏟 🔂	SHARE: 🖂	🚭 획 🔟	
------------------	----------	-------	--



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

#### SIGN IN for Full Access User Name Password » Forgot Password?

» Create an ACM Web Account

SIGN IN

#### ARTICLE CONTENTS: Introduction What's In a Graph? Design Decisions Challenges Ahead Other Key Challenges Conclusion References Authors

#### MORE NEWS & OPINIONS

MIT Robot Could Help People



Back to:

## **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.



### Published deep deductive reasoning work

paper	$\log ic$	$\operatorname{transfer}$	generative	scale	performance	DaSe Lab
[12]	RDFS	yes	no	moderate	$\operatorname{high}$	×
[25]	RDFS	no	yes	low	$\operatorname{high}$	
[10]	$\mathcal{EL}^+$	yes	no	$\mathbf{moderate}$	low	
[20]	OWL RL	no*	no	low	$\operatorname{high}$	
[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

## KANSAS STATE



## **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

- [Note: RDF is one of the simplest useful knowledge representation languages that is not propositional.]
- Think knowledge graph.
  - Think node-edge-node triples such asBarackObama rdf:typePresidentBarackObama husbandOfMichelleObamaPresidentrdfs:subClassOfhusbandOfrdfs:subPropertyOf
- 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)



•



### **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.

KANSAS STATE

UNIVERSITY





### **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:

KANSAS STATE

IVERSI

- 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.



### Representation

KANSAS STATE

IVERSI

- 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**

[			Base					Inferred				Invalid		
Test Dataset	#KG	HUnster	Easts   #East   @Class   @Indu   @D   @Axiom				HEaster HEast Of Change of Lader Of D					filvanu #Easta		
		#Pacts	#Ent.	%Class	%INOV	%K.	%AX10III.	#Pacts	#Ent.	%Class	%Indv	%K.	%AX10M.	#Pacts
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		ass	Inv	alid Triples C	lass	Accuracy
Training Dataset	Test Dataset	Precision	Recall /Sensitivity	F-measure	Precision	Recall /Specificity	F-measure	Accuracy
OWL Centric Dataset	Linked Data	03	08	06	08	03	05	96
OWL-Centric Dataset	OWL Cratric Dataset (100)	95	90	90	90	95	95	90
OwL-Centric Dataset (90%)	OwL-Centric Dataset (10%)	66	91	89	90	88	89	90
OWL-Centric Dataset	OWL-Centric Test Set <sup>b</sup>	79	62	68	70	84	76	69
OWL-Centric Dataset	Synthetic Data	65	49	40	52	54	42	52
OWL-Centric Dataset	Linked Data <sup>a</sup>	54	98	70	91	16	27	86
OWL-Centric Dataset a	Linked Data <sup>a</sup>	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 <sup>a</sup>	70	51	40	47	52	38	51
OWL-Centric Dataset a	Synthetic Data <sup>a</sup>	67	23	25	52	80	62	50
		B	aseline					
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

<sup>a</sup> More Tricky Nos & Balanced Dataset

<sup>b</sup> Completely Different Domain.

Table 3: Experimental results of proposed model



## 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**

• 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









Logic	KG Size	Pointer Networ	ks				
		SubWordText	Tokenizer	Normalized	Not-Norm	LSTM	
		Subword lext	TOKEHIZEI	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.





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

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







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

Description	Expression	Semantics
Individual	a	$a \in \Delta^{\mathcal{I}}$
Тор	Т	$\Delta^{\mathcal{I}}$
Bottom	$\perp$	Ø
Concept	C	$C^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$
Role	R	$R^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}  imes \Delta^{\mathcal{I}}$
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	$R_1 \circ \cdots \circ R_n \sqsubseteq R$	$R_1^{\mathcal{I}} \circ \dots \circ R_n^{\mathcal{I}} \subseteq R^{\mathcal{I}}$

with o signifying standard binary composition



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

	Atomic I	Atomic Levenshtein Distance			.evenshteii	n Distance	Prec	licate Dista	ance
	Precision	Recall	F1-score	Precision	Recall	F1-score	Precision	Recall	F1-score
				Syı	nthetic Dat	a			
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
				SN	OMED Da	ta			
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





## 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





	KG Size	Pointer Networ	ks				
Logic		SubWordText	Tokenizer	Normalized	Not-Norm	LSTM	
					SubWordText	Tokenizer	
	40	73%	73%	8%	8%	0.4 %	0%
ER	50	68%	68%	11%	11%	0.3%	0%
	120	49%	49%	15%	NA	NA	0%

