UNIVERSITÄT MANNHEIM

Semantic Web Technologies
The Layer Cake and Beyond

Heiko Paulheim

Previously on Semantic Web Technologies

- What we would like to have:

  daughterOf(X,Y) ← childOf(X,Y) ∧Woman(X) .

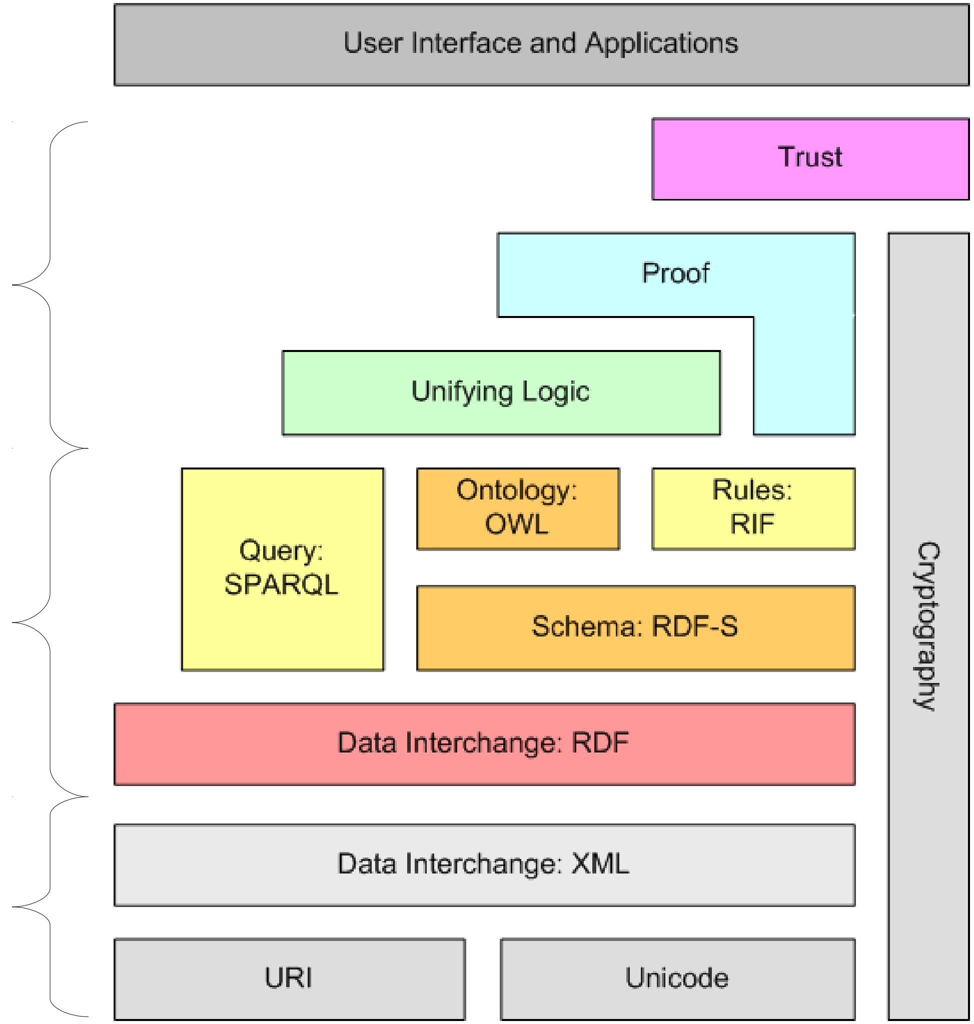
- Rules are flexible
- There are rules in the Semantic Web, e.g.
  - Semantic Web Rule Language (SWRL)
  - Rule Interchange Format (RIF)
  - Some more
- Some reasoners do (partly) support rules

Semantic Web – Architecture

here be dragons...

Semantic Web Technologies (This lecture)

Technical Foundations

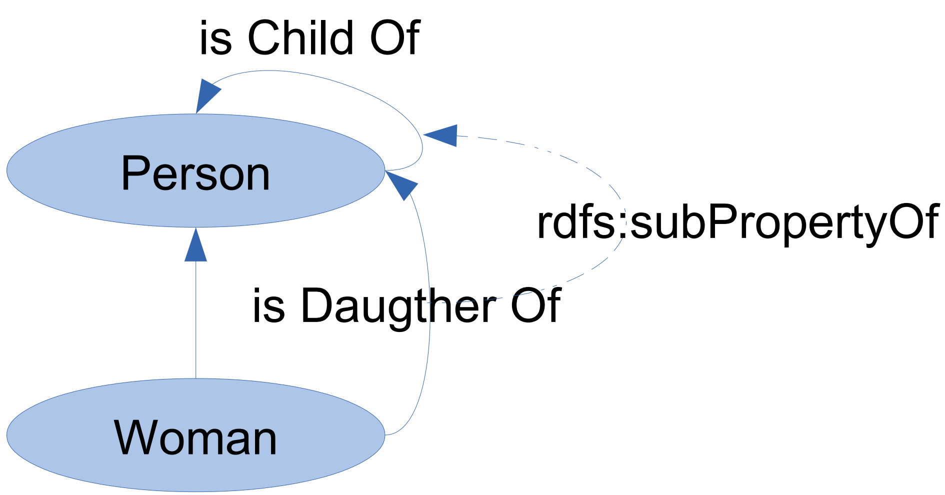


Berners-Lee (2009): *Semantic Web and Linked Data*
http://www.w3.org/2009/Talks/0120-campus-party-tbl/

Towards Rules for the Semantic Web

- What we would like to have:
  - daughterOf(X,Y) ← childOf(X,Y) ∧Woman(X) .

- OWL only gives an approximation:



SWRL

- Semantic Web Rule Language
  - a rule language for the Semantic Web
  - built to be combined with OWL
- W3C Member Submission (2004)
  - not a standard in a strict sense
  - but widely adopted
- Tool support
  - many reasoners
  - Protégé

SWRL Building Blocks

- Classes are defined as *unary predicates*
  - :Peter a :Person . ↔ Person(Peter)

- Properties are defined as *binary predicates*
  - :Peter :hasMother :Julia . ↔ hasMother(Peter,Mary)
  - :Peter :hatAge 24^^xsd:integer . ↔ hasAge(Peter,24)

SWRL Rules

- Basic form:
  - Head (Consequence) ← Body (Condition)
- Body and head are conjunctions of predicates
- Variables are introduced by ?
- Example:
  - daughterOf(?X,?Y) ← childOf(?X,?Y) ∧ Woman(?X)

- There is no
  - disjunction (logical or)
  - negation
  - undbound variables in the rule head
- ...but there are some ways out

Disjunctions in Rule Body

- There is no disjunction

- Example for disjunction in rule body:
  - Female faculty members are students or staff of the faculty
- Intuitive:
  - FemaleFacultyMember(?X) $\leftarrow$ Woman(?X) $\wedge$ Faculty(?Y) $\wedge$ (worksAt(?X,?Y) $\vee$ studentAt(?X,?Y))

Disjunctions in Rule Body

- Solution
  - first step: convert body to disjunctive normal form
    - i.e., disjunction of conjunctions
  - second step: split into individual rules

Disjunctions in Rule Body

- FemaleFacultyMember(?X) ← Woman(?X) ∧ Faculty(?Y) ∧ (worksAt(?X,?Y) ∨ studentAt(?X,?Y))
- turns into
  - FemaleFacultyMember(?X) ←
    (Woman(?X) ∧ Faculty(?Y) ∧ worksAt (?X,?Y))
    ∨ (Woman(?X) ∧ Faculty(?Y) ∧ worksAt (?X,?Y))
- ...which turns into
  - FemaleFacultyMember(?X) ←
    Woman(?X) ∧Faculty(?Y) ∧worksAt (?X,?Y)
  - FemaleFacultyMember(?X) ←
    Woman(?X) ∧Faculty(?Y) ∧studentAt (?X,?Y)

Disjunctions in Rule Head

- Disjunctions in rule head
  - are not so easy to get rid off
- Example
  - Every faculty member is a student or an employee

Student(?X) ∨ Employee(?X) ← FacultyMember(?X)

- On the other hand: what should a reasoner conclude?

  → disjunction in rule head does not make as much sense!

Disjunctions in Rule Head

- SWRL is meant to be used together with OWL
- Idea: build an artificial class for the rule head

  StudentOrEmployee owl:unionOf (Student Employee)

  StudentOrEmployee(?X) ← FacultyMember(?X)

- This way, we can conclude that ?X is in the union of both classes
  - Further reasoning on other axioms might rule out one option

Negation

- Negation can be simulated with a similar trick

- Example:
  - Creatures living in the water are not human.
- Intuitive:

  $\neg$Human(?X) $\leftarrow$ Creature(?X) $\wedge$ habitat(?X,Water)

Simulating Negation

- Again: combining SWRL and OWL
  - NonHuman owl:complementOf Human .
- New Rule:
  - NonHuman(?X) $\leftarrow$ Creature(?X) $\wedge$ habitat(?X,Water)
- Now, a reasoner can find a contradiction between
  - :Nemo a :Creature; habitat :Water .
- and
  - :Nemo a :Human .

