Towards Explaining Neural Networks Through Background Knowledge

Pascal Hitzler
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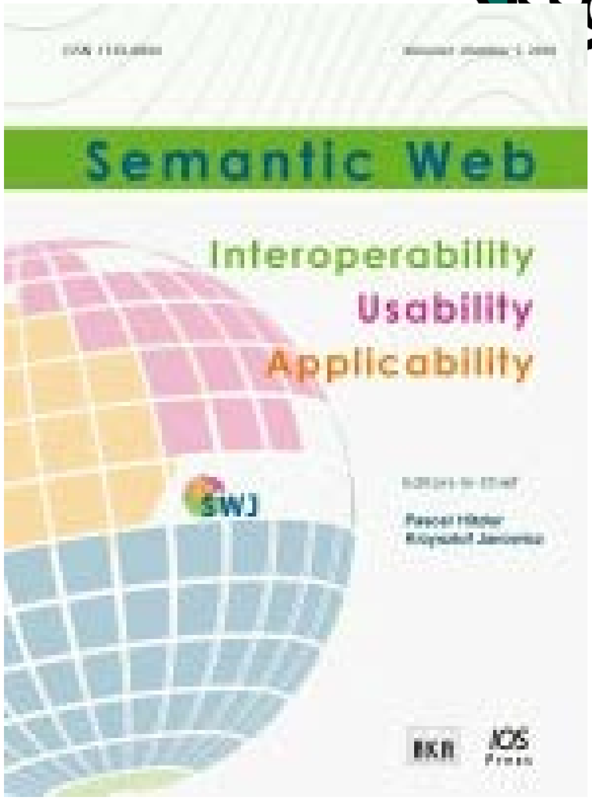
Data Science and Security Cluster (DSSC)
Wright State University
http://www.pascal-hitzler.de

Semantic Web journal

- **EiCs:** **Pascal Hitzler**
  Krzysztof Janowicz
- **Funded 2010**
- **2016 Impact factor of 1.786, top 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/**

Data Semantics Laboratory

Two faculty (Michelle Cheatham, Pascal Hitzler)

1 postdoc (Adila Krisnadhi)

10 graduate students

See http://daselab.org/

Data Science and Security Cluster (DSSC):

Combines 8 faculty, 6 labs (data semantics, bioinformatics, visualization, data science in healthcare, cybersecurity, web and complex systems)

DSSC

Data Science and Security Cluster

Collaborative Research Group

Membership includes 8 faculty and over 40 graduate and undergraduate students across 6 distinct research labs:

- Advanced Visual Data Analysis (AViDA), directed by Thomas Wischgoll.
- Bioinformatics Research Group (BiRG), directed by Travis Doom and Mike Raymer
- Cybersecurity Lab, directed by Junjie Zhang
- Data Science for Healthcare Lab, directed by Tanvi Banerjee
- Data Semantics (DaSe) Lab, directed by Michelle Cheatham and Pascal Hitzler
- Web and Complex Systems (WaCS) Lab, directed by Derek Doran

Semantic Web

- **A research field about methods for:**

Data and Information sharing, discovery, integration, and reuse.

Key paradigms:

- **Representation of information via knowledge graphs in standardized formats (e.g., W3C's RDF).**
- **Typing of the knowledge graphs together with a type logic a.k.a. ontology or schema, represented in standardized/sharable formats (e.g., W3C's OWL)**

Semantic Web

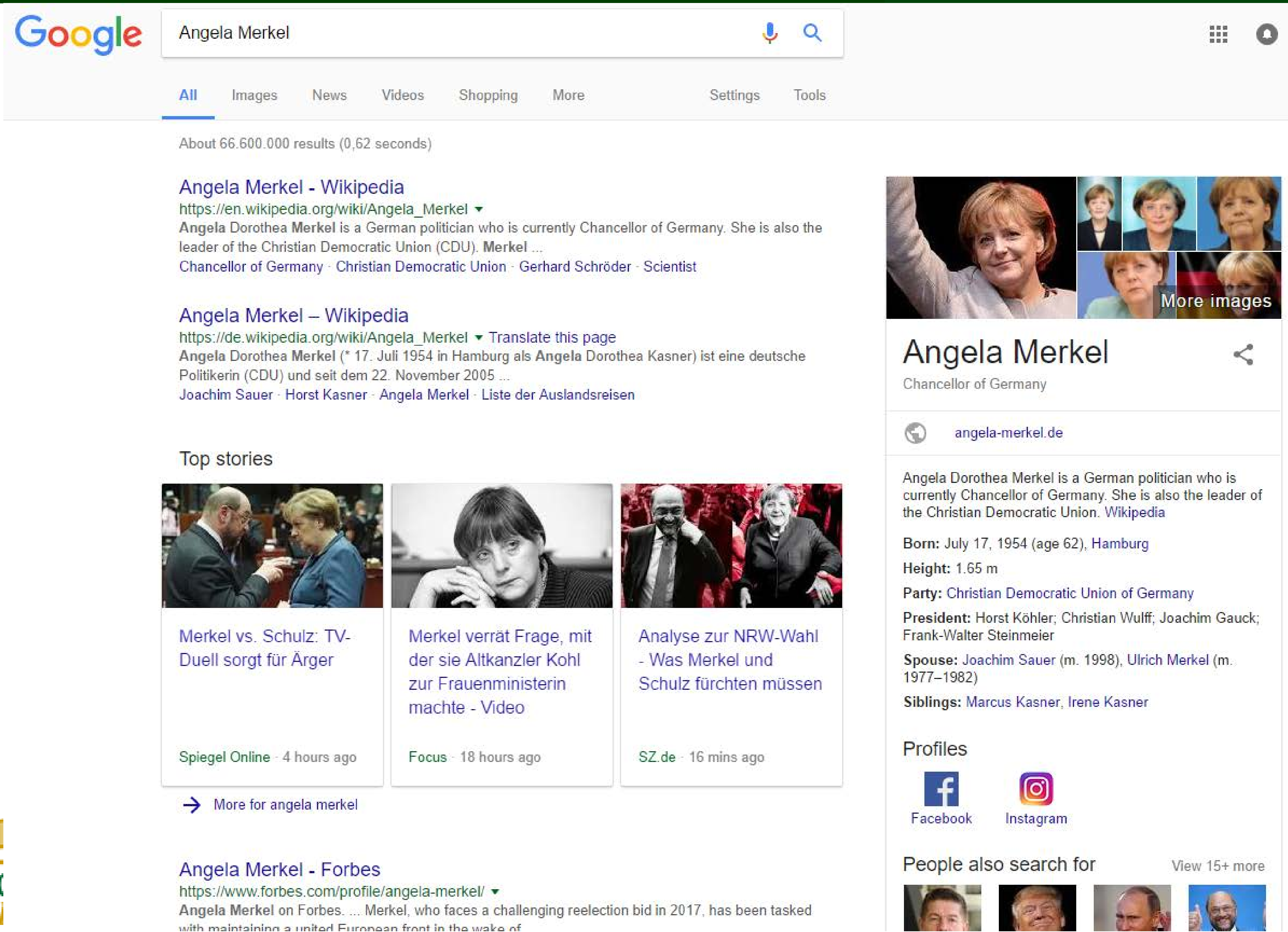
Two major examples of semantic web technologies at work:

- **Google knowledge graph**
  You see a glimpse of it in the boxes to the right of your search results.

- **Schema.org**
  Joint effort by major search engine providers.
  Schema/ontology for annotating Web page content, so that search engines can provide better results.
  In the meantime, schema.org annotations are ubiquitous on the Web.

Google Knowledge Graph

DaSe Lab



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Joachim Sauer

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Angela Merkel › Spouse › Joachim Sauer

Joachim Sauer
m. 1998

Ulrich Merkel
m. 1977–1982

[Joachim Sauer - Wikipedia](https://en.wikipedia.org/wiki/Joachim_Sauer)
https://en.wikipedia.org/wiki/Joachim_Sauer
Joachim Sauer (born 19 April 1949) is a German quantum chemist and full professor at the Humboldt University of Berlin. He is the husband of the Chancellor of ...
Scientific career · Personal life · Public visibility as husband ... · References

Joachim Sauer – Wikipedia
https://de.wikipedia.org/wiki/Joachim_Sauer ▾ Translate this page
Joachim Sauer (* 19. April 1949 in Hosena, Landkreis Oberspreewald-Lausitz, Brandenburg) ist ein deutscher Quantenchemiker sowie Physikochemiker.
Berufliche Laufbahn · Ehrungen und Auszeichnungen · Privates · Werke (Auswahl)

Prof. Dr. Dr. h.c. Joachim Sauer — Quantenchemie der Festkörper ...
https://www.chemie.hu-berlin.de/de/forschung/quantenchemie/Group/js-1 ▾
Year of Birth, 1949. Education, 1967 - 1972, Humboldt University, Berlin. Academic degrees, 1972, Diploma in Chemistry. 1974, Dr. rer. nat. (summa cum laude) ...

Joachim Sauer wird 65: „Der Professor“ statt der Kanzlerin-Gatte
www.handelsblatt.com › Politik › Deutschland ▾ Translate this page
Apr 19, 2014 - Er ist Deutschlands „First Husband“ – aber er tritt nicht als Ehemann der Kanzlerin in Erscheinung: **Joachim Sauer** lebt sein eigenes Leben als ...

Joachim Sauer, Angela Merkel's Husband: 5 Fast Facts | Heavy.com
heavy.com/.../joachim-sauer-angela-merkel-husband-married-germany-chancellor-sci... ▾
Mar 17, 2017 - **Joachim Sauer** is the media-shy husband of German Chancellor Angela Merkel, who is meeting President Donald Trump in Washington today.

Rare sighting of Angela Merkel's publicity-shy husband at G7 summit
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Joachim Sauer

Chemist

Joachim Sauer is a German quantum chemist and full professor at the Humboldt University of Berlin. He is the husband of the Chancellor of Germany, Angela Merkel.
Wikipedia

Born: April 19, 1949 (age 68), Hosena, Senftenberg

Spouse: Angela Merkel (m. 1998)

Education: Humboldt University of Berlin

Children: Adrian Sauer, Daniel Sauer

Parents: Richard Sauer, Elfriede Sauer

Awards: Kolos Medal

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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 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

WRIGHT STATE UNIVERSITY

Representation format

DaSe Lab

Resource Description Framework (RDF), W3C Standard

SSC

- Use URIs to make entities and vocabularies referenceable on the Web.
- Essentially, a labelled and typed graph.

```
@prefix : <https://w3id.org/rdfchess/id/> .
@prefix xsd: <http://www.w3.org/2001/XMLSchema#> .
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix chon: <https://w3id.org/rdfchess/chessonto#> .

:gam19e02 rdf:type chon:ChessGame ;
          chon:subEventOf :tou23as5 ;
          chon:atPlace :pla537es8 ;
          chon:atTime "2013-11-09T00:00:00"^^xsd:dateTime ;
          chon:providesAgentRole :rol88y76c, :rol92z01m ;
          chon:hasResult :res23tu77h ;
          chon:hasOpening :ope662vn2 .

:tou23as5 rdf:type chon:ChessTournament ;
          chon:hasName "WCh 2013"^^xsd:string ;
          chon:atPlace :pla537es8 ;
```

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```
@prefix : <https://w3id.org/rdfchess/id/> .
@prefix xsd: <http://www.w3.org/2001/XMLSchema#> .
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
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          chon:hasOpening :ope662vn2 .

