Neuro-Symbolic Knowledge Representation and Reasoning

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ESSAI 2024 Athens

Preamble

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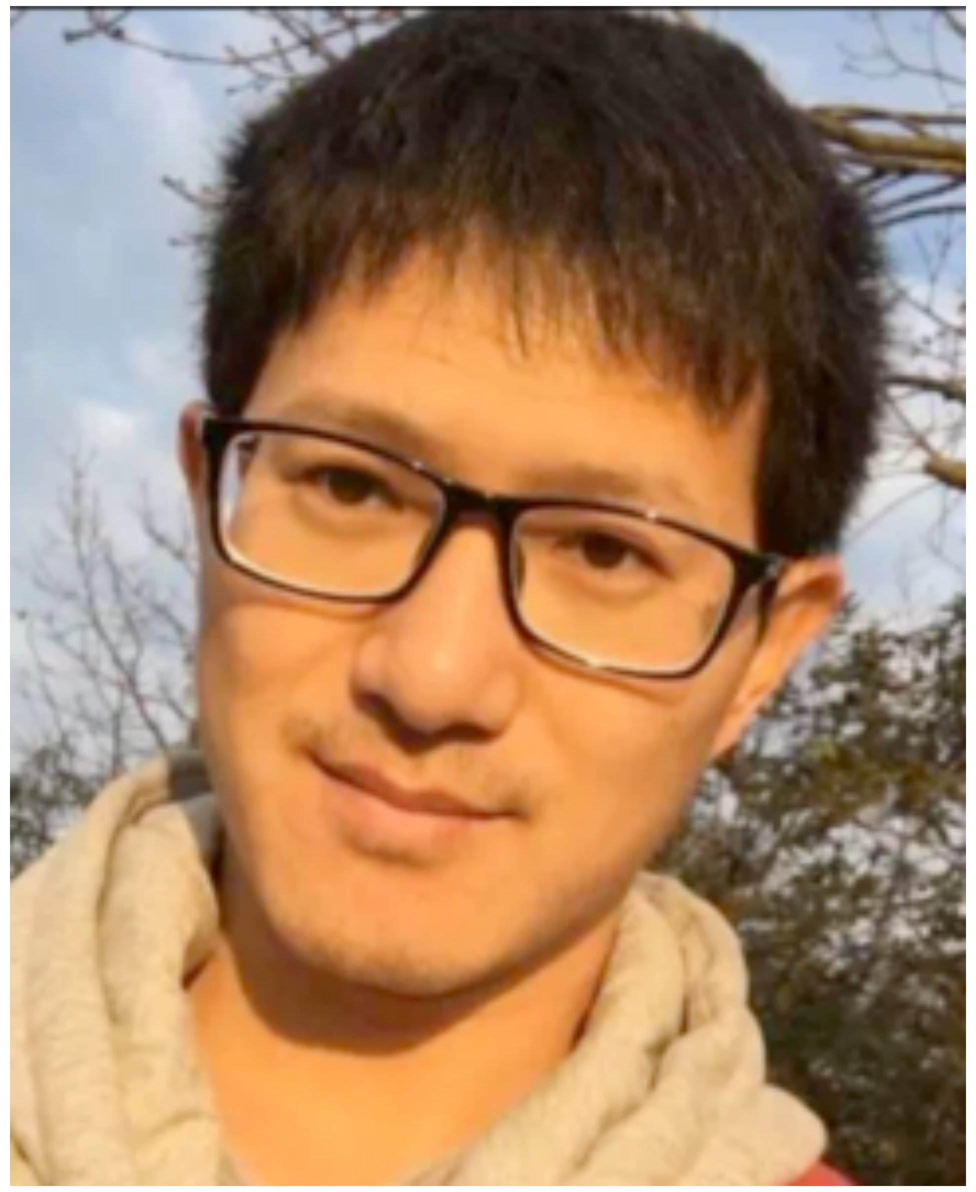
This course is



- introductory
- aimed at general computer scientist

- taught by
  - Jiaoyan Chen - days 3-5
  - Uli Sattler - days 1-2

- explores combination/integration/collaboration of
  - neural &
  - symbolic
    - approaches to knowledge representation, reasoning, ML, …

Overview of this course

Day	Topic	Concepts	Technologies
1	Knowledge Graphs	parsing/serialisation, queries, schemas, validation & reasoning	RDF(S), SPARQL, SHACL,
2	Ontologies	Facts & background knowledge, entailments, reasoning & materialisation	OWL, OWL API, Owlready, Protégé
3	Knowledge Graph Embeddings	Classis Es, literal-aware Es, variants, evaluation	TransE, TransR
4	Ontology Embeddings	Geometric embeddings, literal-aware OEs, soundness & completeness	ELEm, BoxEL, Box^2EL, OWL2Vec*, HiT
5	Applications & Outlook	Preprocessing, materialisation, evaluation	DeepOnto, mOWL

Brief Recap

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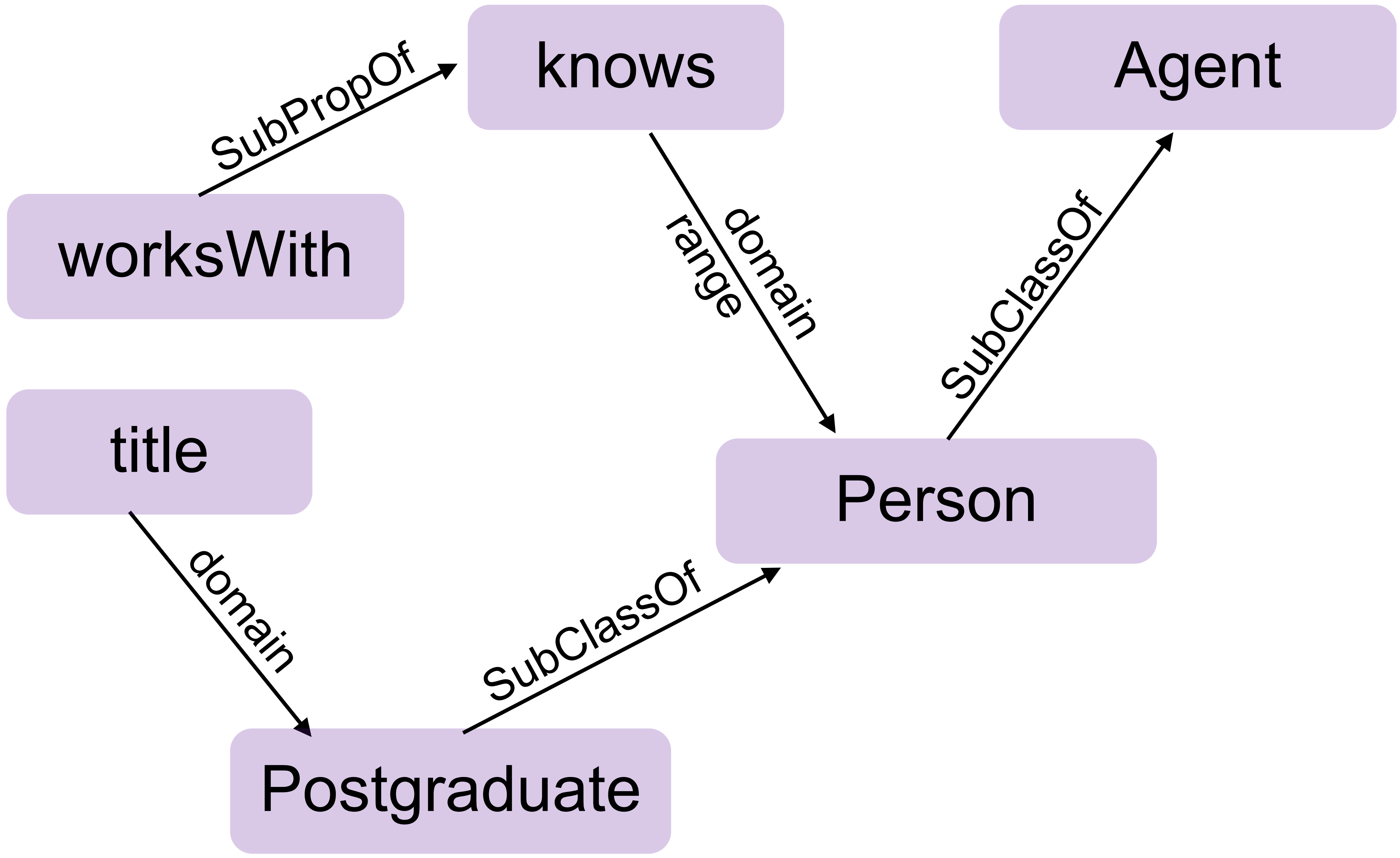
Yesterday:

- Knowledge Graphs
  - RDF
  - factual and conceptual knowledge
- Querying of and Reasoning with KGs
  - SPARQL
  - RDFS
  - SHACL
  - Materialisation of reasoning results
    - making *explicit* the facts we know
    - helps us deal with *incomplete* KGs



Today:

- More on reasoning
  - OWL
    - what we can/can't say
    - why we should
  - materialisation…the many choices!

