

# Knowledge Graphs, Explainable Deep Learning, and What They Have To Do With Each Other

#### **Pascal Hitzler**

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### **Data Semantics Lab**





January 2018 – University of Denver – Pascal Hitzler

### Some Data

- From Germany, dual citizen. PhD in Ireland (in Mathematics)
- Wright State University since 2009.
   Assistant Professor 2009-2012
   Associate Professor 2012-2015
   (Full) Professor since 2015
   Endowed NCR Distinguished Professor since 2016
- Over 400 publications
- Over 8,000 Google Scholar citations
- Previous graduate students and postdocs now at (selection): TU Dresden, Germany
   UG Athens
   U Bonn, Germany
   UN Lisboa, Portugal
   UN Headquarters New York
   GE Global Research
   Nuance
   etc.



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- Redesigned discrete math sequence for computer scientists with focus on underprepared students, and increased their retention rate from 6% to 24%.
- Most of my classes have an additional distance learning section.
- I am teaching most of my classes as flipped classrooms.
- I received specific funding from my host institution for my teaching innovations.



### **Textbook: Syntax & Semantics**

Pascal Hitzler, Markus Krötzsch, Sebastian Rudolph

Foundations of Semantic Web Technologies

Chapman & Hall/CRC, 2010

Choice Magazine Outstanding Academic Title 2010 (one out of seven in Information & Computer Science)



Foundations of Semantic Web Technologies

> Pascal Hitzler Markus Krötzsch Sebastian Rudolph

CRC Press classification

### http://www.semantic-web-book.org



### Semantic Web journal

- EiCs: Pascal Hitzler Krzysztof Janowicz
- Funded 2010

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- 2017 Impact factor of 2.889, top (with 1.3 distance) of all journals with "Web" in the title
- We very much welcome contributions at the "rim" of traditional Semantic Web research – e.g., work which is strongly inspired by a different field.
- Non-standard (open & transparent) review process.



# http://www.semantic-web-journal.net/



# **Knowledge Graphs**





### Theresa May

British Prime Minister



tmay.co.uk

Theresa Mary May is a British politician who has served as Prime Minister of the United Kingdom and Leader of the Conservative Party since July 2016, the second woman to hold both positions. Wikipedia

Born: October 1, 1956 (age 60), Eastbourne, United Kingdom

Height: 5' 8"

Party: Conservative Party

Spouse: Philip May (m. 1980)

Education: St Hugh's College, Oxford (1974 - 1977)

Previous offices: Home Secretary (2010-2016), MORE ~

#### Profiles

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### St Hugh's College, Oxford \*

Website

College in Oxford. England

Directions

St Hugh's College is one of the constituent colleges of the University of Oxford, It is located on a 14.5-acre site on St Margaret's Road, to the north of the city centre. Wikipedia

Address: St Margaret's Rd, Oxford OX2 6LE, UK

Principal: Elish Angiolini Phone: +44 1865 274900 Founder: Elizabeth Wordsworth Founded: 1886 Named for: Hugh of Lincoln Undergraduates: 432 (2011-2012)

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Reviews from the web

4.1/5 University Rooms · 2,310 votes

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#### Notable alumni

View 40+



Theresa

Mav





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### Hugh of Lincoln

Saint

Hugh of Lincoln, also known as Hugh of Avalon, was a French noble, Benedictine and Carthusian monk, bishop of Lincoln in the Kingdom of England, and Catholic saint. Wikipedia

Born: 1140, Avalon, France

Died: November 16, 1200, London, United Kinadom

Feast: 16 November (R.C.C.): 17 November (Anglican)

Major shrine: Lincoln Cathedral

Attributes: a white swan

Patronage: sick children, sick people, shoemakers and swans

#### People also search for



Little Saint

Huah of

Lincoln



Thomas More

William Howard. 1st Visco...