:tou23as5 rdf:type chon:ChessTournament ;
          chon:hasName "WCh 2013"^^xsd:string ;
          chon:atPlace :pla537es8 ;
          chon:atTime "2013-11-09T00:00:00"^^xsd:dateTime .

:pla537es8 rdf:type chon:Place ;
           chon:hasName "Chennai"^^xsd:string .

:rol88y76c rdf:type chon:WhitePlayerRole ; chon:performedBy :ag422yt6 .

:ag422yt6 rdf:type chon:Agent ;
          chon:hasName "Carlsen, Magnus"^^xsd:string .

:rol92z01m rdf:type chon:BlackPlayerRole ; chon:performedBy :ag79yy12 .

:ag79yy12 rdf:type chon:Agent ;
          chon:hasName "Anand, Viswanathan"^^xsd:string .

:res23tu77h rdf:type chon:ChessGameResult ;
            chon:encodedAsSAN "1/2-1/2"^^xsd:string .

:ope662vn2 rdf:type chon:ChessOpening ;
           chon:hasECOCode "A07"^^xsd:string .

:cgr448uy6 rdf:type chon:ChessGameReport ;
     chon:providesAgentRole :rol08ij2a ;
```
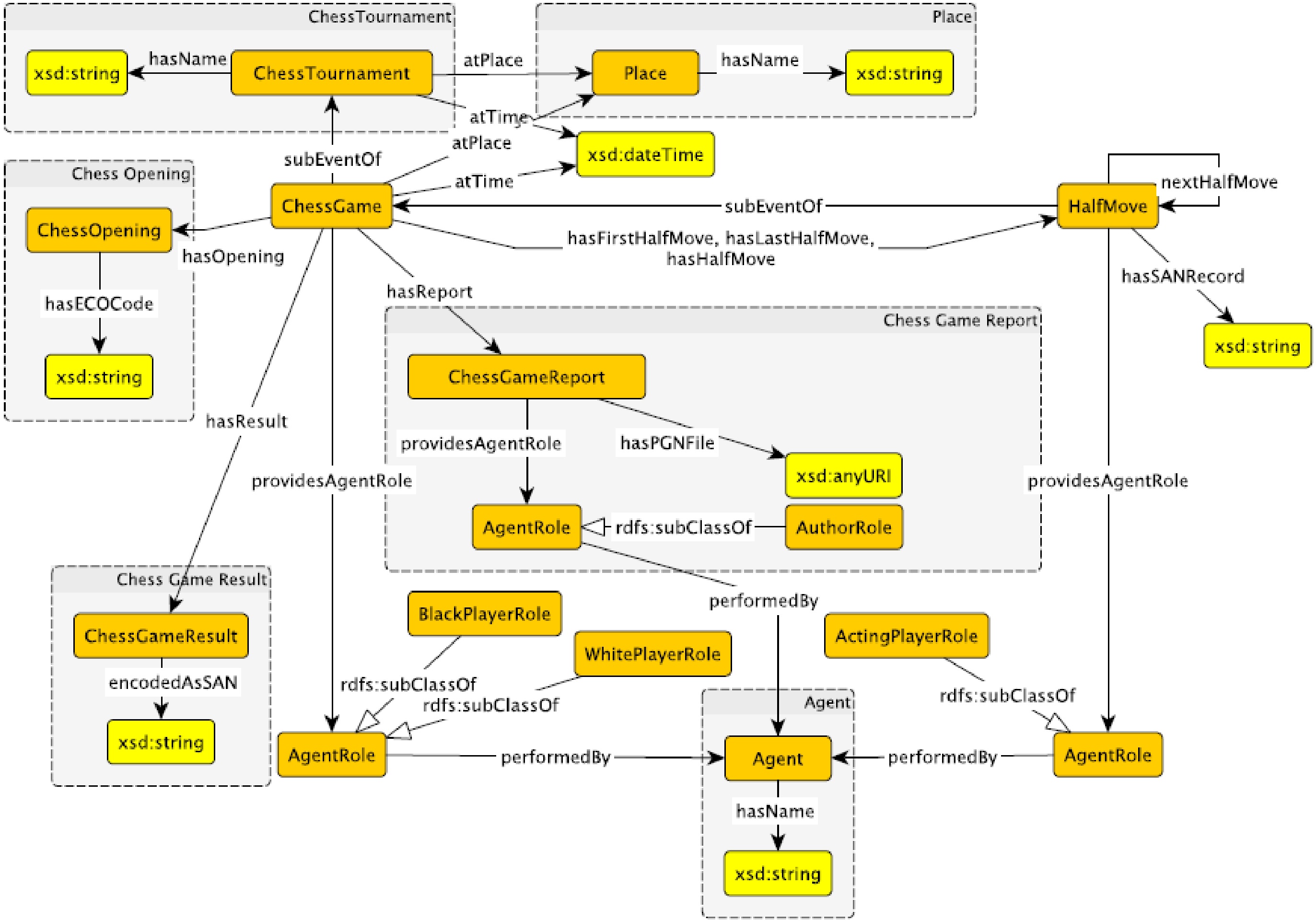

Representation format

Web Ontology Language (OWL), W3C Standard

- **Essentially, a type logic over the types in the RDF graph**
- **Based on description logics, enables automated reasoning.**



$$\text{AgentRole} \sqsubseteq (=1\ \text{performedBy.Agent}) \sqcap \forall\text{performedBy.Agent} \tag{10.1}$$

$$\exists\text{performedBy.Agent} \sqsubseteq \text{AgentRole} \tag{10.2}$$

$$\top \sqsubseteq \forall\text{pAR.AgentRole} \tag{10.3}$$

$$\text{ChessGame} \sqsubseteq \exists\text{atPlace.Place} \sqcap \forall\text{atPlace.Place} \tag{10.4}$$

$$\text{ChessGame} \sqsubseteq \exists\text{atTime.xsd:dateTime} \sqcap \forall\text{atTime.xsd:dateTime} \tag{10.5}$$

$$\text{ChessGame} \sqsubseteq \exists\text{pAR.BlackPlayerRole} \sqcap \exists\text{pAR.WhitePlayerRole} \tag{10.6}$$