• same architecture as before





## Explaining Deep Learning via Symbolic Background Knowledge

Md. Kamruzzaman Sarker, Ning Xie, Derek Doran, Michael Raymer, Pascal Hitzler, Explaining Trained Neural Networks with Semantic Web Technologies: First Steps. In: Tarek R. Besold, Artur S. d'Avila Garcez, Isaac Noble (eds.), Proceedings of the Twelfth International Workshop on Neural-Symbolic Learning and Reasoning, NeSy 2017, London, UK, July 17-18, 2017. CEUR Workshop Proceedings 2003, CEUR-WS.org 2017

Md Kamruzzaman Sarker, Pascal Hitzler, Efficient Concept Induction for Description Logics. In: The Thirty-Third AAAI Conference on Artificial Intelligence, AAAI 2019, The Thirty-First Innovative Applications of Artificial Intelligence Conference, IAAI 2019, The Ninth AAAI Symposium on Educational Advances in Artificial Intelligence, EAAI 2019, Honolulu, Hawaii, USA, January 27 – February 1, 2019. AAAI Press 2019, pp. 3036-3043.

Md Kamruzzaman Sarker, Joshua Schwartz, Pascal Hitzler, Lu Zhou, Srikanth Nadella, Brandon Minnery, Ion Juvina, Michael L. Raymer, William R. Aue, Wikipedia Knowledge Graph for Explainable AI. In: Boris Villazón-Terrazas, Fernando Ortiz-Rodríguez, Sanju M. Tiwari, Shishir K. Shandilya (eds.), Knowledge Graphs and Semantic Web. Second Iberoamerican Conference and First Indo-American Conference, KGSWC 2020, Mérida, Mexico, November 26-27, 2020, Proceedings. Communications in Computer and Information Science, vol. 1232, Springer, Heidelberg, 2020, pp. 72-87.

### KANSAS STATE

### **Explainable Al**

• Explain behavior of trained (deep) NNs.



- Idea:
  - Use background knowledge in the form of linked data and ontologies to help explain.
  - Link inputs and outputs to background knowledge.
  - Use a symbolic learning system to generate an explanatory theory.

• We have key components for this now, but it's still early stages.



#### Concept





## **DL-Learner** [Lehmann, Hitzler]

Approach similar to inductive logic programming, but using Description Logics (the logic underlying OWL).

**Positive examples:** 

KANSAS STATE

UNIVERSITY

negative examples:



- ᠈ᢩᢩᢩ᠐᠋ᢩ᠆ᢣᢩᠵᡝ᠊ᢩ᠘ᢩ᠘᠆᠋ᢩᡌᢆ᠆ᡱ
- ᠈᠂┎╤┰╌ᢩᢩᢙ᠆ᡶᢩ᠐ᢩ᠆ᠮᡛ᠆ᡱ
- ▖▐▆ᡰ᠊ᢒᡄ᠊ᠮᡨ᠆ᡧ᠆ᡛᡛ᠊ᡱ
- ᠈ᢆᢩᢙᡗ᠊ᢩᠧ᠋ᢩᠴ᠆ᢩ᠘᠘ᢩᡰ᠊ᢆᡛ᠋ᢩ᠆ᡱ

2.

₄ୣୢ୲୰ଽ୳ୣ⊒୳ୖୖୣୖୖୖୖୖ

₅ <u>Loohtoh</u>

Task: find a class description (logical formula) which separates positive and negative examples.





#### **DL-Learner**

**Positive examples:** 

- ▖▐ਰᢪҤᡱᡱᠲᡱᠣᡖᡰ᠊ᢆᠿᠼ
- ᠈ᢩᡂ᠆ᢣᢩᠳ᠆ᢩ᠘ᢩ᠘᠊ᢩᡛ
- ᠈᠂┎╤┰╌ᢩᢩᢙ᠆ᡶᢩᢩ᠐᠊ᡰ᠊ᡛᡛ᠆ᡱ
- ▖└═┟╱╗╁┻╣╲╬╱╶╠╧╝
- ᠈ᢩᢩᢩᡋ᠆ᢩ<del>ᡄᢩ</del>ᢩᠴ᠆ᢩᡰᢩᢩᢩᢩᢣ᠆ᢩᡛ

**DL-Learner result:** 

∃hasCar.(Closed⊓Short)