Day 2: Brief RDFS Recap and OWL Warm-Up

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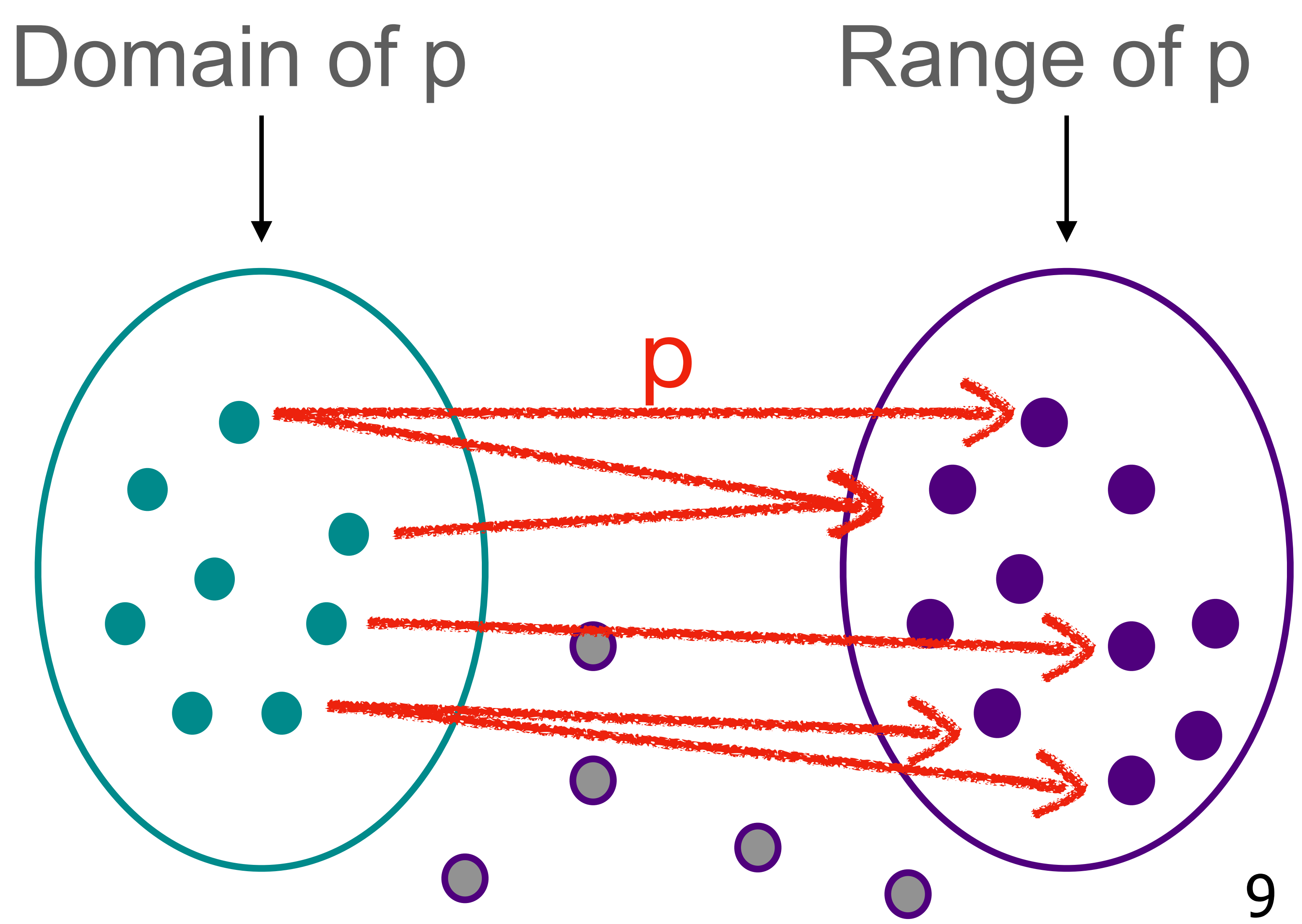
In RDFS, we can state *conceptual knowledge*:

- rdfs:**subClassOf**
  - e.g. (foaf:Person, rdfs:subClassOf, foaf:Agent)
  - (ex:Woman, rdfs:subClassOf, foaf:Person)
- rdfs:**subPropertyOf**
  - e.g. (ex:worksWith, rdfs:subPropertyOf, foaf:knows)
- rdfs:**domain**
  - e.g. (ex:hasChild, rdfs:domain, foaf:Person)
    (foaf:currentProject, rdfs:domain, foaf:Person)
- rdfs:**range**
  - e.g. (ex:hasChild, rdfs:range, foaf:Person)
    (foaf:currentProject, rdfs:range, foaf:Project)