$$\exists\text{subEventOf.ChessTournament} \sqcup \exists\text{hasOpening.ChessOpening} \sqsubseteq \text{ChessGame} \tag{10.7}$$

$$\exists\text{hasResult.ChessGameResult} \sqcup \exists\text{hasReport.ChessGameReport} \sqsubseteq \text{ChessGame} \tag{10.8}$$

$$\text{ChessGame} \sqsubseteq \forall\text{subEventOf.ChessTournament} \sqcap \forall\text{hasOpening.ChessOpening} \tag{10.9}$$

$$\text{ChessGame} \sqsubseteq \forall\text{hasResult.ChessGameResult} \sqcap \forall\text{hasReport.ChessGameReport} \tag{10.10}$$

$$\text{BlackPlayerRole} \sqcup \text{WhitePlayerRole} \sqsubseteq \text{AgentRole} \sqcap (=1\ \text{pAR}^{-}.\text{ChessGame}) \tag{10.11}$$

$$\text{ChessGame} \sqsubseteq (=1\ \text{hasFirstHalfMove.HalfMove}) \sqcap (=1\ \text{hasLastHalfMove.HalfMove}) \tag{10.12}$$

$$\text{ChessGame} \sqsubseteq (=1\ \text{hasLastHalfMove.HalfMove}) \tag{10.13}$$

$$\text{hasHalfMove} \sqsubseteq \text{subEventOf}^{-} \tag{10.14}$$

$$\text{hasFirstHalfMove} \sqsubseteq \text{hasHalfMove} \tag{10.15}$$

$$\text{hasLastHalfMove} \sqsubseteq \text{hasHalfMove} \tag{10.16}$$

$$\text{HalfMove} \sqsubseteq \text{Event} \sqcap \exists\text{pAR.ActingPlayerRole} \sqcap (=1\ \text{hasHalfMove}^{-}.\text{ChessGame}) \tag{10.17}$$

$$\text{ActingPlayerRole} \sqsubseteq \text{AgentRole} \sqcap (=1\ \text{pAR}^{-}.\text{HalfMove}) \tag{10.18}$$

$$\text{HalfMove} \sqsubseteq (\leq 1\ \text{nextHalfMove.HalfMove}) \sqcap \neg\exists\text{nextHalfMove.Self} \tag{10.19}$$

$$\exists\text{subEventOf.ChessGame} \sqcup \exists\text{nextHalfMove.HalfMove} \sqsubseteq \text{HalfMove} \tag{10.20}$$

$$\exists\text{hasSANRecord.xsd:string} \sqsubseteq \text{HalfMove} \tag{10.21}$$

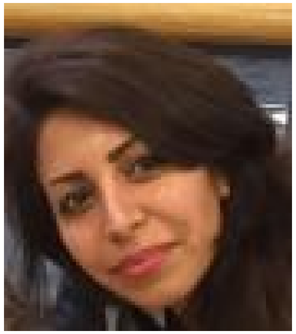
$$\text{HalfMove} \sqsubseteq \forall\text{subEventOf.ChessGame} \sqcap \forall\text{nextHalfMove.HalfMove} \tag{10.22}$$