enver -





Suu Kvi

Barbara Castle

#### From <a href="https://www.nitrd.gov/news/Open\_Knowledge\_Network.aspx">https://www.nitrd.gov/news/Open\_Knowledge\_Network.aspx</a>:

Starting in July 2016, the <u>Big Data Interagency Working Group (BD IWG</u>) leadership has been involved in two meetings to discuss the viability, and possible first steps to creating a joint public/private open data network infrastructure, the Open Knowledge Network (OKN). The vision of OKN is to create an open knowledge graph of all known entities and their relationships, ranging from the macro (have there been unusual clusters of earthquakes in the US in the past six months?) to the micro (what is the best combination of chemotherapeutic drugs for a 56 y/o female with stage 3 glioblastoma and an FLT3 mutation but no symptoms of AML?). OKN is meant to be an inclusive, open, community activity resulting in a knowledge infrastructure that could facilitate and empower a host of applications and open new research avenues including how to create trustworthy knowledge networks/graphs.



- Often, a hype is created because something new has been established.
- In this case, the hype is often over before the technology has really matured to the level of application development.

 The current knowledge graph hype is different. Because there was already a pre-maturity hype 15 years ago, under a different name ...



### Schema.org

- Collaboratively launched in 2011 by Google, • Microsoft, Yahoo, Yandex. 2011: 297 classes, 187 relations 2015: 638 classes, 965 relations
- Simple schema, request to web site providers to • annotate their content with schema.org markup. Promise: They will make better searches based on this.
- 2015: 31.3% of Web pages have schema.org  $\bullet$ markup, on average 26 assertions per page.

Ramanathan V. Guha, Dan Brickley, Steve Macbeth: Schema.org: Evolution of Structured Data on the Web. ACM Queue 13(9): 10 (2015)





- TrainTrip Organization
- Airline
  - Corporation
  - EducationalOrganization
    - CollegeOrUniversity
    - ElementarySchool
    - HighSchool
    - MiddleSchool
    - Preschool
    - School
- GovernmentOrganization
- LocalBusiness
  - AnimalShelter
  - AutomotiveBusiness
    - AutoBodyShop
      - AutoDealer
    - AutoPartsStore
    - AutoRental
    - AutoRepair
    - AutoWash
    - GasStation
    - MotorcycleDealer
    - MotorcycleRepair
    - ChildCare
  - Dentist
  - DryCleaningOrLaundry EmergencyService
    - FireStation
    - Hospital
    - PoliceStation
    - EmploymentAgency
  - EntertainmentBusiness
    - AdultEntertainment
    - AmusementPark
    - ArtGallery
    - Casino
    - ComedyClub
    - MovieTheater
    - NightClub
    - FinancialService
    - AccountingService
    - AutomatedTeller
    - **BankOrCreditUnion**
  - InsuranceAgency FoodEstablishment
    - Bakery
    - BarOrPub
    - Brewery
    - CafeOrCoffeeShop
    - FastFoodRestaurant



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#### Welcome!

Wikidata is a free and open knowledge base that can be read and edited by both humans and machines.

Wikidata acts as central storage for the **structured data** of its Wikimedia sister projects including Wikipedia, Wikivoyage, Wikisource, and others.

Wikidata also provides support to many other sites and services beyond just Wikimedia projects! The content of Wikidata is available under a free license , exported using standard formats, and can be interlinked to other open data sets on the linked data web.

#### Learn about data

New to the wonderful world of data? Develop and improve your data literacy through content designed to get you up to speed and feeling comfortable with the fundamentals in no time.