Simulating Negation

- Negation in the rule body:

  FlightlessBird(?X) ← Bird(?X) ∧ ¬habitat(?X,Air)

- Define class:

```
NotAirHabitat owl:equivalentClass [
   a owl:Restriction ;
   owl:onProperty :habitat ;
   owl:allValuesFrom [
     owl:complementOf [ owl:oneOf (:Air) ] ] ]
```

FlightlessBird(?X) ← Bird(?X) ∧ NotAirHabitat(?X)

Unbound Variables

- All variables appearing in the rule head must also appear in the body
  - those are *bound* variables

- Example: every human has a (human) father
  - Human(?Y) $\wedge$ hasFather(?X,?Y) $\leftarrow$ Human(?X)

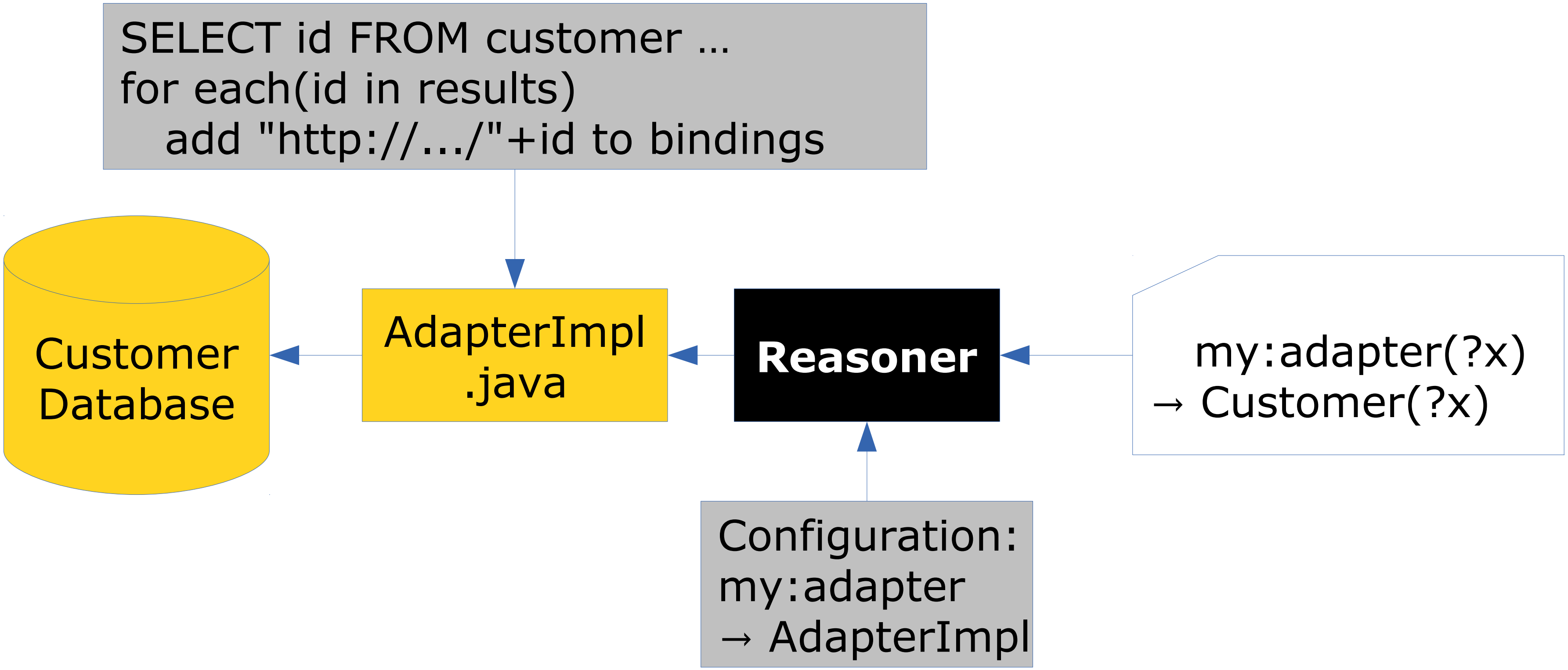
- In that case, the reasoner would have to create *new* instances for Y
  - Possible issue: termination
  - No easy solution in SWRL+OWL

SWRL Extensions and Built-Ins

- Comparison
  - olderThan(?X,?Y) ← hasBirthdate(?X,?BX) ∧ hasBirthdate(?Y,?BY) ∧ swrlb:lessThan(?BX,?BY)
- Arithmetics
  - twiceAsOld(?X,?Y) ← hasAge(?X,?AX) ∧ hasAge(?Y,?AY) ∧ swrlb:multiply(?AX,?AY,2)
- String operations
  - PeopleWithS(?X) ← hasName(?X,?N) ∧ swrlb:startsWith(?N,"S")

SWRL Extensions and Built-Ins

- Some reasoners also allow for custom built-ins
- E.g., for wiring a reasoner to external systems



SWRL Extensions and Built-Ins

- More use cases for custom built-ins
- Live data
  - Weather
  - Stock exchange
  - Product availability

- Complex computations
  - Trip duration from A to B (e.g., Google Maps API)
  - Simulations and predictions
  - ...

Monotonic Reasoning with SWRL

- Recap: monotonous vs. non-monotonous reasoning
  - monotonous: every consequence derived is true forever
  - non-monotonous: consequences may be revoked

- SWRL is monotonous
  - i.e., consequences of all rules add up
  - allows for efficient reasoning
  - may lead to contradictions

Safety of Rules

- Termination guarantee of reasoning

- So far
  - no new instances, classes, and properties are generated
- This constrains the set of consequences which can be derived:
  - C*I type assertions
  - I*O*I object property assertions
  - I*D*L datatype property assertions

→ in monotonous reasoning, the reasoner eventually terminates

Safety of Rules

- Consider this example:

```
:Person rdfs:subClassOf [
  a owl:Restriction ;
  owl:onProperty :hasFather ;
  owl:cardinality 1^^xsd:integer ] .
:hasFather rdfs:range :Person .
:Grandchild rdfs:subClassOf :Person .
```

hasFather(?x,?y) ∧ hasFather(?y,?z) → Grandchild(?x)

- Given

  :Peter a :Person .

- Do we derive GrandChild(Peter)?

Safety of Rules

- Possible solution:
  - We know that each person has a father
  - therefore:

    `:Peter :hasFather _:p0 . _:p0 :hasFather _:p1 . :p1 …`
  - and thus

    `:Peter a :Grandchild .`

- What is the price of that solution?
  - We allow for the creation of new instances
  - i.e., we sacrifice guaranteed termination

Safety of Rules

- DL safe rules:
  - Variables are only bound to *existing* instances
  - No new instances are created
- Thus, we *cannot* derive

```
:Peter a :Grandchild .
```

- Once more: trading off
  - expressivity
  - decidability

Production Rules

- Sometimes, monotonous rules are not desirable
  - consider: if a student passes SWT, his/her credit increases by 6 ECTS

- A first attempt with SWRL + built-ins:

  Student(?X) ∧hasPassed(?X,:SWT)
  ∧hasCredits(?X,?C) ∧swrlb:add(?NC,?C,6)
  → hasCredits(?X,?NC) .

Production Rules

- Consider:

```
:Peter a :Student .
:Peter :hasCredits 26^^xsd:integer .
:Peter :hasPassed :SWT .
```

- After applying the rule:

```
:Peter :hasCredits 32^^xsd:integer .
```

- But rules are monotonous, so the following holds as well:

```
:Peter :hasCredits 26^^xsd:integer .
```

- ...and the reasoner is done yet

Production Rules

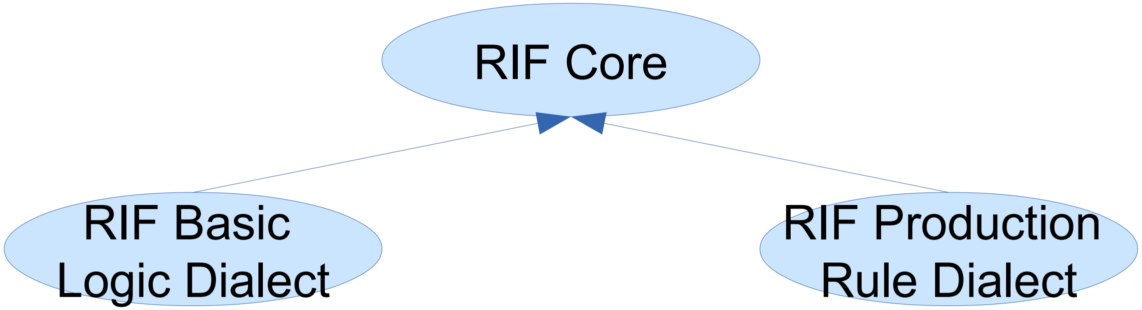
- What happens:

```
:Peter :hasCredits 26^^xsd:integer .
:Peter :hasCredits 32^^xsd:integer .
:Peter :hasCredits 38^^xsd:integer .
:Peter :hasCredits 44^^xsd:integer .
:Peter :hasCredits 50^^xsd:integer .
...
```

- We need to
  - revoke/overwrite statements
    - in contrast to monotonous reasoning!
  - define new criteria for termination