In FOL:

$$\{x \mid \exists y(\operatorname{hasCar}(x, y) \land \operatorname{Closed}(y) \land \operatorname{Short}(y))\}\$$



negative examples:

- ᠈᠂᠋ᢅᡎ᠁᠁ᡝᢩ᠘ᢩ᠘ᡃ᠊ᢩᡶᢒᢩ᠘ᡰᢆᢓᠴ᠋
- ▖৻ᢩᢩ᠘᠊ᡗᢩ᠊᠋᠊᠊ᢩᠴ
- · \ulertertertert





### **ECII** algorithm and system



 We thus implemented our own system, ECII (Efficient Concept Induction from Instances) which trades some correctness for speed. [Sarker, Hitzler, AAAI-19]

Experiment Name	Number of	Runtime (sec)				Accuracy $(\alpha_3)$		Accuracy $\alpha_2$				
	Logical Axioms	DLa	DL FIC(1) <sup>b</sup>	DL FIC(2) <sup>c</sup>	ECII DF <sup>d</sup>	ECII KCT <sup>e</sup>	DLa	ECII DF <sup>d</sup>	DL FIC(1) <sup>b</sup>	DL FIC(2) <sup>c</sup>	ECII DF <sup>d</sup>	ECII KCT <sup>e</sup>
Yinyang_examples	157	0.065	0.0131	0.019	0.089	0.143	1.000	0.610	1.000	1.000	0.799	1.000
Trains	273	0.01	0.020	0.047	0.05	0.095	1.000	1.000	1.000	1.000	1.000	1.000
Forte	341	2.5	1.169	6.145	0.95	0.331	0.965	0.642	0.875	0.875	0.733	1.000
Poker	1,368	0.066	0.714	0.817	1	0.281	1.000	1.000	0.981	0.984	1.000	1.000
Moral Reasoner	4,666	0.1	3.106	4.154	5.47	6.873	1.000	0.785	1.000	1.000	1.000	1.000
ADE20k I	4,714	577.3 <sup>t</sup>	4.268	31.887	1.966	23.775	0.926	0.416	0.263	0.814	0.744	1.000
ADE20k II	7,300	983.4 <sup>t</sup>	16.187	307.65	20.8	293.44	1.000	0.673	0.413	0.413	0.846	0.900
ADE20k III	12,193	4,500 <sup>g</sup>	13.202	263.217	51	238.8	0.375	0.937	0.375	0.375	0.930	0.937
ADE20k IV	47,468	4,500 <sup>g</sup>	93.658	523.673	116	423.349	0.375	NA	0.608	0.608	0.660	0.608

a DL : DL-Learner

<sup>b</sup> DL FIC (1) : DL-Learner fast instance check with runtime capped at execution time of ECII DF

° DL FIC (2): DL-Learner fast instance check with runtime capped at execution time of ECII KCT

d ECII DF : ECII default parameters

e ECII KCT : ECII keep common types and other default parameters

f Runtimes for DL-Learner were capped at 600 seconds.

<sup>8</sup> Runtimes for DL-Learner were capped at 4,500 seconds.



#### **ECII vs. DL-Learner**



IV



Figure 1: Runtime comparison between DL-Learner and ECII. The vertical scale is logarithmic in hundredths of seconds, and note that DL-Learner runtime has been capped at 4.500 seconds for ADE20k III and IV. For ADE20k I it was capped at each run at 600 seconds.

Figure 2: Accuracy  $(\alpha_3)$  comparison between DL-Learner and ECII. For ADE20k IV it was not possible to compute an accuracy score within 3 hours for ECII as the input ontology was too large.

#### KANSAS STATE UNIVERSITY

## **Proof of Concept Experiment**





**Negative:** 







le Graph-Based ML @ AKBC, October 2021

#### Images



#### Come from the MIT ADE20k dataset <u>http://groups.csail.mit.edu/vision/datasets/ADE20K/</u> They come with annotations of objects in the picture:

001 # 0 # 0 # sky # sky # ""
002 # 0 # 0 # road, route # road # ""
005 # 0 # 0 # sidewalk, pavement # sidewalk # ""
006 # 0 # 0 # building, edifice # building # ""
007 # 0 # 0 # truck, motortruck # truck # ""
008 # 0 # 0 # hovel, hut, hutch, shack, shanty # hut # ""
009 # 0 # 0 # pallet # pallet # ""
001 # 1 # 0 # door # door # ""
002 # 1 # 0 # window # window # ""



## KANSAS STATE

### Mapping to SUMO

Simple approach: for each known object in image, create an individual for the ontology which is in the appropriate SUMO class:

contains road1 contains window1 contains door1 contains wheel1 contains sidewalk1 contains truck1 contains box1 contains building1







### **SUMO**

- Suggested Merged Upper Ontology
   <u>http://www.adampease.org/OP/</u>
- Approx. 25,000 common terms covering a wide range of domains
- Centrally, a relatively naïve class hierarchy.
- Objects in image annotations became individuals (constants), which were then typed using SUMO classes.