A bit older but somewhat more expressive: Linked Data on the Web

Number of Datasets in the connected "LOD Cloud"

1,146	2017-01-26
570	2014-08-30
295	2011-09-19
203	2010-09-22
95	2009-07-14
45	2008-09-18
25	2007-10-08
12	2007-05-01
08.854 triples and counting!	38.606.4



LOD Laundromat

### Linked Data: Volume

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Geoindexed Linked Data – courtesy of Krzysztof Janowicz, 2012 http://stko.geog.ucsb.edu/location\_linked\_data



## A bit of history

Before the current hype (stimulated by Google), knowledge graphs

- have been a core artefact of study and deployment since 2007, as part of the maturing "Semantic Web Technologies" field.
- have been based on maturing methods and tools around the use of ontologies in the Semantic Web field, since at least 2001.
- have even older roots in
  - Artificial Intelligence, in particular related to knowledge representation and logical (deductive) reasoning
  - the study of terminologies (and ontologies) pre-dating the Semantic Web era





### What makes a good knowledge graph?



### **Principles**

Goal: Easy sharing, discovery, integration, reuse

Key aspects of knowledge graphs:

- Syntax
- Semantics
- Graph structure
- Tools

Standards for syntax and semantics have been in place since at least 2004, developed by the World Wide Web Consortium (W3C).



### **Graph Structure**

- A schema for a knowledge graph is actually also a knowledge graph, just using more abstract terms, like
  - Classes (or types) of things (like, Person, or Material, or Role)
  - Possible relationships between things (like, persons may have daughters)
  - Complex relationship assertions
     (like, every cube has 6 sides which are squares).
- A quality schema (or ontology) serves as an intermediary between data/graph structure and human conceptualization.
- A quality schema simplifies understanding and reuseability of the knowledge graph.



### **Ontology and Knowledge Graph**



# Schema as a knowledge graph

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### Use of well-constructed patterns minimizes risk of "naïve"

**Ontology Design Pattern:** A reusable ontology-piece

constituting a high-quality, highly reuseable model for a

E.g., "Trajectory", "Activity", "Role (of an Agent)", etc.

**Modular Ontology Architecture** 

commonly recurring notion.

- modeling mistakes, thus increases reusability and repurposing of the ontology.
- Such ontologies are naturally made up of conceptual "modules" – these make understanding and maintenance of the ontology considerably easier.



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# Schema as a knowledge graph

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	AgentRole $\sqsubseteq$ (=1 performedBy.Agent) $\sqcap \forall$ performedBy.Agent	(10.1)
	$\exists performedBy.Agent \sqsubseteq AgentRole$	(10.2)
	$\top \sqsubseteq \forall pAR.AgentRole$	(10.3)
	ChessGame $\sqsubseteq \exists atPlace.Place \sqcap \forall atPlace.Place$	(10.4)
	ChessGame ⊑ ∃atTime.xsd:dateTime □ ∀atTime.xsd:dateTime	(10.5)
	ChessGame ⊑ ∃pAR.BlackPlayerRole ⊓ ∃pAR.WhitePlayerRole	(10.6)
	$\exists subEventOf.ChessTournament \sqcup \exists hasOpening.ChessOpening \sqsubseteq ChessGame$	(10.7)
	$\exists hasResult.ChessGameResult \sqcup \exists hasReport.ChessGameReport \sqsubseteq ChessGame$	(10.8)
	$ChessGame \sqsubseteq \forall subEventOf. ChessTournament \sqcap \forall hasOpening. ChessOpening$	(10.9)
	$ChessGame \sqsubseteq \forall hasResult.ChessGameResult \sqcap \forall hasReport.ChessGameReport$	(10.10)
	$BlackPlayerRole \sqcup WhitePlayerRole \sqsubseteq AgentRole \sqcap (=1 \ pAR^ChessGame)$	(10.11)
	$ChessGame \sqsubseteq (=1  hasFirstHalfMove.HalfMove) \sqcap (=1  hasLastHalfMove.HalfMove)$	(10.12)
	$ChessGame \sqsubseteq (=1  hasLastHalfMove.HalfMove)$	(10.13)
	$hasHalfMove \sqsubseteq subEventOf^-$	(10.14)
	$hasFirstHalfMove \sqsubseteq hasHalfMove$	(10.15)
	$hasLastHalfMove \sqsubseteq hasHalfMove$	(10.16)
	$HalfMove \sqsubseteq Event \sqcap \exists pAR.ActingPlayerRole \sqcap (=1  hasHalfMove^ChessGame)$	(10.17)
	$ActingPlayerRole \sqsubseteq AgentRole \sqcap (=1 \ pAR^HalfMove)$	(10.18)
	$HalfMove \sqsubseteq (\leq 1  nextHalfMove.HalfMove) \sqcap \neg \exists nextHalfMove.Self$	(10.19)
I	$\exists$ subEventOf.ChessGame $\sqcup \exists$ nextHalfMove.HalfMove $\sqsubseteq$ HalfMove	(10.20)
Wi	$\exists has SANRecord.xsd:string \sqsubseteq HalfMove$	(10.21)
U	HalfMove 🗆 \subEventOf ChessGame 🗆 \nextHalfMove HalfMove	$(10.22)^{3}$