Only statements between *atoms*



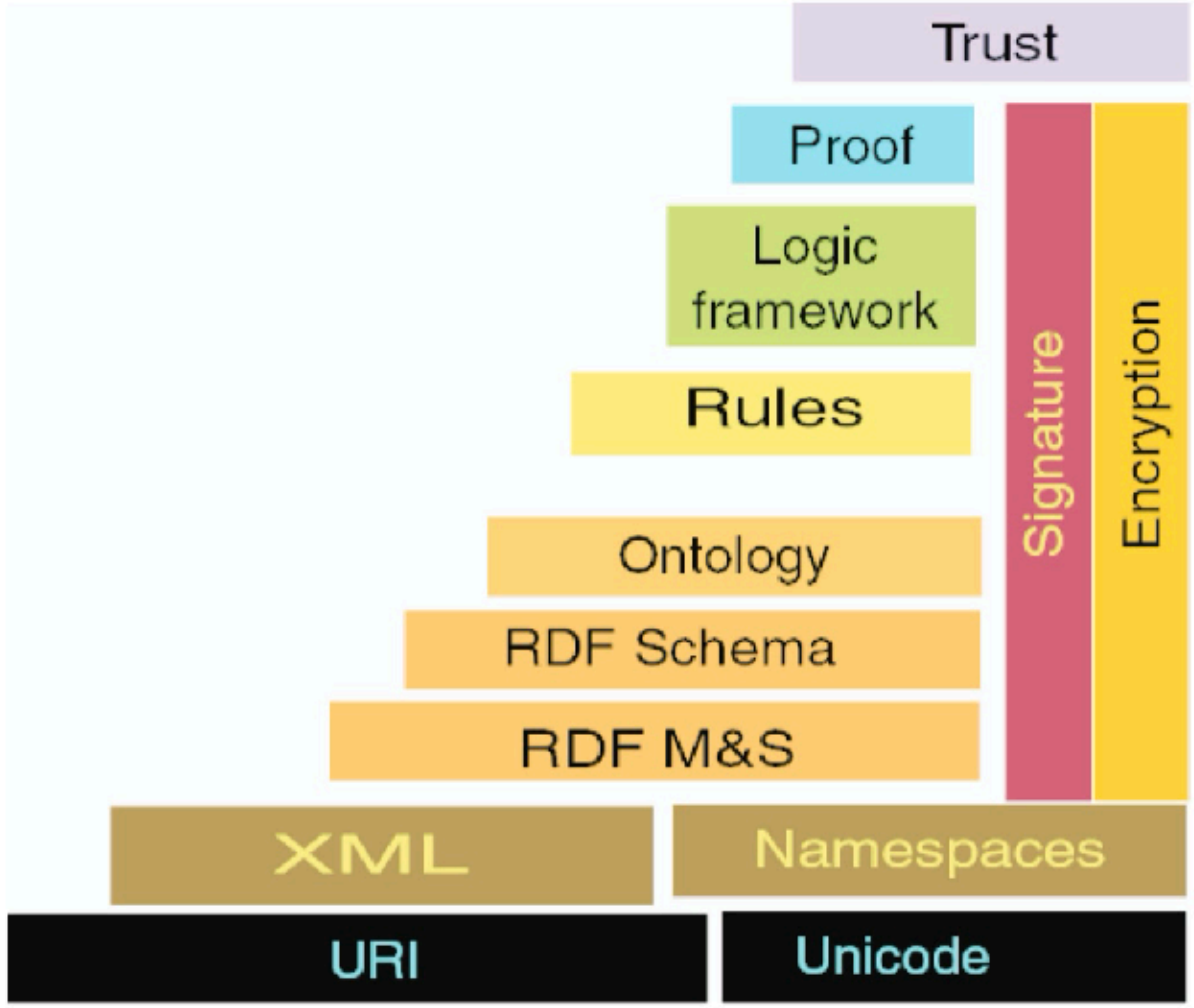
Background/Conceptual Knowledge

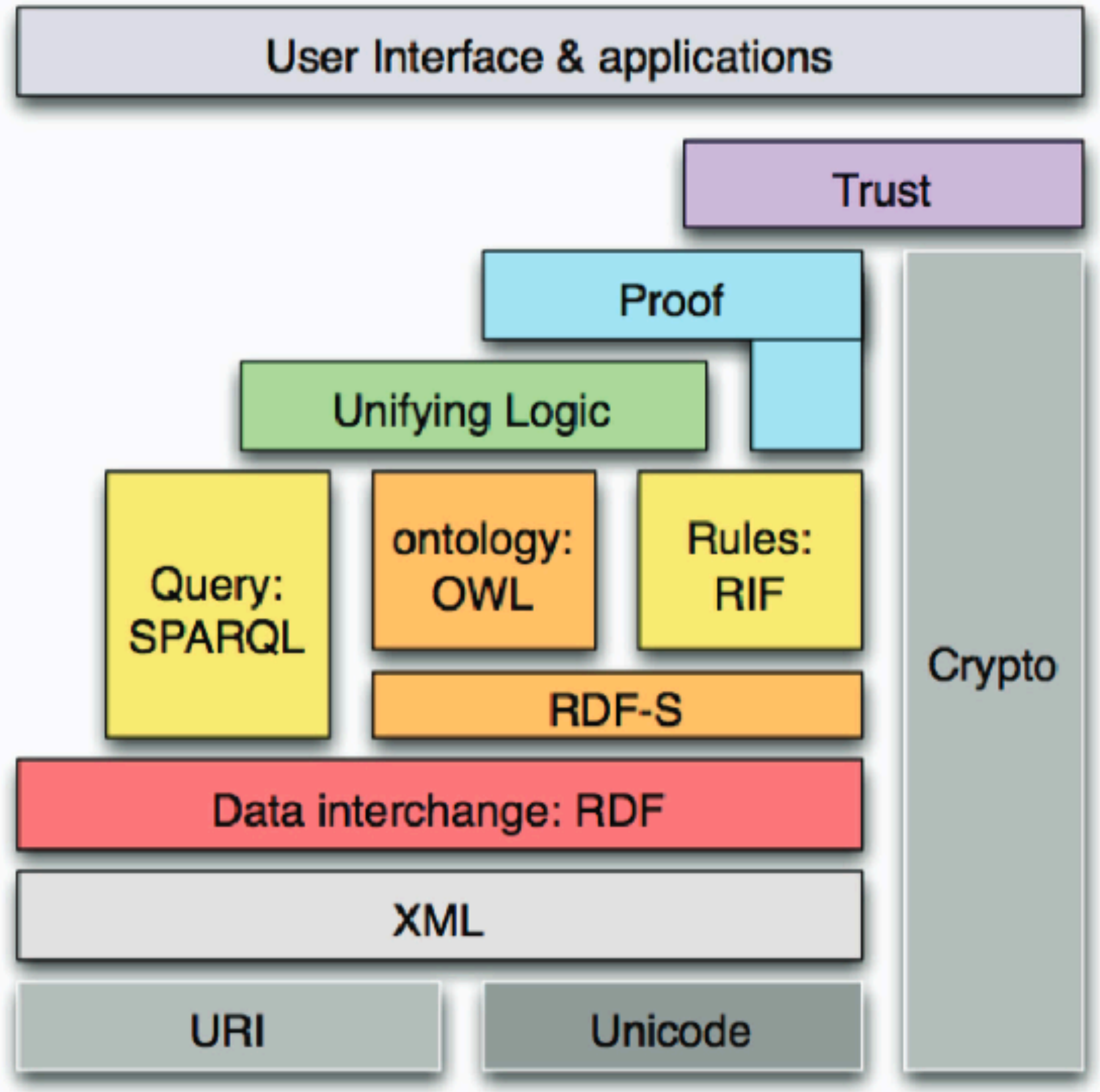
- can be *richer*
  - eg “hasChild is the inverse of isChildOf”
  - eg “isRelatedTo is transitive”
- may involve *expressions*
  - eg “Parents are those Persons who have a child”
  - eg “All children of a Person are also Persons”

- …we need a richer, more expressive language

The Semantic (Web) Layer Cake

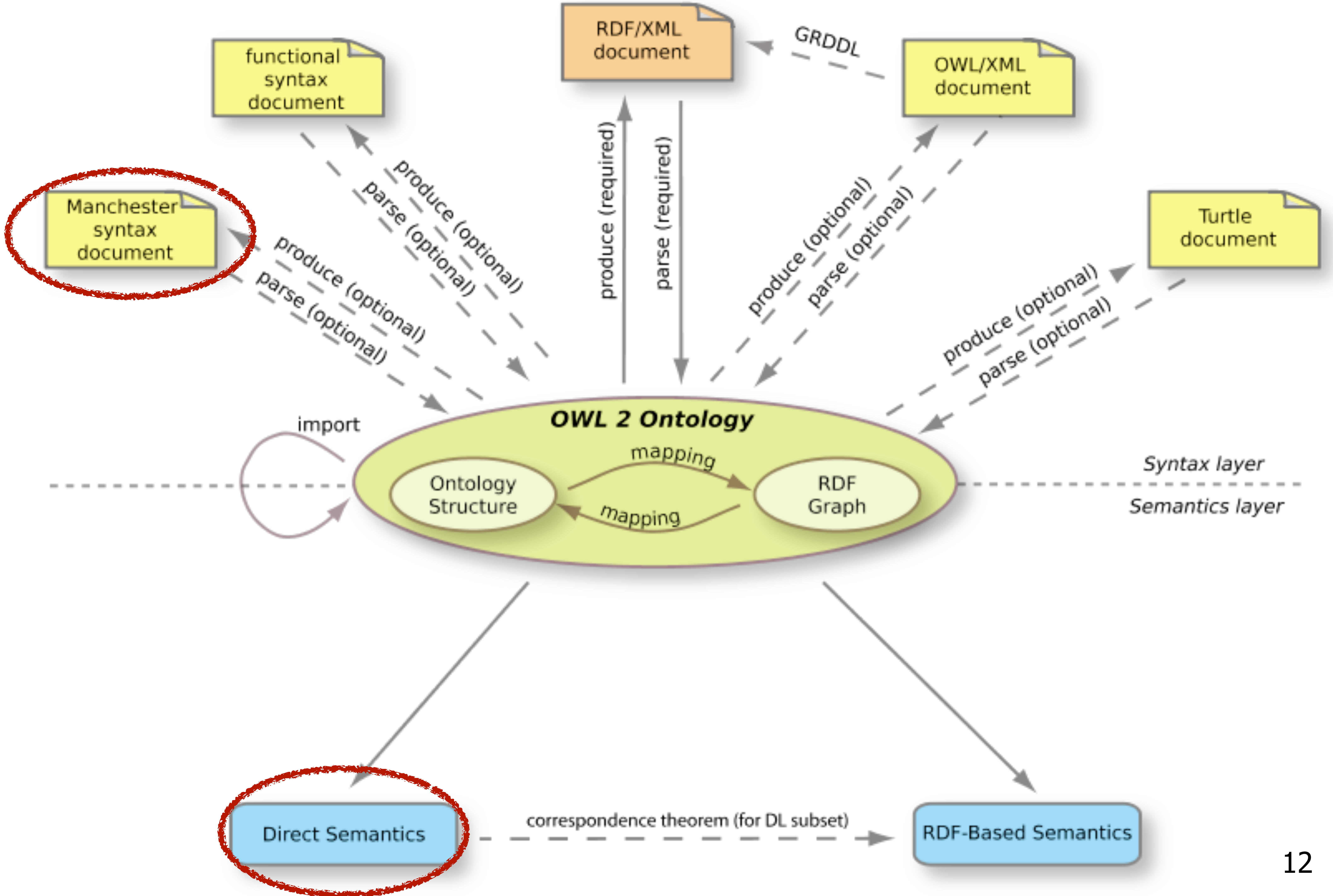
- To describe knowledge, we need a richer, more expressive language
  - background
  - conceptual
  - ontological
  - …
-





OWL is a *Web* Ontology Language

- entity names are IRIs
  - various syntaxes
    - RDF/XML
    - OWL/XML
    - Manchester syntax
    - …
- import mechanism
- version mechanism
- annotations of
  - entities
  - axioms
  - …



Different kinds of knowledge

RDFS

Controlled Vocabulary = {terms for concepts}

Taxonomy = CV + hierarchy

Classification system = Taxonomy + principles

Thesaurus = Taxonomy + more labels

Terminology = … + glossary/explanations

OWL

Ontology = … + logical axioms
+ well-defined semantics
+ reasoning
+ ….

Interlude

Concept

- denotes a set things
- class in RDF(S) or OWL
- 1 concept can have
  - more than 1 terms
    - Person, Human, Peo
  - different terms in diffe
    or contexts

Term

- is a string
  - in a language
- of many strings

In RDFS/OWL

- use class names as you like
- use annotations for
  - labels
  - preferred labels
  - labels in different languages/contexts

What is an OWL ontology?

- A set of *statements* about *entities*
  - eg, Person is a subclass of Agent
  - eg, worksFor is a subProperty of knows
- with a well-defined, logic-based *semantics*
  - directly or
  - via a translation:
    - $\forall x\,.\,\text{Person}(x) \Rightarrow \text{Agent}(x)$
    - $\forall x, y\,.\,\text{worksFor}(x, y) \Rightarrow \text{knows}(x, y)$
- and (usable) (reasoning) services required to
  - design, evolve, maintain, and use ontologies.

