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### **Uli Sattler**

Professor in Computer Science University of Manchester

Neuro-Symbolic **Knowledge Representation** and Reasoning

ESSAI 2024 Athens



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# 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, …





## This course

- is rather intensive
  - 5 \* 90mins
  - no coursework, example classes, exercises
- requires a lot of attention
  - please ask if something is unclear...
- is selective
  - we cannot cover all approaches/applications/views





## 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, Proté	
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 <sup>2</sup> EL, OWL2Vec*, HiT	
5	Applications & Outlook	Preprocessing, materialisation, evaluation	DeepOnto, mOWL	







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Professor in Computer Science University of Manchester

# Motivation

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## How do we store/access data?

## in relational database

- manipulation via SQL
- ✓ very fast access
- highly optimised DBMSs
- proven technology, well understood properties
- with ACID guarantees
- requires schema, certain normal forms, joins
- tricky for
  - sharing/spontaneous usage
  - many many-to-many relations
  - navigational/path queries

1	name	company	addre
2	Aleshia Tomkiewicz	Alan D Rosenburg Cpa Pc	14 Tay
3	Evan Zigomalas	Cap Gemini America	5 Binr
4	France Andrade	Elliott, John W Esq	8 Moo
5	Ulysses Mcwalters	Mcmahan, Ben L	505 E
6	Tyisha Veness	Champagne Room	5396
7	Eric Rampy	Thompson, Michael C Esq	9472
8	Marg Grasmick	Wrangle Hill Auto Auct & Slvg	7457
9	Laquita Hisaw	In Communications Inc	20 Glo
10	Lura Manzella	Bizerba Usa Inc	929 A
11	Yuette Klapec	Max Video	45 Bra
12	Fernanda Writer	K & R Associates Inc	620 N





## How do we store/access data?

as graphs/in graph database

- for objects and their relations
- manipulation:
  - programmatically
  - via query languages
- relatively new, but powerful DBMSs available
  - often built 'on top' of RDMSs
- doesn't require schema or normal forms or joins •
- suitable for
  - data with many many-to-many relations
  - navigational/path queries
  - sharing/integrating data





## Data Graph or Knowledge Graph?

- objects + relations = knowledge?
  - context
  - meaning
  - understanding
- data: factual, about individuals
- knowledge: conceptual, about
  - concepts
  - their relations







## **Knowledge Representation & Reasoning**

- store/access knowledge
  - factual, about individuals
  - conceptual
    - relevant concepts
    - their relations
      - hierachical/logical
      - domain dependent
- reason about it
  - draw conclusions from the explicitly stated knowledge





## Reasoning

- draw conclusions from the explicitly stated knowledge
- E.g.,

. . .

- jchen is of type Person
- sattler is of type Person
- sattler knows npaton
- npaton is of type Person
- jchen is of type Postgraduate
- sattler is of type Agent

# via well-understood *algorithms* implemented in powerful *reasoners*





## **KR&R** and symbolic Al

- in KR&R, we use symbols for
  - concepts
    - eg Person, Postgraduate, ... •
  - relations
    - eg title, knows •
  - individuals
  - ...and build intelligent systems to deal with these
- where does our knowledge (graph) come from?
  - domain experts, database, ...
- what do we do with our knowledge?
  - use them to *harmonise KGs*

capable of reasoning

add inferred types & links



## Harmonise KGs to...



## Sub-symbolic AI — Machine Learning

In sub-symbolic AI, we

- build/train a model
  - artificial/deep/graph neural networks
  - statistical methods

to spot/learn regularities/patterns from data

don't need to

. . .

- formulate explicit rules
- identify the right terms/symbols
- get amazing results/performance





## Sub-symbolic AI — Machine Learning

In sub-symbolic AI, we

- need huge amounts of data for training
  - costly
  - not always available
- bias in training data goes into model
- find it hard to analyse behaviour
  - other than testing it
  - independent on data



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## Neuro-symbolic KR&R

### combines approaches neural/sub-symbolic and

- symbolic

### • symbolic $\Rightarrow$ sub-symbolic

- inject background knowledge into ML models
- informed embeddings





## Today:

- Knowledge Graphs
  - RDF
  - factual and conceptual knowledge
- Querying of and Reasoning with KGs
  - SPARQL
  - RDFS
  - SHACL
  - Materialisation of reasoning results





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# Day 1 Knowledge Graphs

### **Uli Sattler**

Professor in Computer Science University of Manchester ESSAI 2024 Athens

## (Knowledge) Graphs

## come in different shapes

- Google KG
  - both GDB and content
- Neo4J
- Amazon Neptune
- Arango
- RDF

a W3C standard for KGs



- nodes
- edges between nodes
- labels on edges and nodes



## (Knowledge) Graphs

are everywhere

- "knows" on people
  - social networks
- "isRelatedTo" in genealogy
- "interactsWith" on proteins
  - bio-chemistry •
- "educatedAt" etc in Wikidata