### **Research Direction**

- High-Quality Ontology Engineering process well understood by some experts.
- But this is "soft" knowledge. Some missing pieces:
  - Systematic exploration and evaluation of the methodology
  - Providing a powerful tool landscape supporting the methodology – plus evaluations of their effectiveness.
  - Writing it up in tutorials and textbooks, and disseminate.
- Our methods development was supported primarily through two NSF GEO projects. Several follow-on proposals are pending.
- Goal: Practical methods and tools for high-quality knowledge graph schema development.



### Promise

- Data Management (DM) is central for cost-effective / efficient data-intensive solutions, for many application areas and scenarios.
- DM easily takes 80% of the time when data analytics is done.
- Knowledge Graphs are quickly becoming a central DM tool in industry and academia.
- Our methods target lowering the cost of Data Management with Knowledge Graphs.
- I can contribute to large methods- or application-oriented projects which have Data Management components.
- There is also high potential for a company spin-off.



#### Studies on the Semantic Web

#### Studies on the Semantic Web

Karl Hammar, Pascal Hitzler, Adila Krisnadhi, Agnieszka Ławrynowicz, Andrea Giovanni Nuzzolese, Monika Solanki (Editors)

### Ontology Engineering with Ontology Design Patterns

**Foundations and Applications** 

Pascal Hitzler, Aldo Gangemi, Krzysztof Janowicz, Adila Krisnadhi, Valentina Presutti (Eds.)

## Advances in Ontology Design and Patterns

IOS Press







published 2017



Other Aspects of Knowledge Graph management we are (or have recently been) investigating:

- Data/schema merging and integration
- Formal logic as schema representation language
- Deductive (logical) reasoning as KG engineering tool
- Efficient algorithms for deductive reasoning, including cloudbased
- KG compression
- Other aspects of KG quality
- Benchmark generation for different KG tools



- NSF for core new methods projects
- Intelligence/Defense for application-oriented projects with data management component, where effort can be used to improve and evaluate existing methods and tools.
- NIH similar, but haven't tapped into this yet.
- Potential sources also on application domains such as smart cities, data privacy and security, library science, human performance improvements, etc.





### **Explaining Deep Learning**



### Problem

- Connectionist systems are black boxes.
- How can we make sense of what they are doing? E.g. learn from what they encoded?
  - For human consumption.
  - For further processing in application software.
- "Explainable Artificial Intelligence" topic currently significantly on the rise and controversially discussed.
- Not a new topic as such.
   I've been involved in "neural-symbolic integration" research since I was a PhD student.



## **Understanding ANN systems**

• Explain behavior of trained (deep) NNs.

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- 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 (e.g., DL-Learner) to generate an explanatory theory.

• We're just starting on this, I report on very first experiments.