Some key research areas

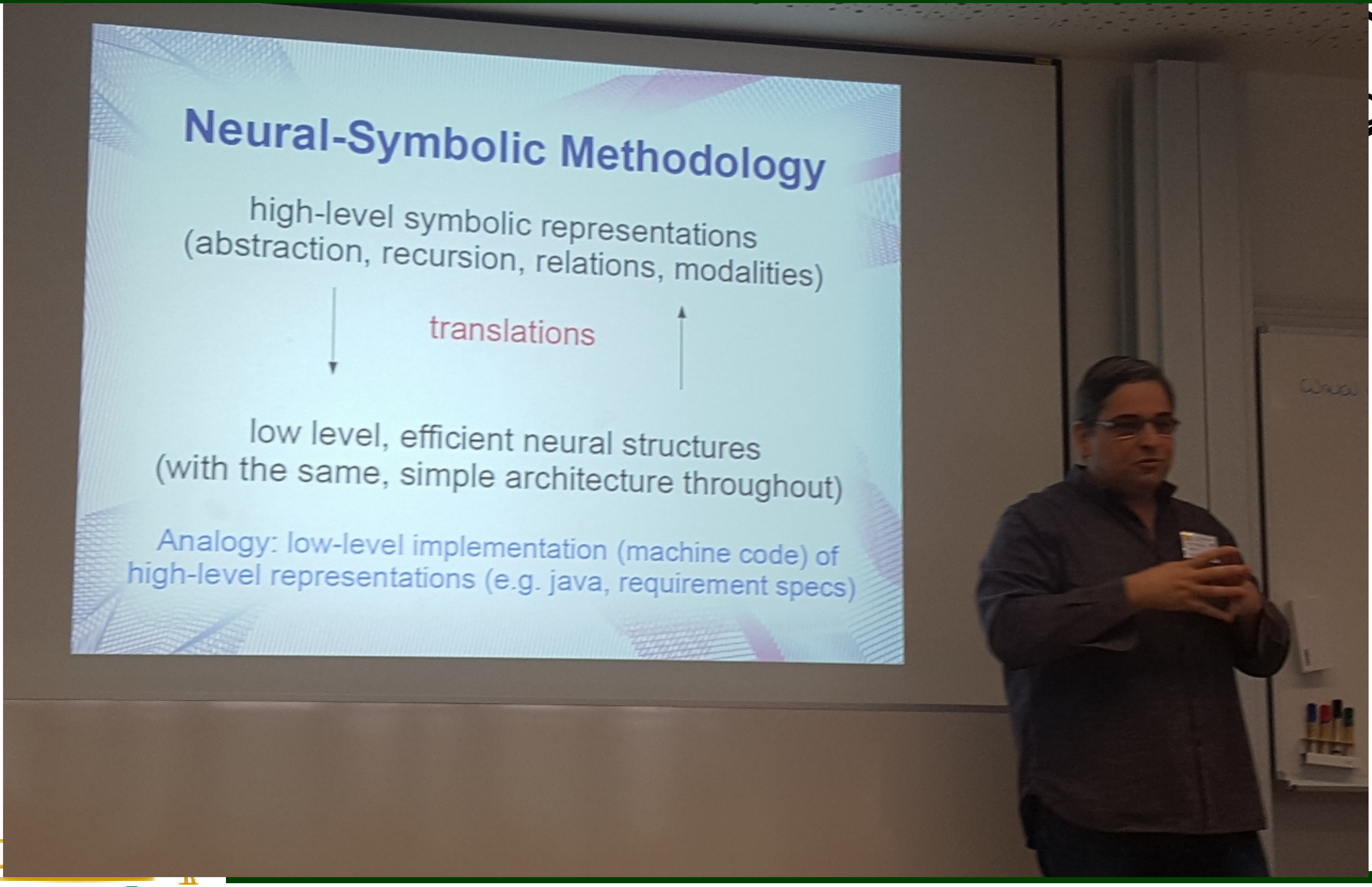
- Given an ontology and some data (or text), how to automatically transform the data such that it will adhere to the schema defined by the ontology? (Ontology/Knowledge base population)
- Given two ontologies, how to map between the ontologies such that data can be integrated? (Ontology alignment)
- How to make ontologies, which make these (and other) data management tasks as simple as possible?

Propositional rule extraction from trained neural networks under background knowledge

(work with Maryam Labaf)



Neural and symbolic



Extraction

In this case: extracting propositional rules.

General idea:

- **Input value 1 interpreted as “true”, value 0 as “false”**
- **Outputs interpreted as true or false according to a threshold**
- **I.e. network function maps binary vectors.**

Garcez et al, 2001: By weight analysis (layer by layer) under differentiable activation functions. Possible in principle but intricate and, arguably, the resulting rule sets are usually rather difficult to understand.

Lehmann, Bader, Hitzler, 2010: Black-box approach (looking at inputs and outputs only).

Lehmann, Bader, Hitzler, 2010

For every monotonic function

$$f : \{0,1\}^n \rightarrow \{0,1\}^k$$

there is a unique reduced set of positive propositional rules which capture exactly the function f.

Reduced means: no redundancies, and as small as possible.

Problem: Rule sets can get large and messy, i.e. still very difficult to understand.

Adding Background Knowledge

Can we lift the result just given to include background knowledge?

Given:

- A (reduced) propositional logic program P (extracted from an ANN as above).