Rule Interchange Format

- Rule Interchange Format (RIF)
- Unification of
  - Basic Logic Rules (such as SWRL)
  - Production Rules (e.g., JENA rules)
- Standardized by W3C in 2010

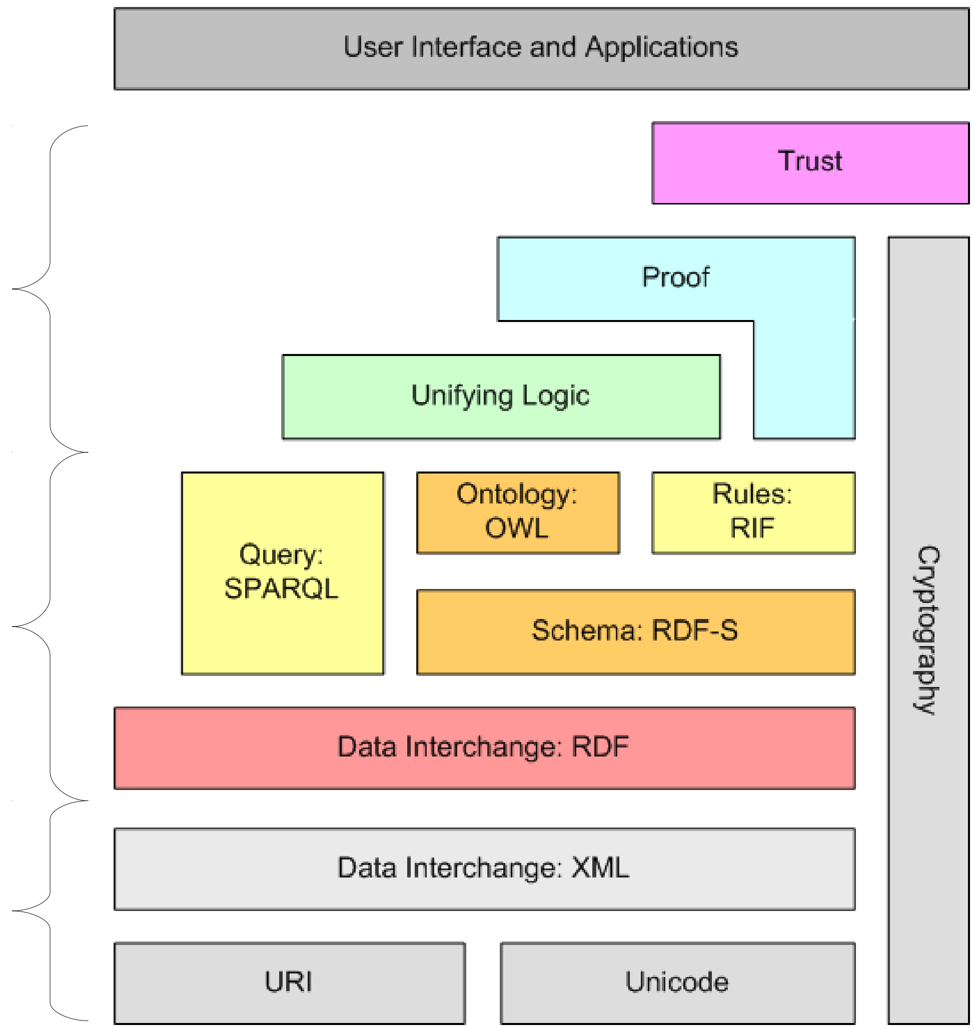


Semantic Web – Architecture

here be dragons...

Semantic Web Technologies (This lecture)

Technical Foundations



Berners-Lee (2009): *Semantic Web and Linked Data*
http://www.w3.org/2009/Talks/0120-campus-party-tbl/

Other Semantic Web Languages

- What else is out there?

>50% non W3C languages

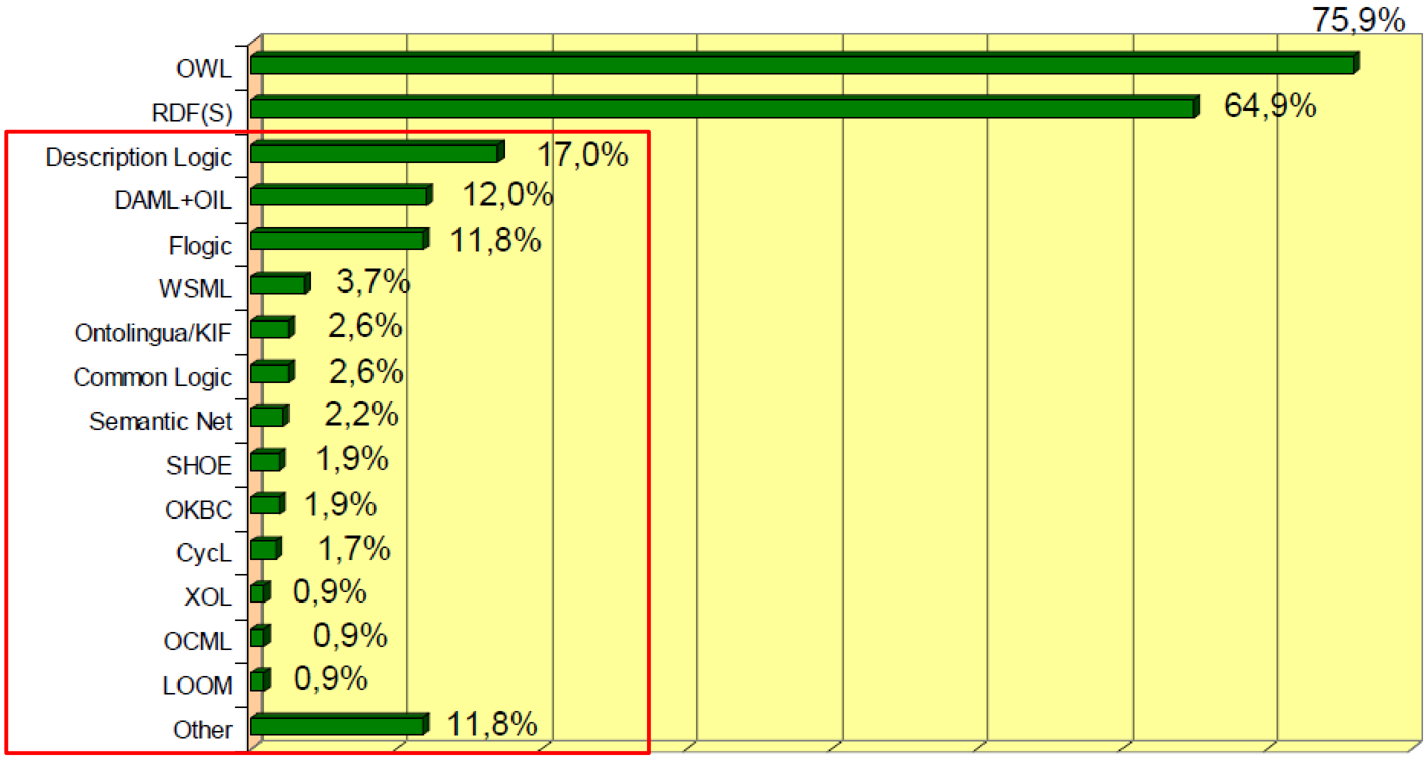


Figure 5. Ontology languages currently used by users.

Cardoso (2006): The Semantic Web Vision – Where are We?

Other Semantic Web Languages

- There is a wild mix
  - of old and new languages
  - of different paradigms
  - of sophisticated languages and pure, low-level logic
- We will look at one example of a radically different language

F-Logic

- Main concept: *frames*
  - collection of properties of a class
  - similar to class and database models

Person	Mother (Person)	Father (Person)	Age (int)
:Paul	:Martha	:Hans	24
:Martha	:Johanna	:Karl	47
...	...	...	...

F-Logic: A First Glance

- First observation:
  - relations are bound to class
  - in RDFS/OWL: first class citizens
- Inheritance
  - Relations are inherited to subclasses
  - Domain and range cannot be restricted any further
- Semantics
  - Closed world semantics
  - Negation can be used

F-Logic: Rules

- Almost everything is expressed in rules

- e.g., property chains:

```
uncleOf(?X,?Z) :-
                  ?X:Man[siblingOf->?Y]
            and ?Z[childOf->?Y] .
```

- Datalog-like syntax
- :- is used for implication ←
- Variables are denoted with ?