Inside an ontology, we find

- classes (unary relations)
  - describing sets of elements, eg, Agent, Person, Course
- properties (binary relations)
  - relating elements, eg, worksFor, knows, hasChild
- individuals
  - describing elements, eg, jchen, sattler
- axioms
  - constraining how we interpret the above:
  - eg, Person is a SubClass of Agent
  - eg, Employee is a SubClass of Person and works for some Company
- annotations
  - to record information about terms, axioms, …

Next:

- Dive into OWL
  - what we can see
  - how we can write it down
  - what it means
  - how to reason about it
- Back to materialisation of reasoning results

Day 2: OWL Syntax

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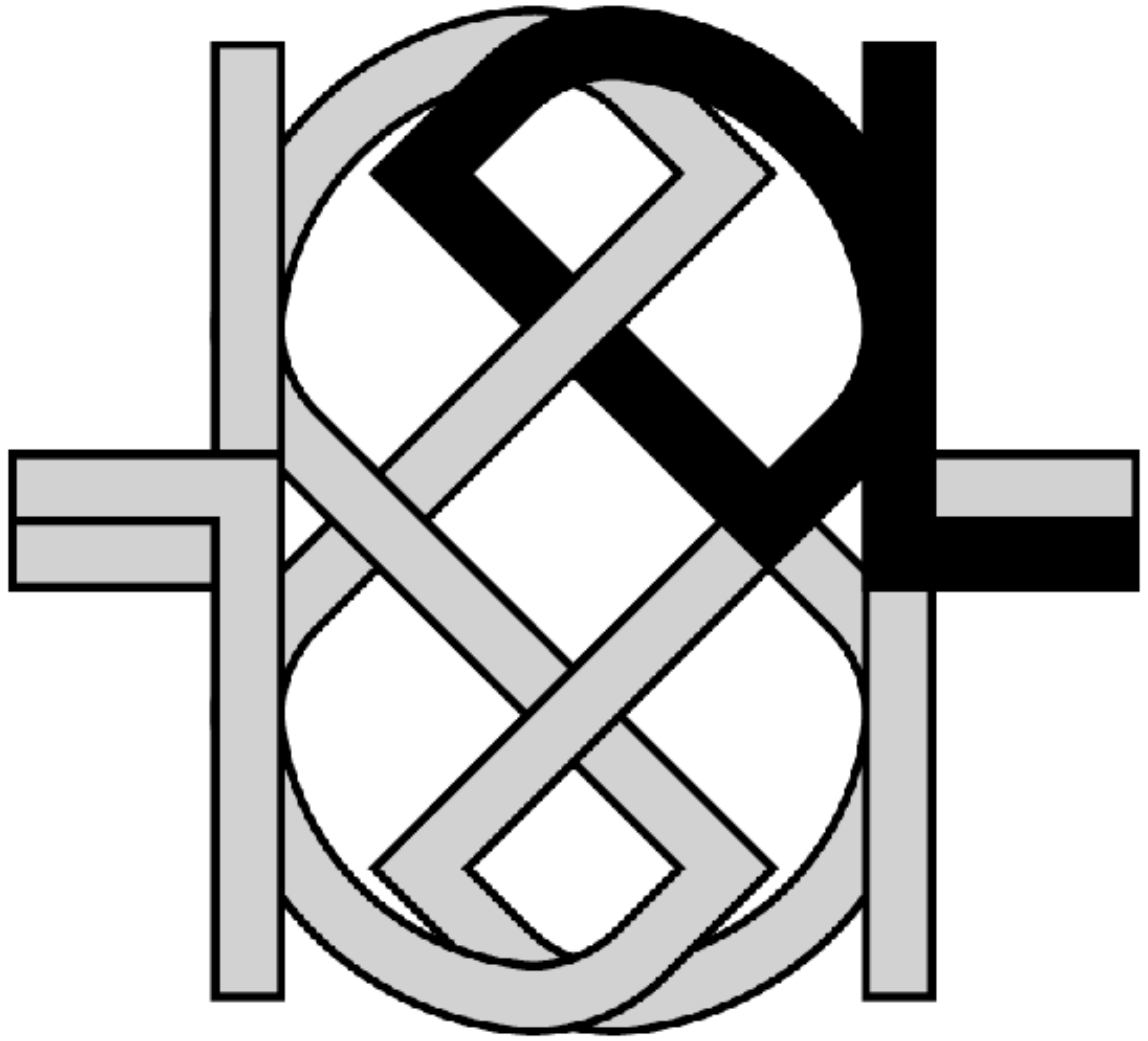
OWL

- is based on *description logics*
  - a well-understood family of logic for KR&R
  - with *nice* properties:
    - decidable reasoning problems with
    - known computational complexity
- comes in 3 flavours/*profiles*
  - for different applications
- comes in many different syntaxes
  - so far, I used mainly “English”…

Description Logics

- decidable fragments of First Order Logic
  - more expressive than Boolean Logic
  - less than FOL
- closely related to
  - modal logics, guarded fragments
  - hybrid logics
- capture monotonic aspects of
  - frame-based systems
  - semantic networks
- complexity of reasoning ranges
  - from AC_0 via polynomial to ExpTime and NExpTime



OWL Axioms - an example

Manchester syntax

Inflammation	*SubClassOf*	Disease
HeartDisease	*EquivalentClass*	Disease *and* hasLoc *some* Heart
Endocarditis	*EquivalentClass*	Inflammation *and* hasLoc *some* Endocardium

- NCI Thesaurus
  - ~300K terms/classes
  - since 2000
  - since 2003 in OWL, monthly version, +800 terms/month
- …in OWL, published both
  - as a thesaurus ~ inferred concept hierarchy
  - in OWL, including underlying logical axioms, see BioPortal

Inflammation *SubClassOf* Disease

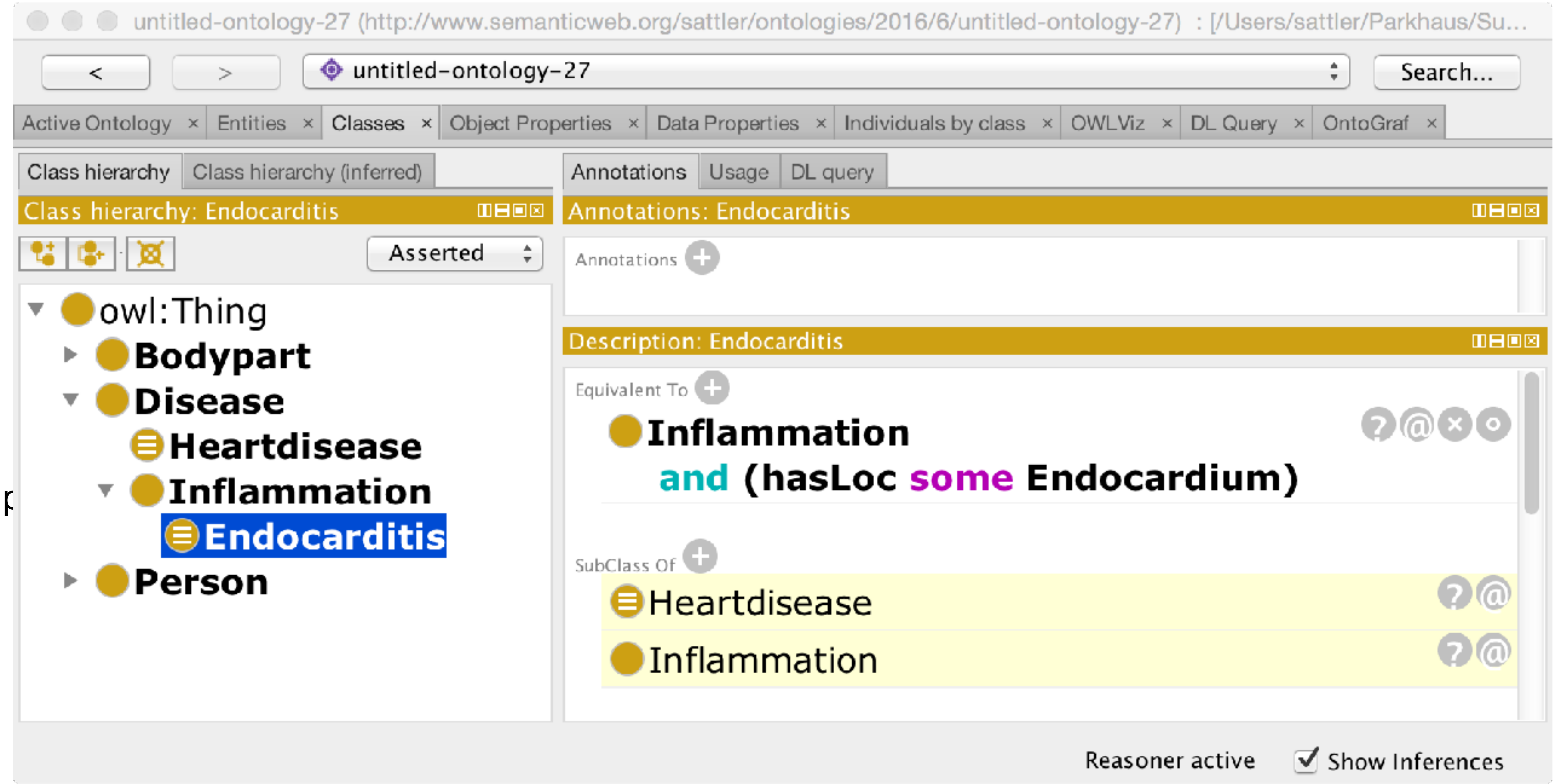
HeartDisease *EquivalentClass* Disease *and* hasLoc *some* Heart