- Set I of prop. variables representing ANN inputs.
- Set O of prop. variables representing ANN outputs.
- A background knowledge base K (a propositional logic program).

We then seek a logic program P' (simpler than P) s.t. for all subsets i in I and each o in O we have

$$P \wedge i \models o \qquad \text{iff} \qquad P' \wedge K \wedge i \models o.$$

Adding Background Knowledge

It turns out that

- P' is no longer unique in general
  (even under reduction).
- P' may not even exist
  (unless I is restricted to the left-hand side of rules in K).

- But with suitable K you can get P' which are simpler than P.
  Typical case:

P: $p_1 \wedge q \rightarrow o$, $p_2 \wedge q \rightarrow o$

K: $p_1 \rightarrow r$, $p_2 \rightarrow r$

P': $r \wedge q \rightarrow o$

Adding Background Knowledge

P: $p_1 \wedge q \rightarrow o$

$p_2 \wedge q \rightarrow o$

K: $p_1 \rightarrow r$

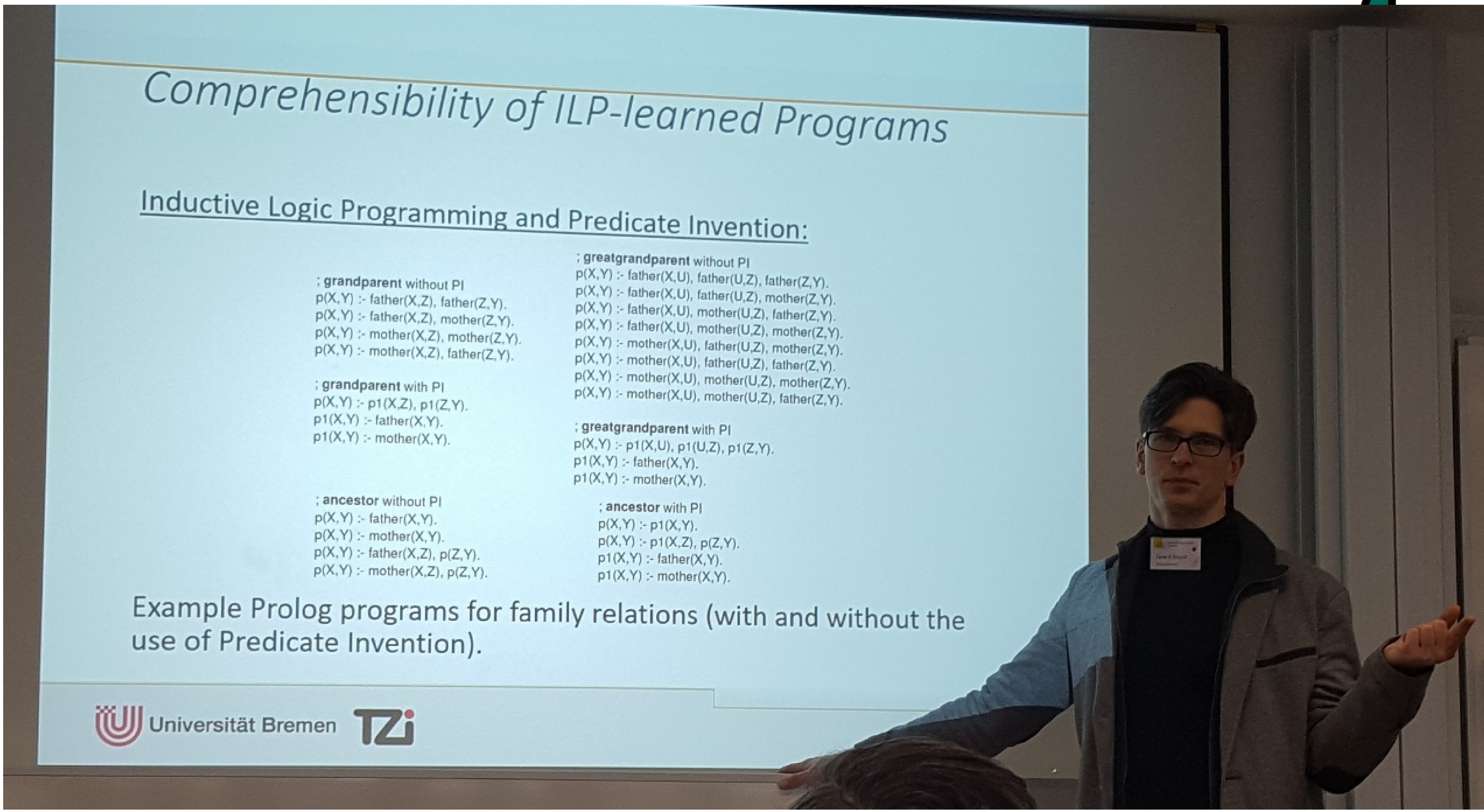
$p_2 \rightarrow r$

P': $r \wedge q \rightarrow o$

Note that K essentially groups input variables. Once could think of r being a "more general concept" than either p1 and p2.

Of course, we have only discussed the propositional case so far, but in order to obtain strong explanations for the input-output behavior of ANNs we need to go beyond propositional.

Comprehensibility!



Description Logic extraction from trained neural networks under background knowledge

(work with Md Kamruzzaman Sarker, Derek Doran, Ning Xie, Mike Raymer)




DL Extraction from ANNs

- **Explain input-output 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 (e.g., DL-Learner) to generate an explanatory theory.**
- **We're just starting on this, experiments (below) just came out.**

DL Extraction from ANNs

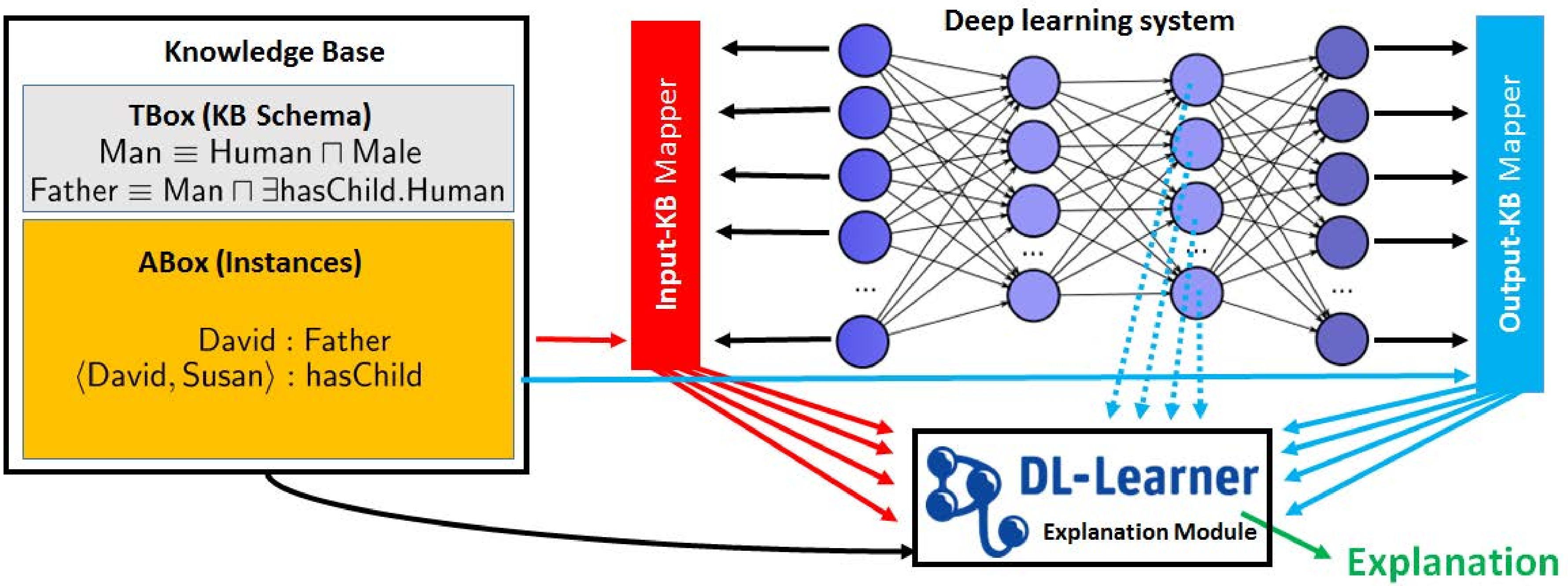
Possible data sources:

- **Linked data / semantic web data**
  - **I.e. structured data on the web, organized in so-called RDF graphs.**
- **Cross-domain ontologies (e.g., SUMO, Proton)**
- **Wikidata**
- **schema.org**

Essentially, all content already readily and publicly available in structured form.

If further domain knowledge is needed: use state-of-the-art approaches for knowledge graph generation in order to obtain structured data from suitable text corpora.

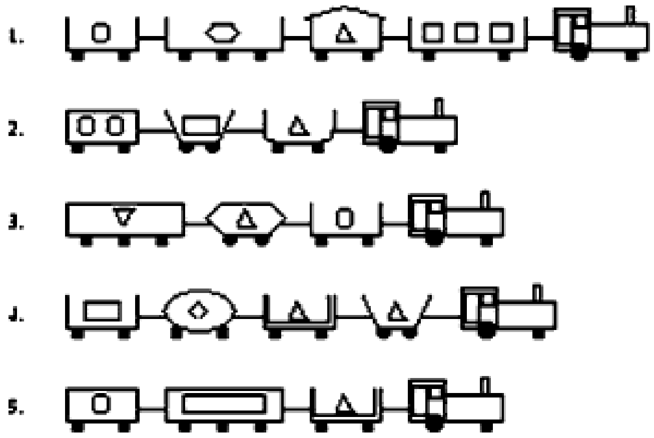
DL Extraction from ANNs

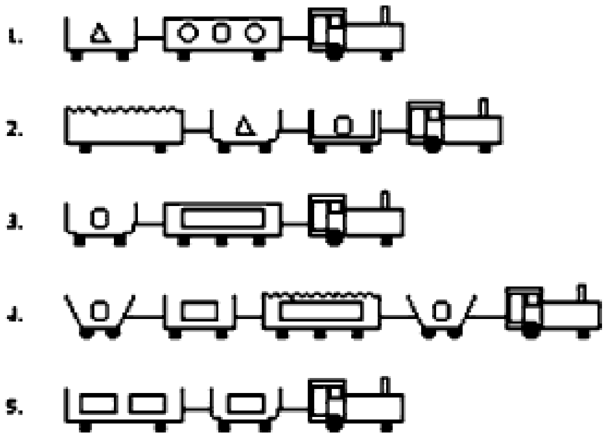


DL-Learner

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

Positive examples: **negative examples:**

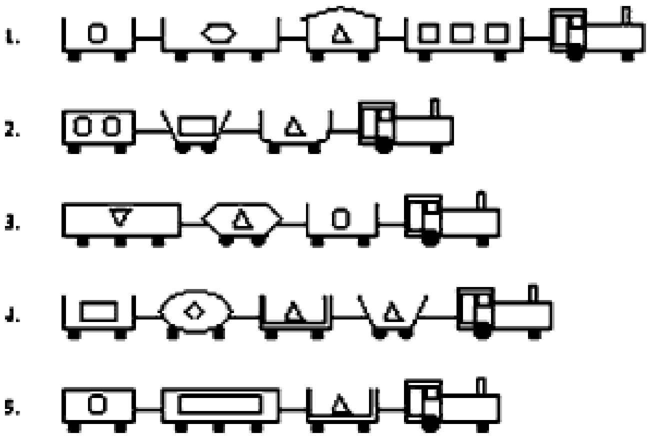




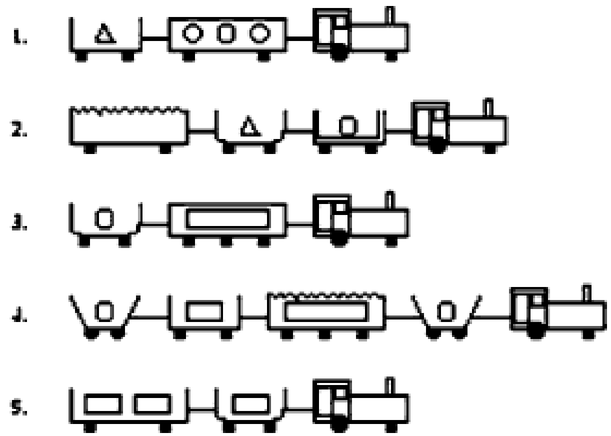
Task: find a class description (logical formula) which separates positive and negative examples.

DL-Learner

Positive examples:



negative examples:



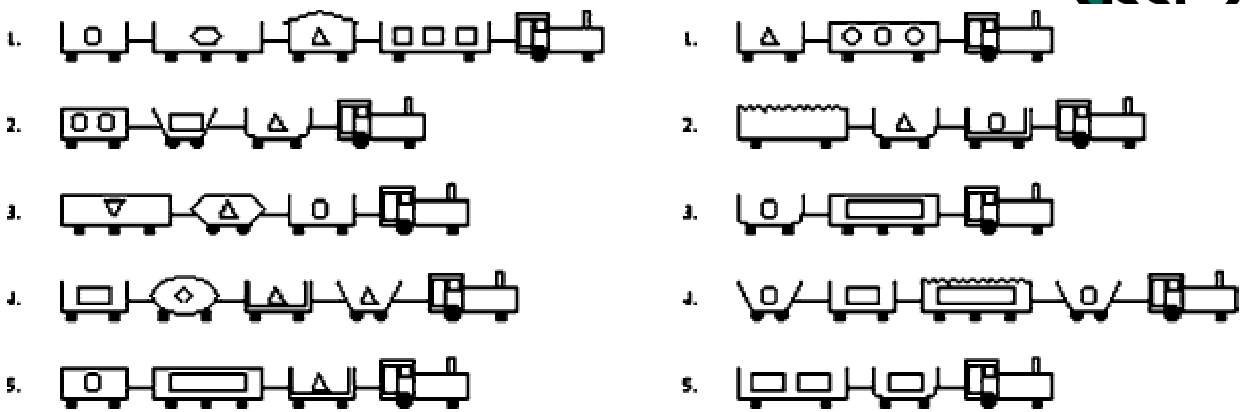
DL-Learner result: $\exists \text{hasCar}.(\text{Closed} \sqcap \text{Short})$

In FOL:

$$\{x \mid \exists y(\text{hasCar}(x, y) \wedge \text{Closed}(y) \wedge \text{Short}(y))\}$$

DL-Learner

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



$\top$

Train – covers all examples.

$\exists$hasCar.$\top$

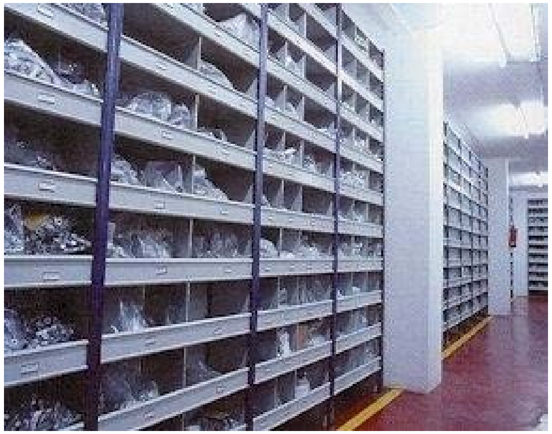
$\exists$hasCar.Closed – covers all positives, two negatives

$\exists$hasCar(Closed $\sqcap$ Short) – solution

Proof of Concept Experiment

Positive:

Negative:



Images

Come from the MIT ADE20k dataset
http://groups.csail.mit.edu/vision/datasets/ADE20K/
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 # ""
011 # 0 # 0 # box # boxes # ""
001 # 1 # 0 # door # door # ""
002 # 1 # 0 # window # window # ""
009 # 1 # 0 # wheel # wheel # ""
```