F-Logic: Quantifiers

- There are extensional and universal quantifiers

- Authors are persons who have written at least one book

```
?X:Author :- ?X:Person
  AND (EXIST ?Y ?Y:Book and ?X[hasWritten->?Y]).
```

- A non-author is a person who has not written any book

```
?X:NonAuthor :- ?X:Person
  AND NOT(EXIST ?Y ?Y:Book and ?X[hasWritten ->?Y]).
```

- A star author is an author who as *only* written bestsellers

```
?X[isStarAuthor->true] :- ?X:Author AND
  (FORALL ?Y
    (?X[hasWritten->?Y] --> ?Y:Bestseller) ) .
```

F-Logic: Negation

- Negation may have unwanted consequences
- Consider this example:
-
```
?X[hates->?Y] :-
  not(?X[likes->?Y] or ?X[doesntCare->?Y])) .
?X[likes->?Y] :- ?X[knows->?Y] and not(?X[hates->?Y]) .
```

- Assume, the reasoner wants to prove `?X[likes->Stefan] .`

- Possible plan:

```
?X[likes->Stefan] .

?X[knows->Stefan] and not(?X[hates->Stefan])) .

?X[knows->Stefan] and not(not(?X[likes->Stefan] or
                              ?X[doesntCare->Stefan)) .

?X[knows->Stefan] and not(not(?X[knows->Stefan] and ...
```

F-Logic: Decidability and Stratification

- F-Logic ontologies with negations can be undecidable
- Underyling problem:
  - Cycles of rules containing negations
- Simplest case
  - `p(X) :- not(p(X)) .`

- Test: Stratification
  - lat. *Stratum* (pl.: *Strata*): *Layer*
- Divide ontology into layers
- Each predicate is assigned to a layer
  - Classes are treated as unary predicates

F-Logic: Decidability and Stratification

- Assign a layer S(p) to each predicate p
- Two conditions must be fulfilled:
  - for all rules which have p in their head and a non-negated predicate q in the body:

    $S(q) \leq S(p)$
  - for all rules which have p in their head and a negated predicate q in their body

    $S(q) < S(p)$
- If such an assignment can be found, the ontology is decidable

F-Logic: Decidability and Stratification

- Simple case:
- ```
  ?X[hates->?Y] :- not(?X[likes->?Y]) .
  ?X[knows->?Y] :- ?X[likes->?Y] .
  ```

- We have to ensure
  - S(likes) < S(hates)
  - S(likes) ≤ S(knows)

- For those two rules, we can assign
  - S(likes) = 0
  - S(hates) = 1
  - S(knows) = 0
  ```

F-Logic: Decidability and Stratification

- We obtain the following layers

`?X[hates->?Y] :- not(?X[likes->?Y]) .`	*Layer 1*
`?X[knows->?Y] :- ?X[likes->?Y] .`	*Layer 0*

- Trivial observation
  - For ontologies without negation, one layer is enough!

F-Logic: Decidability and Stratification

- Back to the original example

```
?X[hates->?Y] :-
  not(?X[likes->?Y] or ?X[doesntCare->?Y])) .
?X[likes->?Y] :- ?X[knows->?Y] and not(?X[hates->?Y])
.
```

- Can we find a stratification?
- We would need
  - S(likes) < S(hates)
  - S(hates) < S(likes)

- This is not possible!

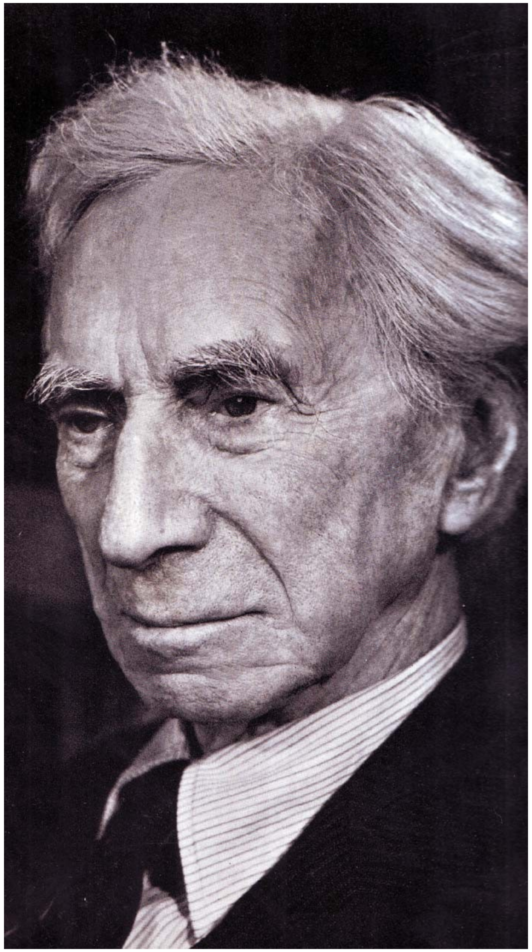
  → The ontology cannot be stratified, i.e., it is undecidable!

Recap: Russell's Paradox

- A classic paradox by
  Bertrand Russell, 1918

- In a city, there is exactly one barber who shaves everybody who does not shave themselves.

  Who shaves the barber?



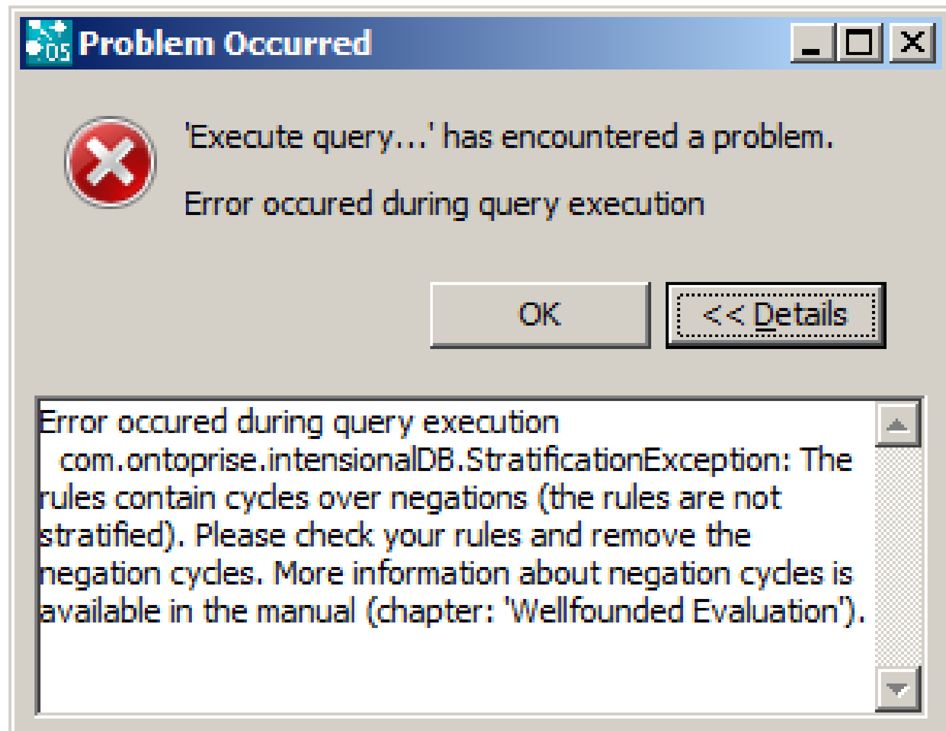
F-Logic: Decidability and Stratification

- Russell's paradox in F-Logic:

  theBarber[shaves->?X] :- not(?X[shaves->?X]) .

- We would need

  S(shaves) < S(shaves)



Validating Datasets with RDF Shapes

- Ontology reasoning is good for semantic validation
  - but sometimes problematic due to semantic properties
  - i.e., closed world assumption, non unique name assumption

- To validate data quality
  - we want to ensure certain data is there
    - e.g., every person has a name
  - we want to ensure that data is not duplicated
    - e.g., every person has exactly one birth place
  - etc.

Validating Datasets with RDF Shapes

- Example dataset:

```
:Mary a :Person .
:Mary :birthPlace :Mannheim .
:Mary :birthPlace :Berlin .
```

- Constraints in OWL:

```
Person rdfs:subClassOf [
  a owl:Restriction .
  owl:onProperty :name .
  owl:minCardinality 1 . ]
Person rdfs:subClassOf [
  a owl:Restriction .
  owl:onProperty :birthPlace .
  owl:maxCardinality 1 . ]
```

Shapes Constraint Language (SHACL)

- A W3C Standard since 2017
- For RDF *validation*
- Differences to reasoning
  - Closed world evaluation
  - Counting is possible
  - More fine-grained checks (see later)

Shapes Constraint Language (SHACL)

- Example dataset:

```
:Mary a :Person .
:Mary :birthPlace :Mannheim .
:Mary :birthPlace :Berlin .
```

- Constraints in SHACL:

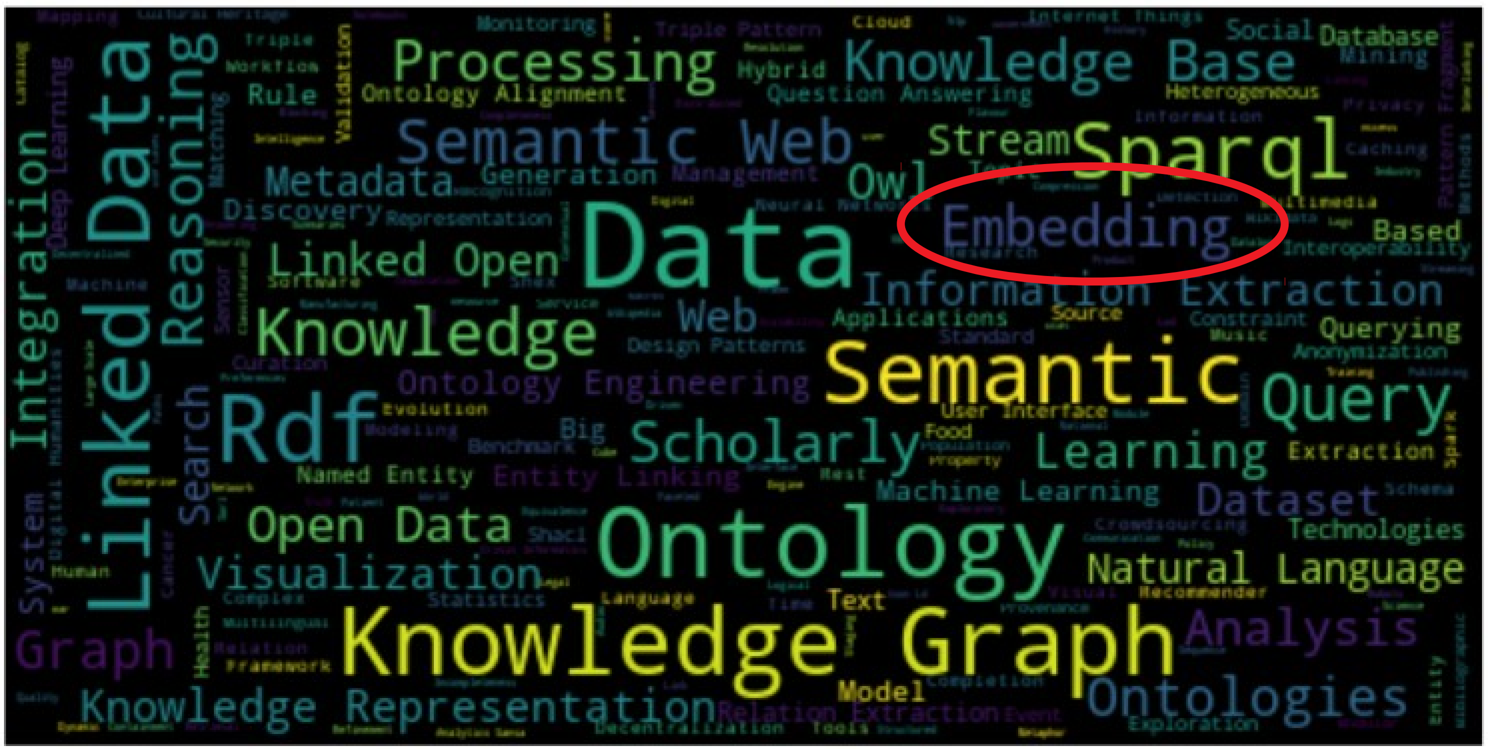
```
:PersonShape
    a sh:NodeShape ;
    sh:targetClass :Person ;
    sh:property [
        sh:path :name ;
        sh:minCount 1 ;
        sh:datatype xsd:string ] ;
    sh:property [
        sh:path :birthPlace ;
        sh:maxCount 1 ;
        sh:class :City ] .
```

Shapes Constraint Languages

- Further possibilities
  - Dependencies between attributes
    - e.g., given name and first name are equivalent
  - Complex expressions involving paths and even SPARQL queries
  - Checking strings against regex patterns (e.g., phone numbers)
  - ...

RDF Embeddings

- One of the current hot topics in Semantic Web research:
  - Embeddings



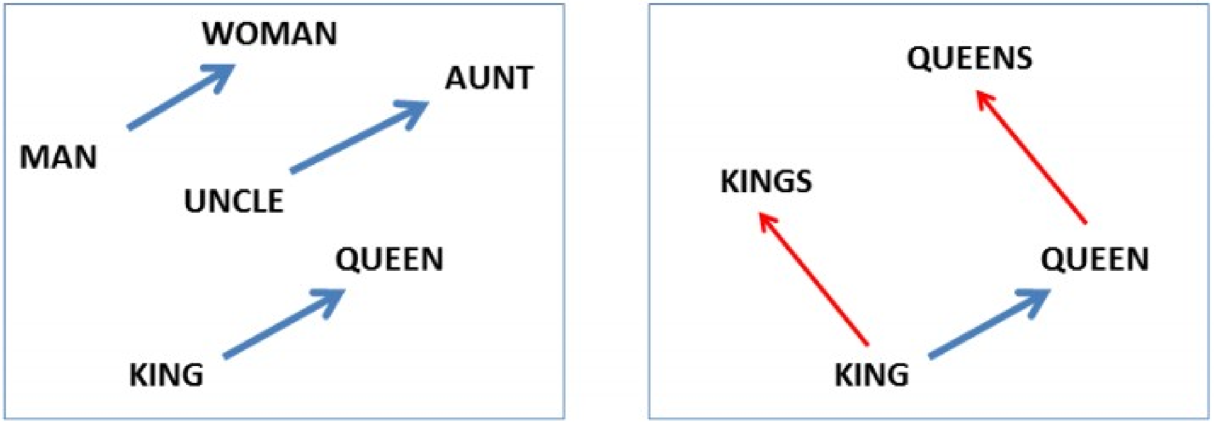
RDF Embeddings

- Challenge in RDF/OWL etc.:
  - How similar are two entities?
  - e.g., is Mannheim more similar to Karlsruhe than to Heidelberg?

- Application scenarios:
  - Recommender systems
  - Information retrieval

Excursion: word2vec

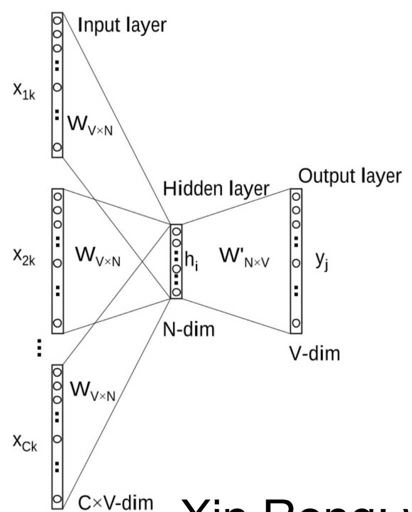
- Such approaches exist for words
  - aka, *word embeddings*
  - each word becomes a vector in a low-dimensional vector space
  - similar words are close in that vector space
  - semantic relations have a similar direction and length
    - allows for arithmetics, e.g., King – Man + Woman = Queen

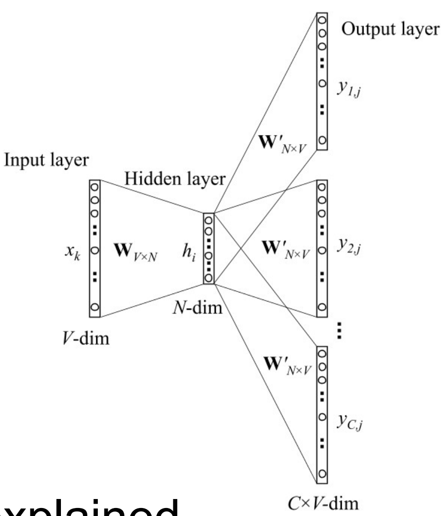


(Mikolov et al., NAACL HLT, 2013)

word2vec

- General idea: similar words appear in similar contexts
- Training set: sequences from a text corpus
- Training method: neural network
- Training variants:
  - Continuous bag of words (CBOW): predict a word from its context