Endocarditis *EquivalentClass* Inflammation *and* hasLoc *some* Endocardium

OWL Axioms - in Protégé

an OWL editor

see http://protege.stanford.edu/products.p



OWL Axioms in First Order Predicate Logic

Inflammation *SubClassOf* Disease

HeartDisease *EquivalentClass* Disease *and*
hasLoc *some* Heart

Endocarditis *EquivalentClass* Inflammation *and*
hasLoc *some* Endocardium

$$\forall x.\mathrm{Inflammation}(x) \Rightarrow \mathrm{Disease}(x)$$

$$\forall x.\mathrm{HeartDisease}(x) \Leftrightarrow \mathrm{Disease}(x) \wedge \exists y.(\mathrm{hasLoc}(x,y) \wedge \mathrm{Heart}(y))$$

$$\forall x.\mathrm{Endocarditis}(x) \Leftrightarrow \mathrm{Inflammation}(x) \wedge \exists y.(\mathrm{hasLoc}(x,y) \wedge \mathrm{Endocardium}(y))$$

OWL Axioms in Description Logic

Inflammation *SubClassOf* Disease

HeartDisease *EquivalentClass* Disease *and*
hasLoc *some* Heart

Endocarditis *EquivalentClass* Inflammation *and*
hasLoc *some* Endocardium

$$\text{Inflammation} \sqsubseteq \text{Disease}$$

$$\text{HeartDisease} \equiv \text{Disease} \sqcap \exists \text{hasLoc}.\text{Heart}$$

$$\text{Endocarditis} \equiv \text{Inflammation} \sqcap \exists \text{hasLoc}.\text{Endocardium}$$

Entities in OWL

Class Name

Class Expression

Inflammation *SubClassOf* Disease

Axiom

HeartDisease *EquivalentClass* Disease *and*
hasLoc *some* Heart

Endocarditis *EquivalentClass* Inflammation *and*
hasLoc *some* Endocardium

Bob *Types* Person *and*
(suffersFrom *some*
(Inflammation *and* (hasLoc some Endocardium)))

Property Name

Different kinds of OWL axioms

For a complete list, see
OWL 2 Primer
https://www.w3.org/TR/owl2-primer/

- about classes

Inflammation	*SubClassOf*	Disease
HeartDisease	*EquivalentClass*	Disease *and* hasLoc *some* Heart

- about properties

hasDaughter	*SubPropertyOf*	hasChild
hasPart	*InversePropertyOf*	isPartOf

- about individuals

Bob	*Types*	Person *and* (suffersFrom *some* Inflammation)
Bob	*Facts*	hasDaughter Mary

Day 2: OWL Entailments

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Meaning of axioms…

- like in FOL, meaning/semantics
  is defined in terms of *an interpretation* $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$ where
  - $\Delta^{\mathcal{I}}$ is a non-empty set, the *interpretation domain*
  - $\cdot^{\mathcal{I}}$ is a mapping that maps each
    - class name A to a set $A^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$
    - property name p to a binary relation $p^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$
- plus
  - mechanism to interpret class expression, eg $A \sqcap B$
  - specification of what it means for $\mathcal{I}$ to satisfy axioms/an ontology …

Why so complicated?