#### **Positive:**



- img1: road, window, door, wheel, sidewalk, truck, box, building
- img2: tree, road, window, timber, building, lumber
- img3: hand, sidewalk, clock, steps, door, face, building, window, road

**Negative:** 

- img4: shelf, ceiling, floor
- img5: box, floor, wall, ceiling, product
- img6: ceiling, wall, shelf, floor, product

**DL-Learner results include:** 

∃contains.Transitway ∃contains.LandArea



### **Proof of Concept Experiment**



K

HI HE

**Negative:** 





Icontains.Transitway Le Graph-Base Icontains.LandArea

#### **Experiment 5**

DaSe Lab

#### Positive:



#### Negative (selection):









#### $\exists contains.BodyOfWater$





## Wikipedia KG (WKG) : Breaking Cycle

Lost Significant Information

- 50% of the subclass relation
- 50% of the class assertion



Number of entities/facts	SUMO	DBpedia	Wikipedia cyclic	Wikipedia noncyclic
Concepts	4558	1183	1,901,708	$1,\!860,\!342$
Individuals	86,475	1	$6,\!145,\!050$	6,079,748
Object property	778	1144	2	2
Data property	0	1769	0	0
Axioms	$175,\!208$	7228	$71,\!344,\!252$	39,905,216
Class assertion axioms	167381	1	57,335,031	27,991,282
Subclass axioms	5330	769	$5,\!962,\!463$	3,973,845

### KANSAS STATE

### Mapping with Knowledge Graph

#### Model: Resnet-50

#### Data:

image p1: machinery, wall, desk, shelf, pigeonhole, box, projector, computer, screen, monitor, book

image p2: .... image p3: ....

image n1: lumber, sky, road, sidewalk, building, box, window, hutch

image n2: ..... image n3: .....

#### Mapping:

P1 imageContains machinery machinery subClassof DurableGood

•••••











Test images. **Workroom** as positive examples  $p_1$ ,  $p_2$ ,  $p_3$  on the left, **Warehouse** as negative examples  $n_1$ ,  $n_2$ ,  $n_3$  on the right (from top).

KANSAS STATE

## Evaluation : Knowledge Graph in XAI

#### Workroom Explanations

SUMO

- ∃contains.(DurableGood □ ¬ForestProduct) •
- ∃contains.(DurableGood □ ¬Lumber) •
- ∃contains.Entity

#### Wikipedia

- ∃contains.(Wrenches □ Tools □ ¬Lumber) •
- ∃contains.(Mechanicaltools □ ¬Lumber) •
- ∃contains.(Mechanicaltools □ ¬Sky) •











Test images. **Workroom** as positive examples p<sub>1</sub>, p<sub>2</sub>, p<sub>3</sub> on the left, **Warehouse** as negative examples  $n_1$ ,  $n_2$ ,  $n_3$  on the right (from top).

#### Market Explanations

SUMO

- ∃contains.SentientAgent Wikipedia
- ∃contains.(Structure □ Life )

#### Mountain Explanations SUMO

- ∃contains.BodyOfWater

#### Wikipedia

contains.((Life  $\sqcap$  Branches of botany)  $\sqcap$ (Nature))

#### KANSAS STATE UNIVERSITY

### Evaluation : Knowledge Graph in XAI

- Wikipedia Knowledge graph producing better coverage score.
  - Reason behind this is the large number of concepts it has.

Experiment name	#Images	#Positive images	Wikipedia		SUMO	
			#Solution	Coverage	#Solution	Coverage
Market vs. WorkRoom and wareHouse	96	37	286	.72	240	.72
Mountain vs. Market and workRoom	181	85	195	.61	190	.53
OutdoorWarehouse vs. IndoorWarehouse	55	3	128	.94	102	.89
Warehouse vs. Workroom	59	55	268	.56	84	.24
Workroom vs. Warehouse	59	4	128	.93	93	.84



### KANSAS STATE



## Conclusions



### Conclusions

• Bridging the neuro-symbolic gap is still a major quest.