### **DL Extraction from ANNs**

WRIGI



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

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

**Positive examples:** 

negative examples:

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- ₅ <u>Lachtat</u>

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



### **DL-Learner**

**Positive examples:** 

- ▖▐ਰᢪᡰᠮᡱᡀᡂᡀᡛᠼ
- ᠈ᢩᡂ᠆ᢣᢩᠳ᠆ᡶᢩᢩᢘ᠆ᢩᡌ
- ᠈<u>ᢏᢩᠵ</u>ᠴ᠆ᢩᢙ᠆ᡶᢩᢩᢩᠥ᠆ᡛᢩ
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- ᠈ᢩᢩᢩᡋ᠆ᢩ<del>ᡄᢩ</del>ᢩᠴ᠂ᢩᡰᢩᢩᢩᢩᢣ

negative examples:

- ▖▐ᄛᡨ᠊᠖ᢆᡂᢤ
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- ᠈᠂ᡁ᠘᠆ᢏ══┚᠆ᡛᡛ᠆ᡱ
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- י נססאפא**ני**א

DL-Learner result: ∃hasCar.(Closed □ Short)

In FOL:

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



### **DL-Learner**

DL-Learner uses refinement operators to construct ever better approximations of a solution.





• Loohoh

```
\top
Train – covers all examples.
\exists hasCar. \top
\exists hasCar. Closed – covers all positives, two negatives
\exists hasCar(Closed \sqcap Short) - solution
```



### **Proof of Concept Experiment**



**Negative:** 





### 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 # ""





### 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**

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**Negative:** 









 $\exists contains. Transitway$ 

Econtains.LandArea

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- $\exists \text{contains.Transitway}$  (2)
- $\exists$ contains.SelfConnectedObject (3)
  - $\exists$ contains.Roadway (4)
    - $\exists$ contains.Road (5)

$\exists {\rm contains.LandTransitway}$	(6)
$\exists contains.LandArea$	(7)
$\exists contains. Building$	(8)
$\forall contains. \neg Floor$	(9)
$\forall \text{contains.} \neg \text{Ceiling}$	(10)



### **Positive (selection):**





WRIGH

Negative (selection):

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 $\exists contains.(DurableGood \sqcap \neg ForestProduct)$ 

#### **Positive:**

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 $\forall$ contains.( $\neg$ Furniture  $\sqcap \neg$ IndustrialSupply)

### **Positive (selection):**





**Negative (selection):** 

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 $\exists contains. Sentient Agent$ 



#### **Positive:**

#### Negative (selection):





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### $\exists contains.BodyOfWater$







- Utilize more sophisticated ontology.
- Utilize more sophisticated mappings.
- Explain hidden neurons.
- Then also tune learning algorithms towards easier interpretability.
- Tune DL-Learner better to the specific task.
- Dig deeper on the ADE20k dataset case, or transfer to other datasets of media. E.g. collaboration with IBM has already been established to look into drug-drug-interaction data.



- To the best of our knowledge, nobody else is pursuing explainable deep learning though background knowledge.
- To the best of our knowledge, nobody funded under the DARPA XAI program is pursuing explainable deep learning through background knowledge.





Other Aspects of Deep Learning we are investigating include:

- Deep Learning methods for data integration
- Deep Learning for text analysis
- Deep Learning algorithms to support KG engineering tools (e.g., deductive reasoning and graph completion)
- Explaining other statistical approaches (not only deep learning) by transferring our methods.



# **Target funding agencies**

- NSF for core new methods projects
- Intelligence/Defense for application-oriented projects regarding the use of explainable deep learning.
- NIH similar, but haven't tapped into this yet. We just started a collaboration with IBM TJ Watson on applying our method to drug-drug-interaction.
- Potential sources also on any current or emerging application domain of deep learning, including security, social media analysis, intelligence analysis, etc.



## Summary

- My work has many facets.
- My work is in synch with several current trends, including
  - Knowledge Graphs
  - Deep Learning
  - Big Data
  - Data Science
- Covering methods/foundations and applications; and the transfer between them.
- Broad options for obtaining research funding.
- Easier because of already significant visibility and standing. Since I became a US citizen (summer 2017) I also made significant inroads for defense funding, in particular establishing a network of contacts.





## **Thanks!**