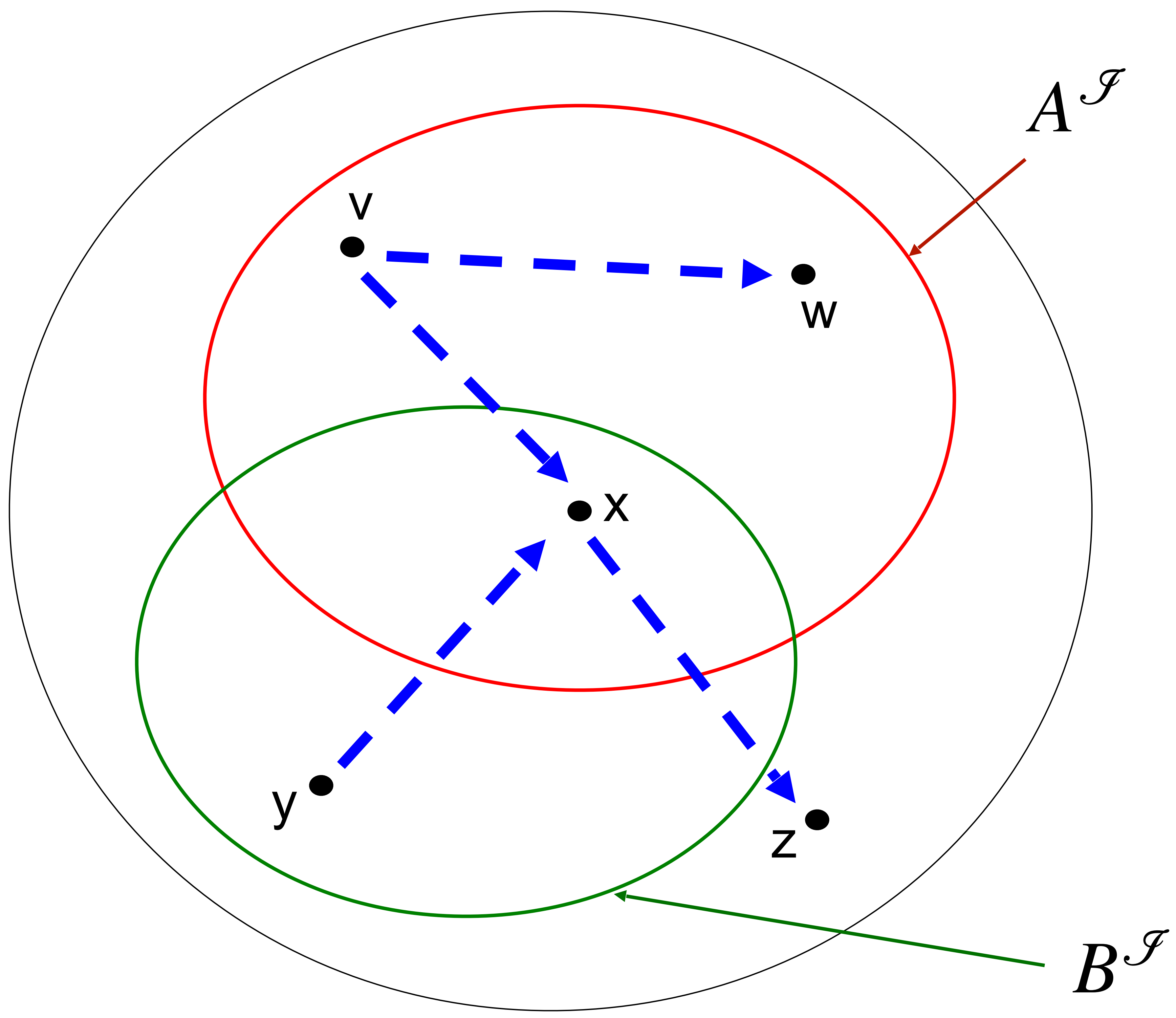
Eg to analyse algorithms

Eg as spec for reasoners

correctness complexity

We can *draw* interpretations

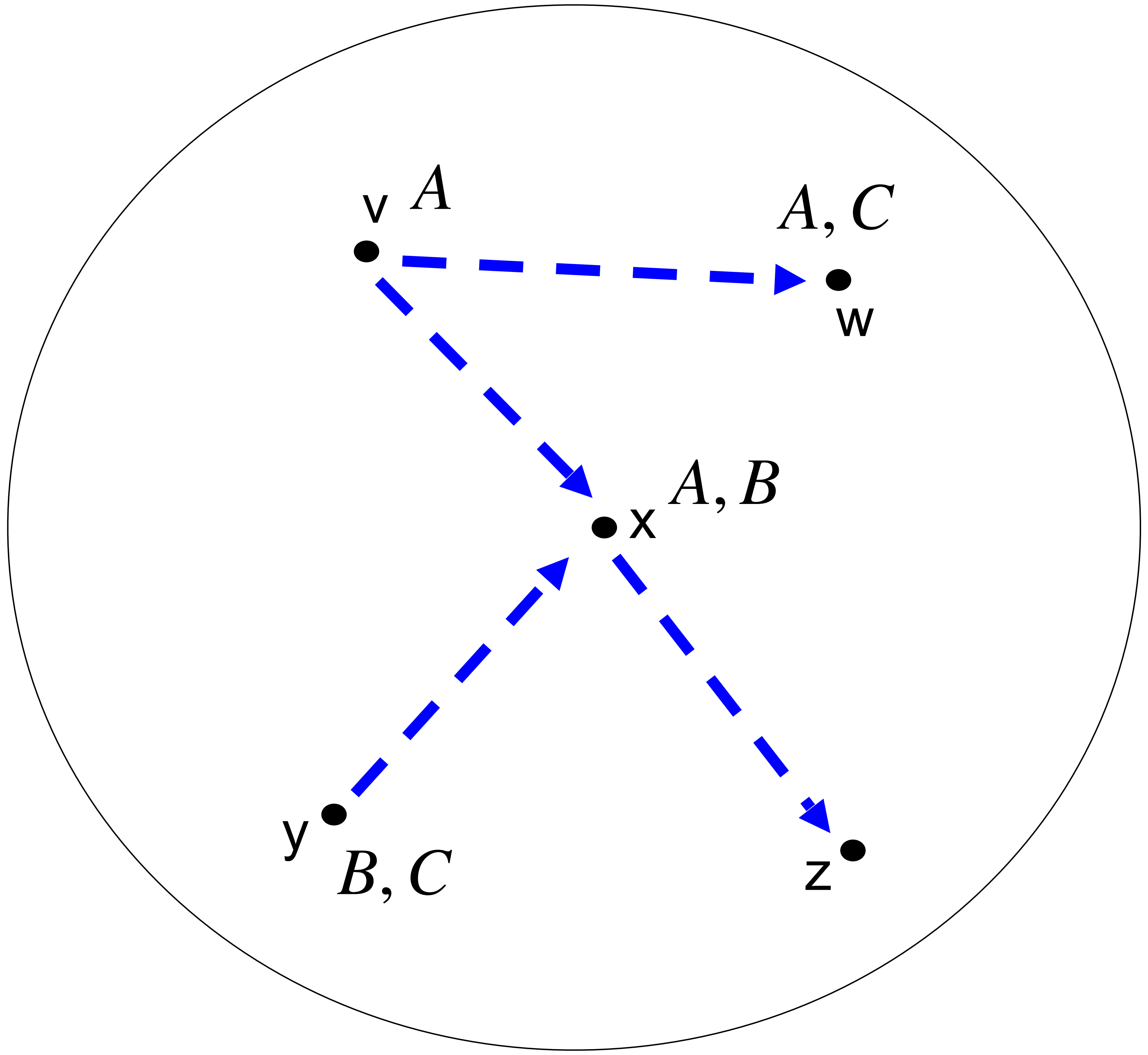
- $\Delta^{\mathcal{I}}$ = {v, w, x, y, z}
- $A^{\mathcal{I}}$ = {v, w, x}
- $B^{\mathcal{I}}$ = {x, y}
- $C^{\mathcal{I}}$ = {w, y}
- $D^{\mathcal{I}} = \emptyset$
- $p^{\mathcal{I}}$ = {(v, w), (v, x), (y, x), (x, z)}



$C^{\mathcal{I}}$???

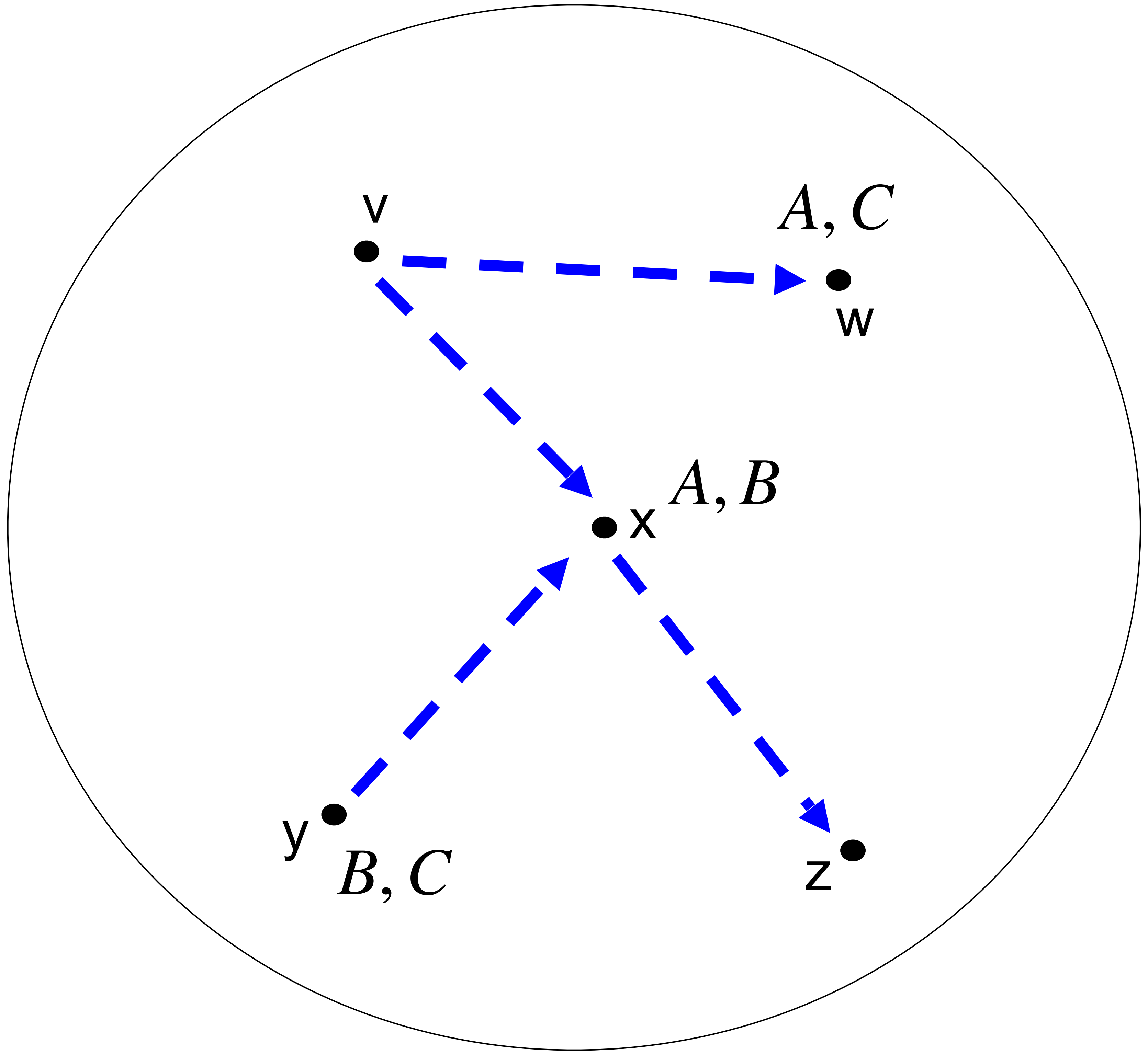
We can *draw* interpretations

- $\Delta^{\mathcal{I}}$ = {v, w, x, y, z}
- $A^{\mathcal{I}}$ = {v, w, x}
- $B^{\mathcal{I}}$ = {x, y}
- $C^{\mathcal{I}}$ = {w, y}
- $D^{\mathcal{I}} = \emptyset$
- $p^{\mathcal{I}}$ = {(v, w), (v, x), (y, x), (x, z)}



Drawing Interpretations

- helps understand semantics of OWL
- check/re-read the definition:
  - what size can the domain have?
  - what size are extensions?
  - which restrictions are on them?
  - what's a really small interpretation?
  - what's a really big interpretation?