  - Skip-Gram: predict context from a word





Xin Rong: word2vec parameter learning explained

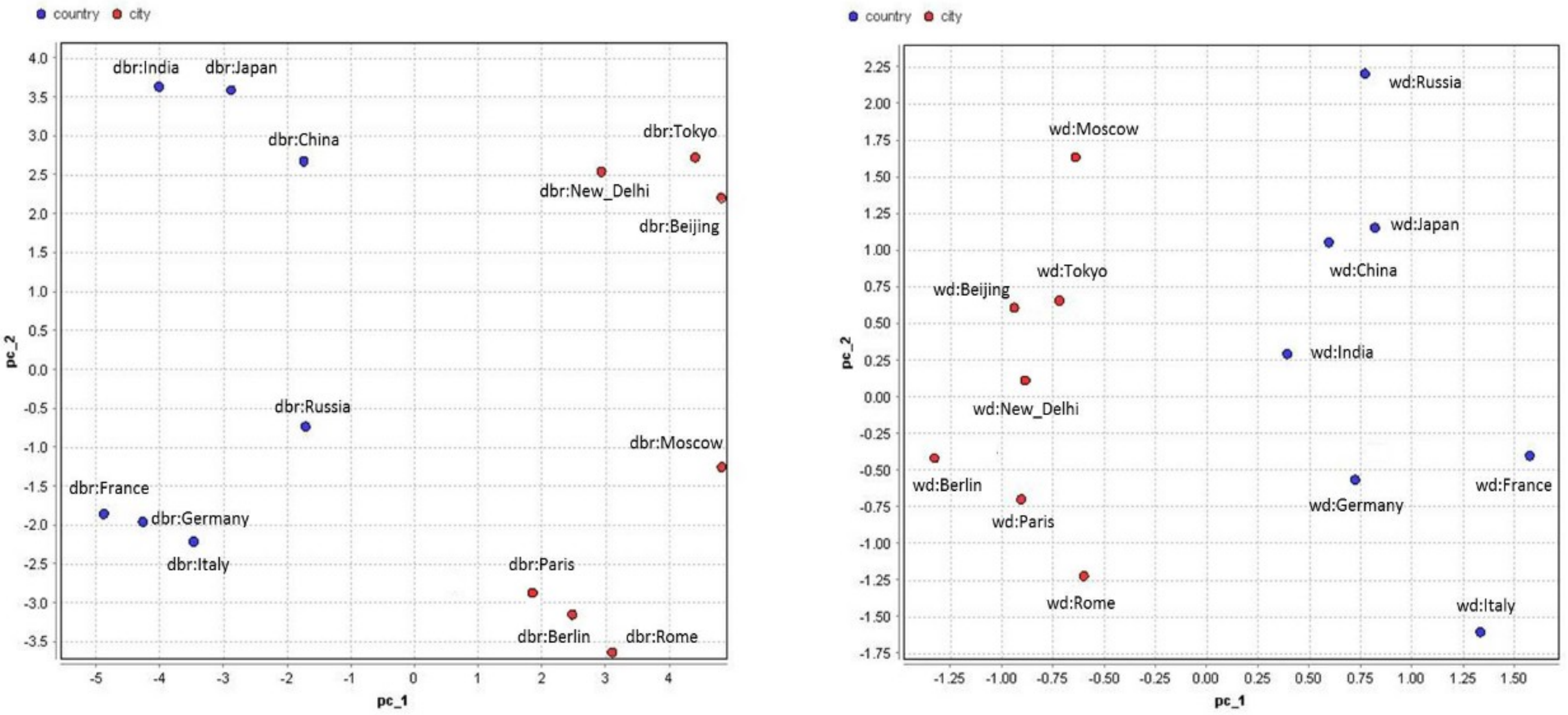
From word2vec to RDF2vec

- Generating sequences from an RDF dataset
  - by starting random walks from each entity
- Example:
  - dbr:Germany dbo:capital dbr:Berlin dbo:mayor dbr:Michael_Mueller
- Those are fed into a word2vec training engine

- Variants (Cochez et al., 2017)
  - replace “random” by “semi-random” walk
  - e.g., weight edges by frequency, PageRank, ...

From word2vec to RDF2vec

- Observation: similar properties hold for RDF2vec

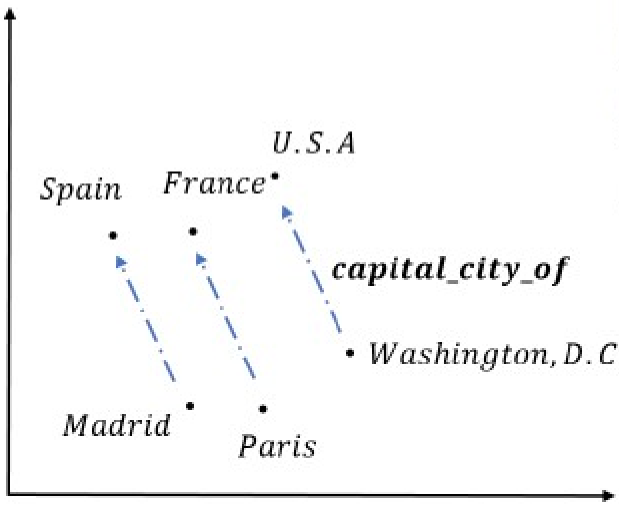


a) *DBpedia vectors* b) *Wikidata vectors*

Ristoski & Paulheim: RDF2vec: RDF Graph Embeddings for Data Mining, 2016

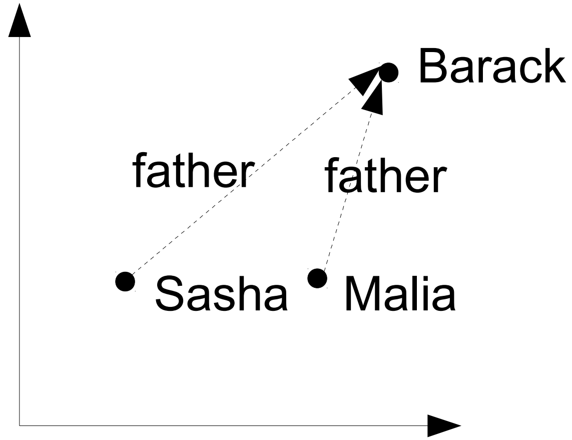
TransE and Descendants

- In RDF2vec, relation preservation is a by-product
- TransE: direct modeling
  - Formulates RDF embedding as an optimization problem
  - Find mapping of entities and relations to R^n so that
    - across all triples <s,p,o>
      Σ ||s+p-o|| is minimized



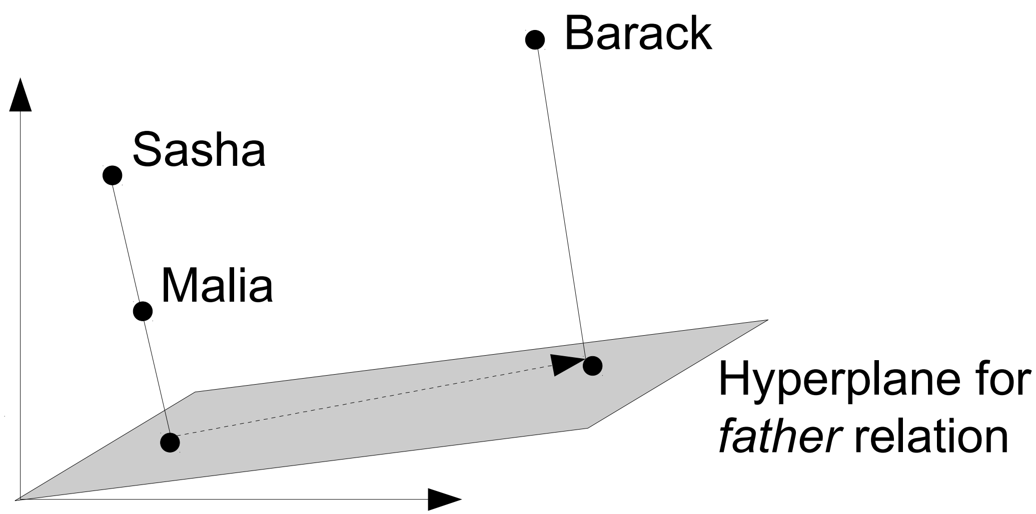
Limitations of TransE

- TransE works fine if we have 1:1 relations
  - But what in case of 1:n or n:m relations?
- Example below:
  - We have to miminize
    ||Malia + father – Barack|| + ||Sasha + father – Barack||
  - This is minimized if ||Malia|| = ||Sasha||
  - i.e., they become indistinguishable



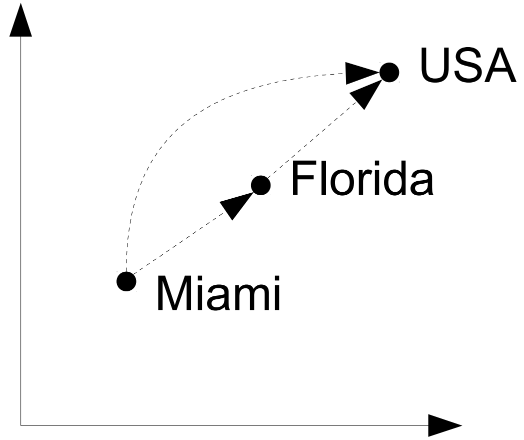
Extension: TransH

- In TransH, there is a hyperplane per relation
  - Subject and object are projected to that hyperplane
  - On each hyperplane, a TransE-like optimization is conducted