- Research is needed to push the envelope with respect to core aspects such as
  - more complex logics
  - higher reasoning accuracy
  - better transfer
  - scalability
- Knowledge Graphs can explain system behavior by means of background knowledge.
  - Key challenges include
    - knowledge graph selection
    - scalability

KANSAS STATE

IVERSI





# Thanks!





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

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

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, Neural-Symbolic Learning and Reasoning: A Survey and Interpretation. https://arxiv.org/abs/1711.03902 (2017)

Md Kamruzzaman Sarker, Lu Zhou, Aaron Eberhart, Pascal Hitzler Neuro-Symbolic Artificial Integration: Current Trends Al Communications, to appear.



DaSe Lab

Federico Bianchi, Pascal Hitzler, On the Capabilities of Logic Tensor Networks for Deductive Reasoning. In: Andreas Martin, Knut Hinkelmann, Aurona Gerber, Doug Lenat, Frank van Harmelen, Peter Clark (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.

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.



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.

DaSe Lab

Bassem Makni, James Hendler, Deep learning for noise-tolerant RDFS reasoning. Semantic Web 10(5): 823-862 (2019)

Monireh Ebrahimi, Aaron Eberhart, Pascal Hitzler, On the Capabilities of Pointer Networks for Deep Deductive Reasoning. June 2021. https://arxiv.org/abs/2106.09225

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

Pascal Hitzler, Federico Bianchi, Monireh Ebrahimi, Md Kamruzzaman Sarker, Neural-Symbolic Integration and the Semantic Web. Semantic Web 11 (1), 2020, 3-11.



DaSe Lab

Federico Bianchi, Matteo Palmonari, Pascal Hitzler, Luciano Serafini, Complementing Logical Reasoning with Sub-symbolic Commonsense. In: Paul Fodor, Marco Montali, Diego Calvanese, Dumitru Roman, Rules and Reasoning - Third International Joint Conference, RuleML+RR 2019, Bolzano, Italy, September 16-19, 2019, Proceedings. Lecture Notes in Computer Science 11784, Springer 2019, pp. 161-170.

Sebastian Bader, Pascal Hitzler, Dimensions of neural-symbolic integration – a structured survey. In: S. Artemov, H. Barringer, A. S. d'Avila Garcez, L. C. Lamb and J. Woods (eds). We Will Show Them: Essays in Honour of Dov Gabbay, Volume 1. International Federation for Computational Logic, College Publications, 2005, pp. 167-194.

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



DaSe Lab

Md. Kamruzzaman Sarker, Ning Xie, Derek Doran, Michael Raymer, Pascal Hitzler, Explaining Trained Neural Networks with Semantic Web Technologies First Steps. In: Tarek R. Besold, Artur S. d'Avila Garcez, Isaac Noble (eds.), Proceedings of the Twelfth International Workshop on Neural-Symbolic Learning and Reasoning, NeSy 2017, London, UK, July 17-18, 2017. CEUR Workshop Proceedings 2003, CEUR-WS.org 2017

Md Kamruzzaman Sarker, Pascal Hitzler, Efficient Concept Induction for Description Logics. In: The Thirty-Third AAAI Conference on Artificial Intelligence, AAAI 2019, The Thirty-First Innovative Applications of Artificial Intelligence Conference, IAAI 2019, The Ninth AAAI Symposium on Educational Advances in Artificial Intelligence, EAAI 2019, Honolulu, Hawaii, USA, January 27 – February 1, 2019. AAAI Press 2019, pp. 3036-3043.

Md Kamruzzaman Sarker, Joshua Schwartz, Pascal Hitzler, Lu Zhou, Srikanth Nadella, Brandon Minnery, Ion Juvina, Michael L. Raymer, William R. Aue, Wikipedia Knowledge Graph for Explainable AI. In: Boris Villazón-Terrazas, Fernando Ortiz-Rodríguez, Sanju M. Tiwari, Shishir K. Shandilya (eds.), Knowledge Graphs and Semantic Web. Second Iberoamerican Conference and First Indo-American Conference, KGSWC 2020, Mérida, Mexico, November 26-27, 2020, Proceedings. Communications in Computer and Information Science, vol. 1232, Springer, Heidelberg, 2020, pp. 72-87.





# Thanks!