Interpretations of Class Expressions

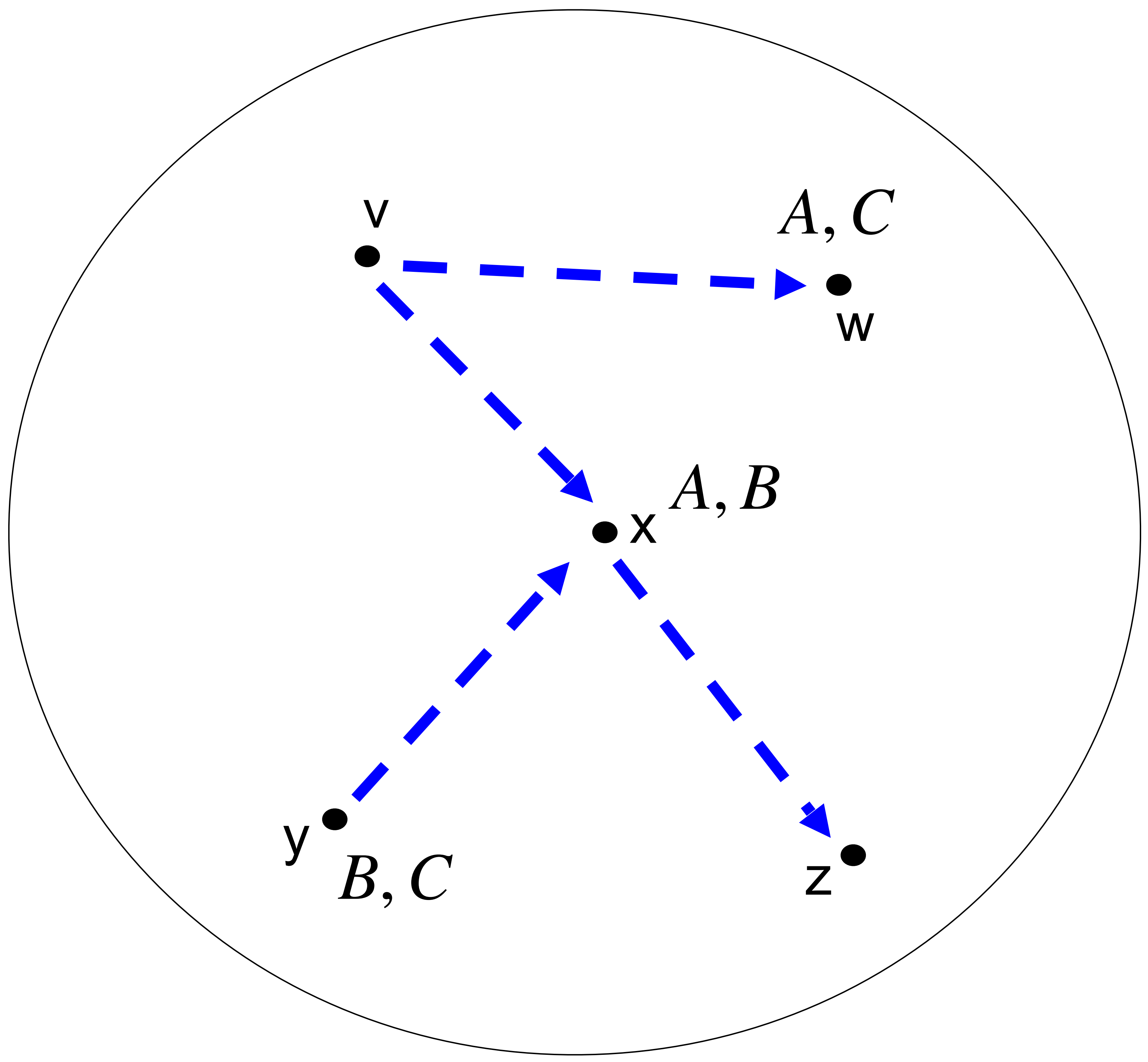
Constructor in Manchester Syntax	**Example**	**Interpretation**
Class name	*Human*	$Human^I \subseteq \Delta$
Thing	n/a	Δ
Nothing	n/a	$\emptyset$
and	*Human* and *Male*	$Human^I \cap Male^I$
or	*Doctor* or *Lawyer*	$Doctor^I \cup Lawyer^I$
not	not *Male*	$\Delta \setminus Male^I$

Interpretations of More Class Expressions

Constructor in Manchester Syntax	**Example**	**Interpretation**
some	*hasChild* some *Lawyer*	$\{e \in \Delta \mid$ there is some f: $(e,f) \in \mathit{hasChild}^I$ and $f \in \mathit{Lawyer}^I\}$
only	*hasChild* only *Doctor*	$\{e \in \Delta \mid$ for all $f \in \Delta$: if $(e,f) \in \mathit{hasChild}^I$ then $f \in \mathit{Doctor}^I\}$
min	*hasChild* min 2 *Tall*	$\{e \in \Delta \mid$ there are at least 2 $f \in \Delta$ with $(e,f) \in \mathit{hasChild}^I$ and $f \in \mathit{Tall}^I\}$
max	*hasChild* max 2 *Tall*	$\{e \in \Delta \mid$ there are at most 2 $f \in \Delta$ with $(e,f) \in \mathit{hasChild}^I$ and $f \in \mathit{Tall}^I\}$

Interpretation of Classes - let's see

- $(\text{not B})^{\mathcal{I}}$ =
- $(\text{A and B})^{\mathcal{I}}$ =
- $((\text{not A}) \text{ or B})^{\mathcal{I}}$ =
- $(\text{R some B})^{\mathcal{I}}$ =
- $(\text{R only B})^{\mathcal{I}}$ =
- $(\text{R some (R some A)})^{\mathcal{I}}$ =
- $(\text{R some not(A or B)})^{\mathcal{I}}$ =
- $(\text{R min 1.Thing})^{\mathcal{I}}$ =
- $(\text{R max 1.Thing})^{\mathcal{I}}$ =



Semantics of Axioms and Ontology

- An interpretation $\mathcal{I}$ *satisfies* an axiom of the form
  - C *SubClassOf* D if $C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$
  - C *EquivalentTo* D if $C^{\mathcal{I}} = D^{\mathcal{I}}$
  - p *SubPropertyOf* q if $p^{\mathcal{I}} \subseteq q^{\mathcal{I}}$
  - …
  - x *Type* C if $x^{\mathcal{I}} \in C^{\mathcal{I}}$
  - $x \; p \; y$ if $(x^{\mathcal{I}}, y^{\mathcal{I}}) \in p^{\mathcal{I}}$
- An interpretation $\mathcal{I}$ *satisfies* an ontology if $\mathcal{I}$ satisfies all axioms in it
  - we call $\mathcal{I}$ a *model* of the ontology

Open World Assumption

An ontology can have *many* models

Model of an ontology = a *fitting* interpretation

Entailments of an Ontology

Let $\mathcal{O}$ be an ontology, α an axiom, and A, B classes, b an individual name:

- $\mathcal{O}$ is *consistent* ______ if there exists some model $\mathcal{I}$ of $\mathcal{O}$
  - i.e., there is an interpretation that satisfies **all** axioms in $\mathcal{O}$
  - i.e., $\mathcal{O}$ isn't self contradictory
- $\mathcal{O}$ *entails* α (written $\mathcal{O} \models \alpha$) ______ if α is satisfied in **all** models of $\mathcal{O}$
  - i.e., α is a consequence of the axioms in $\mathcal{O}$
- A is *satisfiable* w.r.t. $\mathcal{O}$ ______ if $\mathcal{O} \not\models A$ SubClassOf Nothing
  - i.e., there is a model $\mathcal{I}$ of $\mathcal{O}$ with $A^{\mathcal{I}} \neq \emptyset$
- b is an instance of A w.r.t. $\mathcal{O}$ (written $\mathcal{O} \models b : A$) _ if $b^{\mathcal{I}} \in A^{\mathcal{I}}$ in every model $\mathcal{I}$ of $\mathcal{O}$

…let's see this in Protégé!?

Entailment Examples

Patient	*EquivalentClass*	Person *and* suffersFrom *some* Disease
Inflammation	*SubClassOf*	Disease
HeartDisease	*EquivalentClass*	Disease *and* hasLoc *some* Heart
Endocarditis	*EquivalentClass*	Inflammation *and* hasLoc *some* Endocardium
Endocardium	*SubClassOf*	Bodypart *and* isPartOf *some* Heart
hasLoc o isPartOf *SubPropertyOf* hasLoc		

⊨ Endocarditis *SubClassOf* HeartDisease

Entailment Examples

Patient *EquivalentClass* Person *and* suffersFrom *some* Disease

Inflammation *SubClassOf* Disease

HeartDisease *EquivalentClass* Disease *and* hasLoc *some* Heart

Endocarditis *EquivalentClass* Inflammation *and* hasLoc *some* Endocardium

Endocardium *SubClassOf* Bodypart *and* isPartOf *some* Heart

hasLoc o isPartOf *SubPropertyOf* hasLoc

Bob *Type* (Person *and*
suffersFrom *some* (Inflammation *and*
hasLoc *some* Endocardium))

⊨ Bob *Type* Patient

Entailment Examples

Patient *EquivalentClass* Person *and* suffersFrom *some* Disease

Inflammation *SubClassOf* Disease

HeartDisease *EquivalentClass* Disease *and* hasLoc *some* Heart

Endocarditis *EquivalentClass* Inflammation *and* hasLoc *some* Endocardium

Endocardium *SubClassOf* Bodypart *and* isPartOf *some* Heart

hasLoc o isPartOf *SubPropertyOf* hasLoc

Bob *Type* (Person *and*
suffersFrom *some* (Inflammation *and*
hasLoc *some* Endocardium))

⊨ Bob *Type* (Patient *and* suffersFrom *some* HeartDisease)

OWL Reasoning - how?

- OWL reasoners
  - implement *decision procedures* for consistency/entailments, and classify ontologies
- Protégé
  - interacts with reasoners via the OWL API
  - shows results as
    - inferred class hierarchy where
    - unsatisfiable classes are red and you get a
    - warning (red triangle) if O is inconsistent

OWL Reasoning - how?