- *Sasha* and *Malia* become indistinguishable on *father* hyperplane
  - But are still distinguishable in the vector space



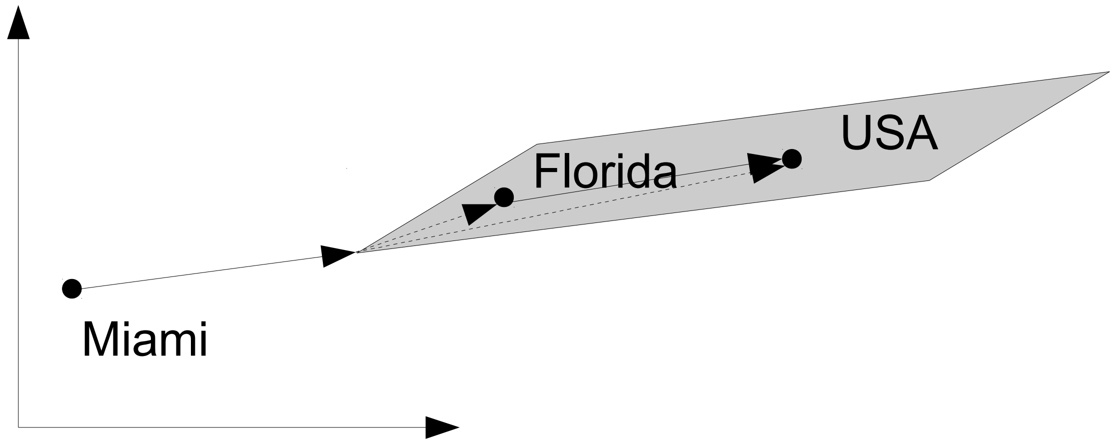
Limitations of TransE

- Transitive Properties
  - we have to minimize
    ||Miami + partOf – Florida|| and ||Florida + partOf – USA||, but also
    ||Miami + partOf – USA||
  - ideally, *Miami + partOf = Florida*, *Florida + partOf = USA*,
    Miami + partOf = USA
    - Again: all three become infinitely close
    - partOf becomes 0 vector



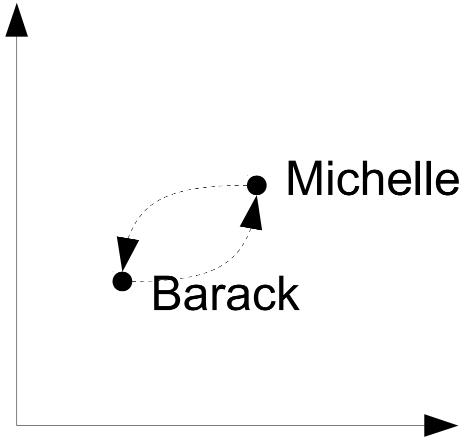
Extension: TransE-DT (2017)

- Entities and relations can be hyperplanes
  - Represented as the vector of the hyperplane plus an individual vector
  - Relations can hold between a point and a hyperplane or two hyperplanes
  - Relations may be hyperplanes themselves



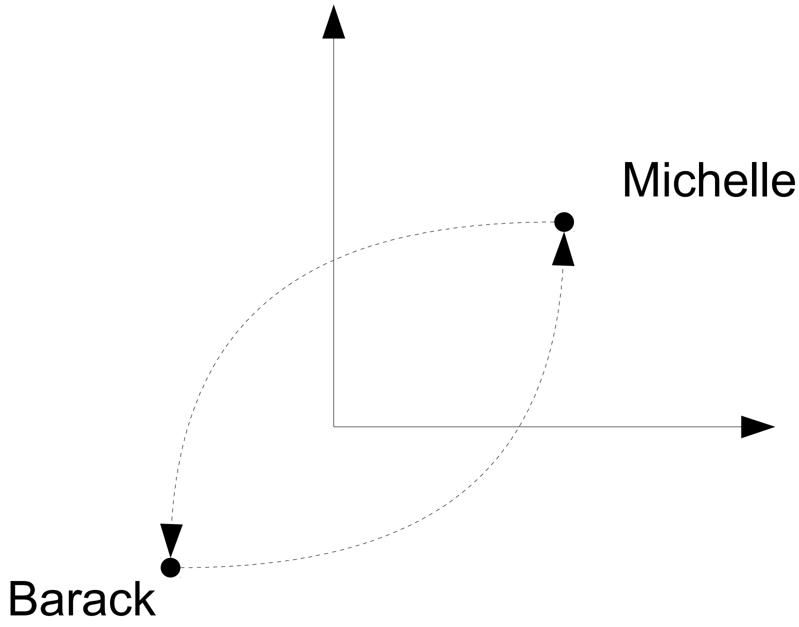
Limitations of TransE

- Symmetric properties
  - we have to minimize
    ||Barack + spouse – Michelle|| and ||Michelle + spouse – Barack||
    simultaneously
  - ideally, *Barack* + *spouse* = *Michelle* and *Michelle* + *spouse* = *Barack*
    - Michelle and Barack become infinitely close
    - spouse becomes 0 vector



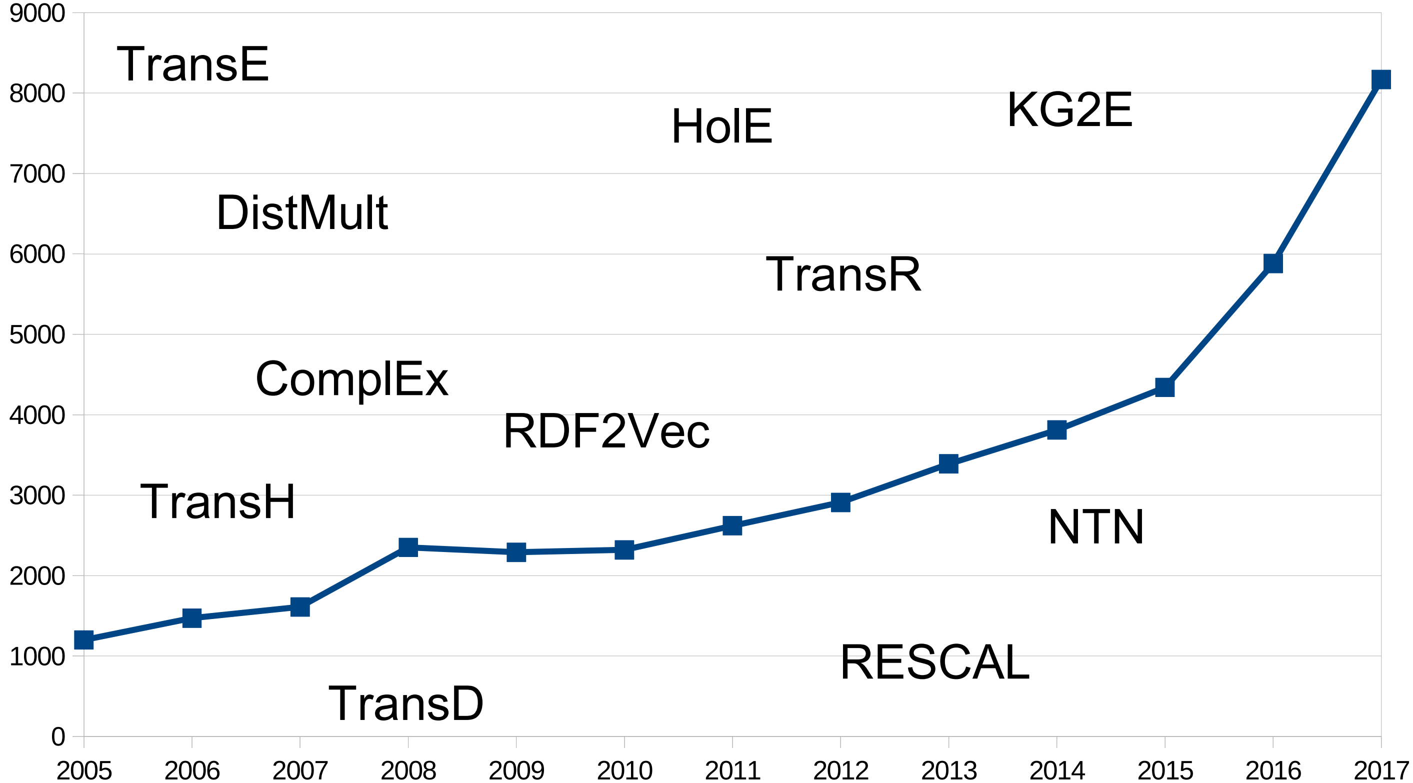
Extension: RotatE (2019)

- Relations are not represented as *straight vectors*, but rotations
  - This allows for symmetric relations
  - Also works for reflexive relations (they become a rotation by 360°)



Limitations of TransE

- Numerous variants of TransE have been proposed to overcome limitations (e.g., TransH, TransR, TransD, …)
- Plus: embedding approaches based on tensor factorization etc.



A Look Back

- This is where we embarked on our Semantic Web Technologies journey in September:

```
<html>
  …
  <b>Dr. Mark Smith</b>
  <i>Physician</i>
  Main St. 14
  Smalltown
  Mon-Fri 9-11 am
  Wed 3-6 pm
  …
</html>
```

In the eyes of a human

Dr. Mark Smith
Physician
Main St. 14
Smalltown
Mon-Fri 9-11 am
Wed 3-6 pm

in the eyes of a computer

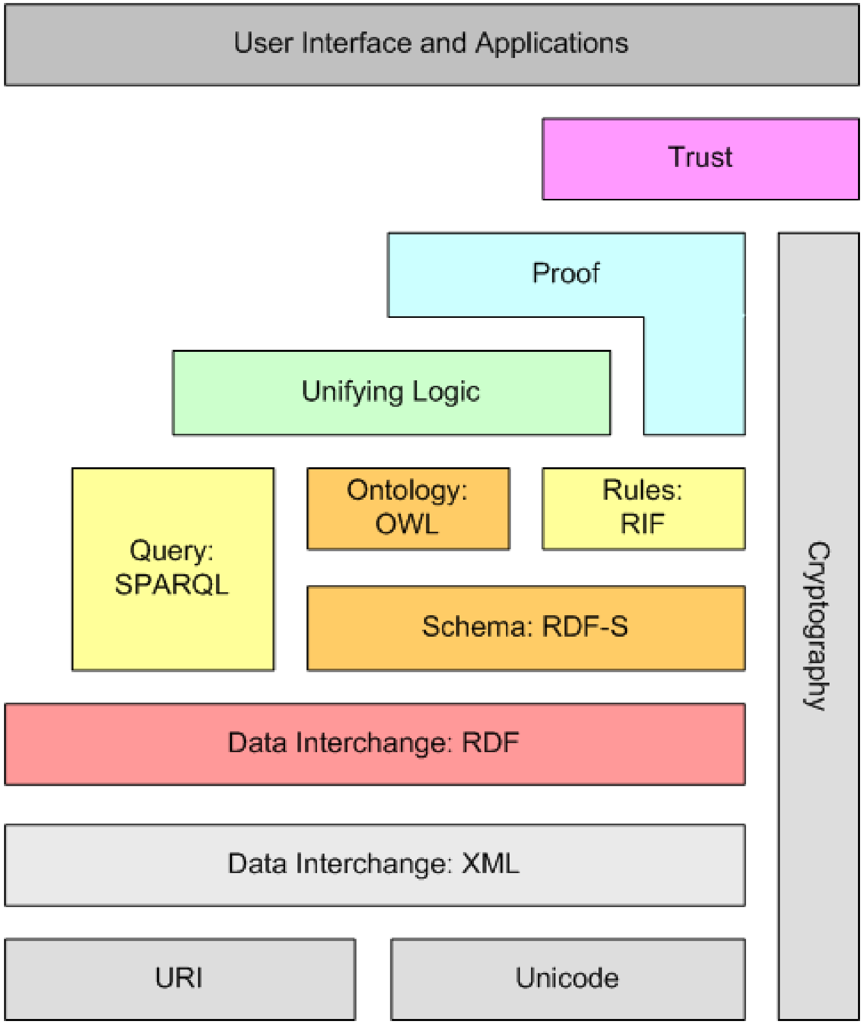
Print in bold: „hmf298hmmhudsa"
Print in italics: „mj2i9ji0"
Print normal: „fdsah 02hfadsh0um2m0adsmf0ihm asdfjköfdsa298ndsfmij32mio lk2mjpoimjiofdpmsajiomjm"

A Look Back

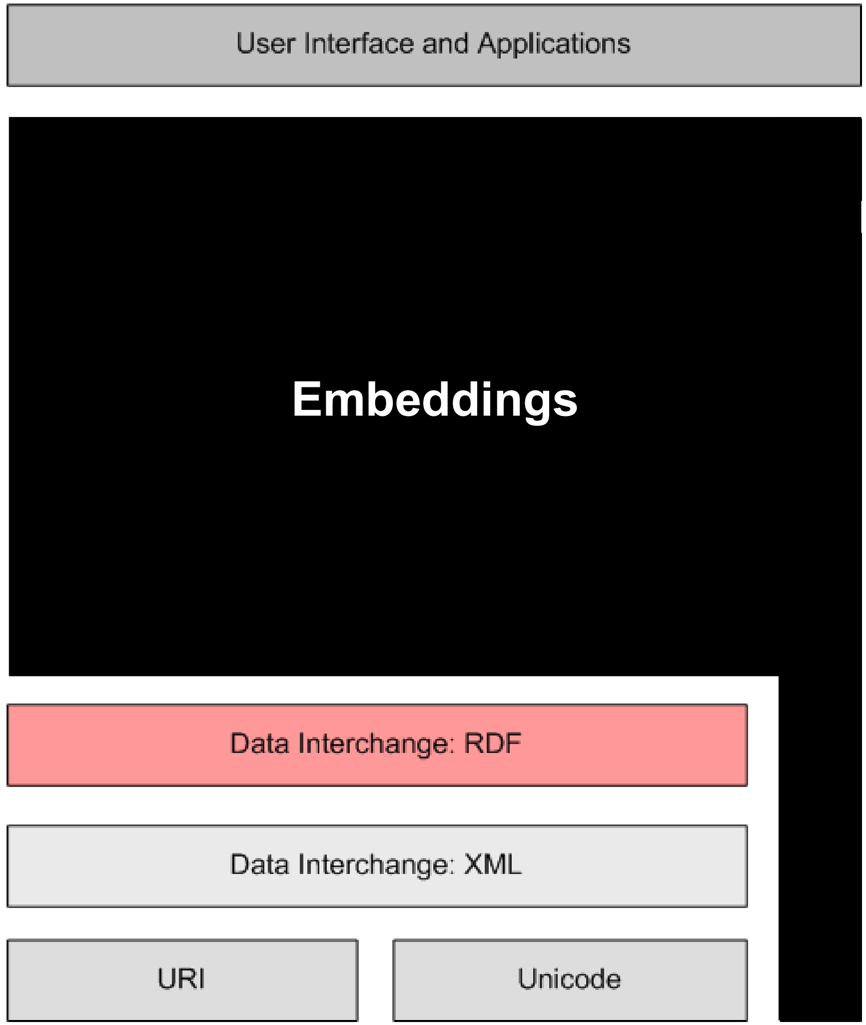
- Formal Semantics
  - Every entity has classes and relations to other entities
  - Those are defined in an ontology
  - Humans and computers can interpret those semantics
  - Computers give justification on reasoning results

- Embeddings
  - Every entity is an n-dimensional vector
  - We do not know about the meaning of the dimensions
  - Results are often good, but hard to justify

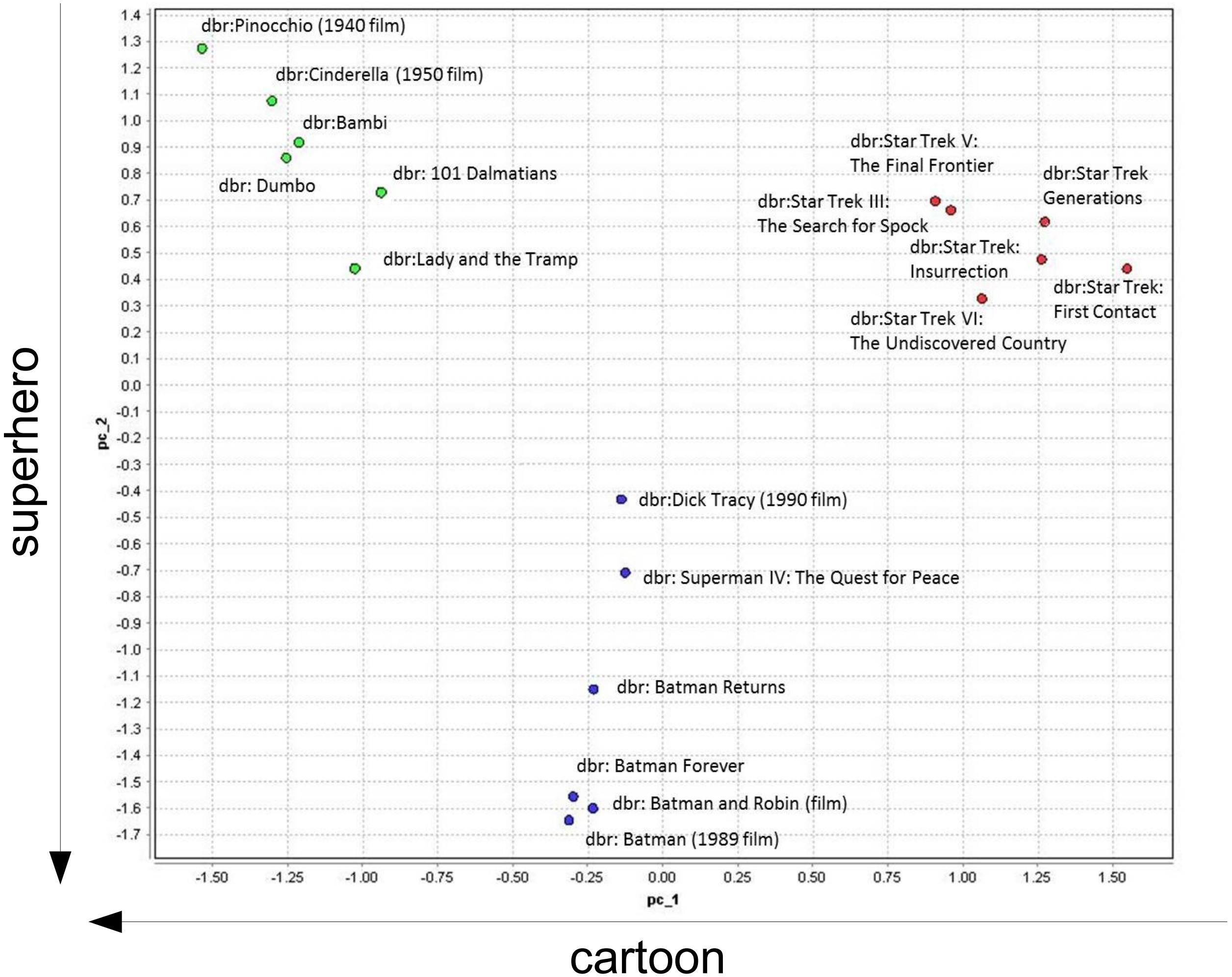
The 2009 Semantic Web Layer Cake



The 2018 Semantic Web Layer Cake



Towards Semantic Vector Space Embeddings



The Holy Grail

- Combine semantics and embeddings
  - e.g., directly create meaningful dimensions
  - e.g., learn interpretation of dimensions a posteriori
  - ...

Summary

- OWL and OWL 2 are not the end
  - Rules create more possibilities
- Other (non W3C standard) languages have also been also proposed
  - different semantic paradigms (e.g., F-Logic)
  - different problem setting (e.g., SHACL)
- Recent trend
  - using vector space embeddings
  - challenge: combine interpretable semantics and embeddings

Questions?