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**
  http://www.adampease.org/OP/

- **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.**

DL-Learner input

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:

$$\exists \text{contains}.\text{Transitway}$$

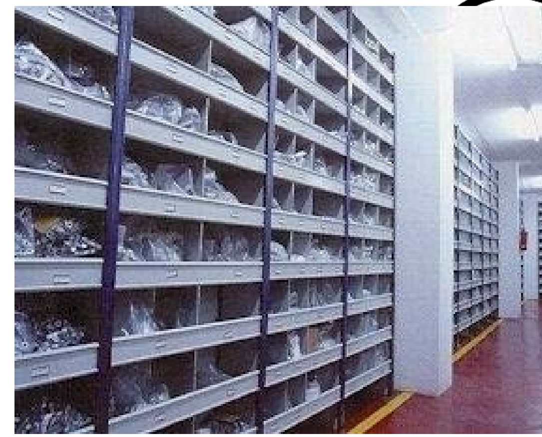
$$\exists \text{contains}.\text{LandArea}$$

Proof of Concept Experiment

DaSe Lab

Positive:

Negative:



$$\exists \text{contains}.\text{Transitway}$$

$$\exists \text{contains}.\text{LandArea}$$

First 10 DL-Learner responses

$$\exists \text{contains}.\text{Window} \quad (1)$$

$$\exists \text{contains}.\text{Transitway} \quad (2)$$

$$\exists \text{contains}.\text{SelfConnectedObject} \quad (3)$$

$$\exists \text{contains}.\text{Roadway} \quad (4)$$

$$\exists \text{contains}.\text{Road} \quad (5)$$

$$\exists \text{contains}.\text{LandTransitway} \quad (6)$$

$$\exists \text{contains}.\text{LandArea} \quad (7)$$

$$\exists \text{contains}.\text{Building} \quad (8)$$

$$\forall \text{contains}.\neg \text{Floor} \quad (9)$$

$$\forall \text{contains}.\neg \text{Ceiling} \quad (10)$$

Experiment 2

Positive (selection):

Negative (selection):

$$\exists \text{contains}.(\text{DurableGood} \sqcap \neg \text{ForestProduct})$$

Experiment 3

Positive:

Negative:

$$\forall \text{contains}.(\neg \text{Furniture} \sqcap \neg \text{IndustrialSupply})$$

Experiment 4

Positive (selection):

Negative (selection):

$\exists \mathrm{contains.SentientAgent}$

Experiment 5

Positive:

Negative (selection):

$\exists$contains.BodyOfWater

Next steps

- Utilize more sophisticated ontology.
- Utilize more sophisticated mappings.
- Explain hidden neurons.
- Tune DL-Learner better to the specific task.

Explaining hidden neurons

Collaborators Derek Doran and Ning Xie (Web and Complex Systems Lab)

They explore how to determine groups of hidden neurons which often fire together and thus may indicate the "detection" of certain features.

We plan to apply the above mentioned DL-Learner approach also to these groups of hidden neurons, in order to determine which features they detect.

Thanks!

References

- Md. Kamruzzaman Sarker, David Carral, Adila A. Krisnadhi, Pascal Hitzler, Modeling OWL with Rules: The ROWL Protege Plugin. In: Takahiro Kawamura, Heiko Paulheim (eds.), Proceedings of the ISWC 2016 Posters & Demonstrations Track co-located with 15th International Semantic Web Conference (ISWC 2016), Kobe, Japan, October 19, 2016. CEUR Workshop Proceedings 1690, CEUR-WS.org 2016.
- Md Kamruzzaman Sarker, Adila A. Krisnadhi, David Carral, Pascal Hitzler, Rule-based OWL Modeling with ROWLTab Protege Plugin. In: Proceedings ESWC 2017. To appear.
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- Adila Krisnadhi, Ontology Pattern-Based Data Integration. Dissertation, Department of Computer Science and Engineering, Wright State University, 2015.

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