- OWL reasoners
  - implement highly optimised algorithms which decide complex logical decision problems
  - for example
    - ELK
    - Hermit
    - JFact
    - Conclude
  - use via
    - OWL API
    - OWL2Ready
    - …

OWL Reasoning - why?

- Take a
  - *factual* KG $\mathscr{K}$
  - *rich* ontology $\mathscr{O}$
- ask reasoner to
  - find all entailments of $\mathscr{K} \cup \mathscr{O}$
  - add these to $\mathscr{K}$
    - so that $\mathscr{K}$ + entailments is *harmonised* & *complete*
- use $\mathscr{K}$ + entailments in downstream tasks

A KG can be completed in different ways

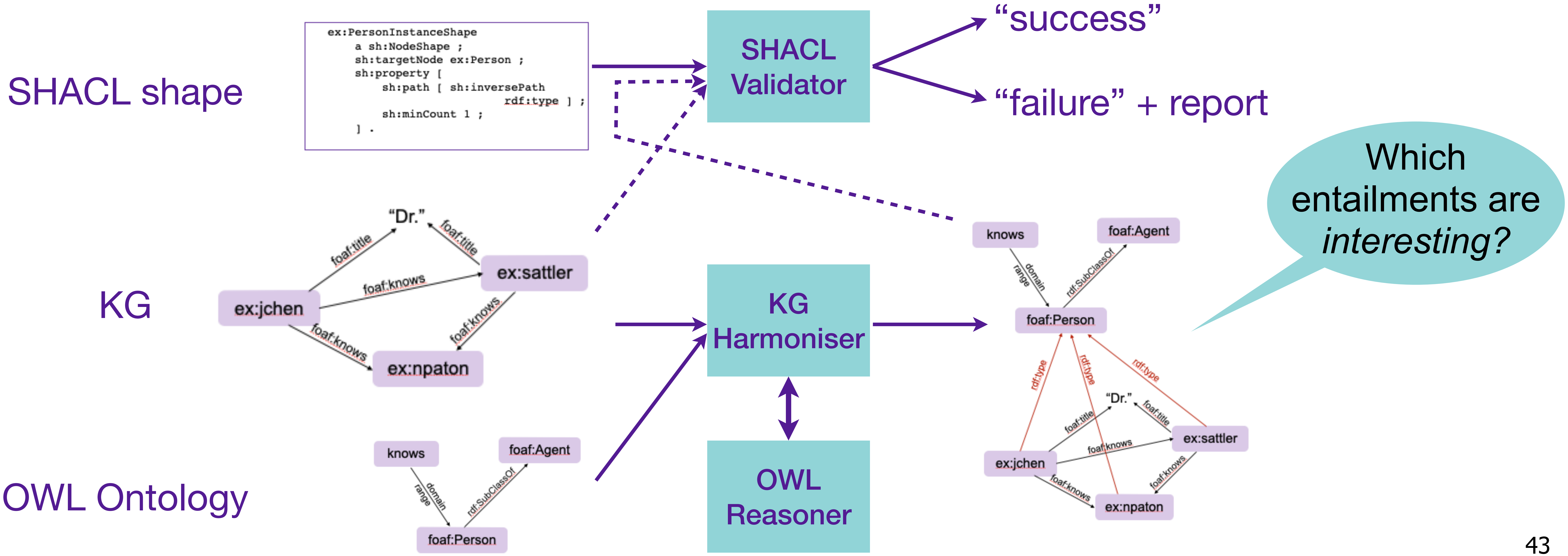
Graph embeddings depend on graph shape!

Only add *interesting* entailments

there are infinitely many entailments

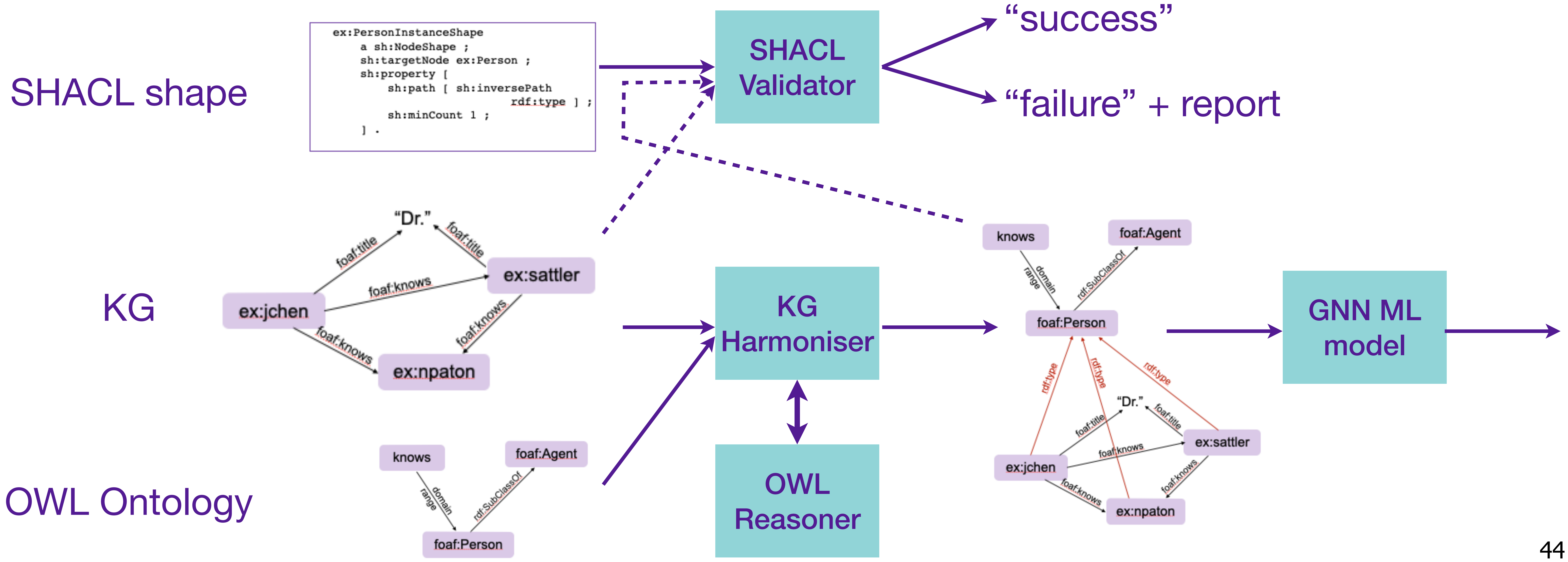
Materialising Ontology Consequences

- Slightly more involved



Materialising Ontology Consequences

- Slightly more involved - but far more powerful



Many things left out…

- how to reason exactly
- computational complexity of reasoning
- model theory of OWL and DL
- profiles
- modularity, module extraction
- explanation of entailments
- relationship with other formalisms
- query answering and rewriting
- …

Summary of today

- Factual KGs can be enhanced with rich conceptual knowledge
  - eg from OWL ontologies
    - with well-defined, logic based semantics and
    - powerful reasoners available
    - no need to reason yourself!
- Many ontologies are available
    - eg in Bioportal
  - that can be used to *harmonise* a factual knowledge graph
  - … in many different ways

Any questions?

Tomorrow: incorporating KG/ontologies in ML models

The End of Today's session

Polyglott persistence

- How can we **vary?**
  - Same core data model, same implementation
    - but different domain models
  - Same core data model, same domain model
    - different implementations, e.g., SQLite vs. MySQL
  - Same shape of core data model, same conceptual model
    - different formalisms!
      - Usually, but not always, implies different implementations
      - e.g. JSON and XML
- We can be **explicitly** or **implicitly** poly-
  - If we **encode** another data model into our home model
    - We are still poly-
    - But only implicitly so
    - Key Cost: Ad hoc implementation
  - If we split our domain model across multiple formalisms/implementations

Key point

- Understand your **domain**
  - What are you trying to represent and manipulate
- Understand your use case
  - including (frequent, relevant) queries, error sources,…
- Understand the **fit** between domain and data model(s)
  - To see where there are sufficiently good fits
- Understand your infrastructure

Question 1

Consider again the Conceptual Model you started to work on last week: can you

- finish/improve/extend it?
- add adjectives?
- add examples?

– format	– domain model	– robust
– formalism	– schema	– extensible
– core data model	– schema language	– scalable
– data model	– application	– self-describing
– database	– system	– valid
– external repr.	– internal repr.	– expressive
– …	– …	– verbose
		– …

Question 2

Consider a format for a reporting system for health & safety incidents, as exemplified by the printed example document:

- sketch a system for
  - gathering this data
  - reporting it monthly
- which kind of schema(s) would you use to describe it?
  - why?
- does this format make good use of XML's

Title Text

Good Bye!

- We hope you have learned a lot!
- It was a pleasure to work with you!
- Speak to us about projects
  - taster/MRes
  - MSc
- Enjoy the rest of your programme
  - COMP62421 query processing
  - COMP62342 rich modelling, inference semantic web, symbolic AI