- University of Cambridge
- Radboud University Nijmegen





## **Graph Basics**

- A graph G = (V, E) is a pair with
  - V a set of vertices (also called) nodes, and
  - $E \subseteq V \times V$  a set of edges
- Variants:
  - (in)finite graphs: V is a (in)finite set
  - (un)directed graphs: E (is) is not a symmetric relation
    - i.e., if G is undirected, then  $(x,y) \in E$  implies  $(y,x) \in E$ .
  - node/edge labelled graphs: a label set S, labelling function(s)
    - L:  $V \rightarrow S$  (node labels)
    - L:  $E \rightarrow S$  (edge labels)



Example:

- $G = ({a,b,c,d},$ 
  - $\{(a,b), (b,c), (b,d), (c,d)\}$
  - where are a,...,d in this graph's picture?



## Graph Basics (2)

• Example: node-labelled graph  $^{/}$ - L: V  $\rightarrow$  {A,P}

• Example: edge-labelled graph • P-  $L: E \rightarrow \{p,r,s\}$ 

• Example: node-and-edge-labelled graph  $A_{\bullet}$ .  $-L: V \rightarrow \{A, P\}$  $-L: E \rightarrow \{p, r, s\}$ 









## Knowledge Graph

- Nodes ~ entities
  - possibly with attributes for features of nodes
- Edges ~ relations between entities
  - edge labels to describe kind
- Great for
  - many-to-many relations
  - cyclic relations
  - path queries





## Graph Basics: External Representation

• Pictures are a bad external representations for graphs



$$G = (\{a,b,c,d\} \\ \{(a,b), (| \\ L: \lor \rightarrow d \\ L: a \mapsto A \}$$



(b,c), (b,d), (b,c)},  $\{A,P\}$ A,  $b \mapsto P$ ,  $c \mapsto A$ ,  $d \mapsto A$ )

. . .



## Graph Basics: External Representation

- Pictures are a bad external representations for graphs capture loads of irrelevant information
- - colour
  - location, geometry,
  - shapes, strokes, ...
  - what if labels are more complex/structured?
  - how do we parse a picture into an internal representation?
    - what is a good internal representation?







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# Day 1: RDF a graph-shaped data model

### **Uli Sattler**

Professor in Computer Science University of Manchester ESSAI 2024 Athens

## A Graph Formalism: RDF...why?

- RDF is an
  - *independent* data model
  - standardised by W3C
  - supported by various of the about GBDMSs
- other graph formalisms/data models are available, eg
  - Neo4J
  - GraphDB
  - MongoDB





## A Graph Formalism: RDF

- Resource Description Framework
- a graph-based data structure formalism
- a W3C standard for the representation of graphs
- comes with various syntaxes for External Representation
- is based on **triples** (subject, predicate, object)









## **RDF:** basics

- an RDF graph G is a set of triples  $\{(S_i, p_i, O_i) | 1 \le i \le n\}$
- where each
  - $S_i \in U \cup B$
  - $p_i \in U$
  - $O_i \in U \cup B \cup L$

**U**: URIs, incl. rdf:type,

U: URIs (for resources), incl. rdf:type **B:** Blank nodes L: Literals





## **RDF:** basics

- an RDF graph G is a set of triples  $\{(S_i, p_i, O_i) \mid 1 \le i \le n\}$
- where each
  - $S_i \in U \cup B$
  - $p_i \in U$
  - $O_i \in U \cup B \cup L$

a graph ???

U: URIs (for *resources*), incl. rdf:type B: Blank nodes L: Literals

{(ex:jchen, foaf:knows, ex:sattler), (ex:jchen, rdf:type, foaf:Person), (ex:jchen, rdf:type, foaf:Agent), (ex:sattler, foaf:title, "Dr."), (ex:sattler, foaf:lastName, "Sattler"), (ex:jchen, foaf:title, "Dr."), (ex:sattler, foaf:knows, ex:npaton), (ex: jchen, foaf: knows, ex: npaton) }

> abbreviate: ex: for http://www.cs.man.ac.uk/ foaf: for <u>http://xmlns.com/foaf/0.1/</u>



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## **RDF:** basics

• an RDF graph G is a set of triples  $\{(S_i, p_i, O_i) | 1 \le i \le n\}$ 



U: URIs (for *resources*), incl. rdf:type B: Blank nodes L: Literals

```
a graph
   !!!
     "Sattler"
         foaf:title
     ex:sattler
```

{(ex:jchen, foaf:knows, ex:sattler),
(ex:jchen, rdf:type, foaf:Person),
(ex:jchen, rdf:type, foaf:Agent),
(ex:sattler, foaf:title, "Dr."),
(ex:sattler, foaf:lastName, "Sattler"),
(ex:jchen, foaf:title, "Dr."),
(ex:sattler, foaf:knows, ex:npaton),
(ex:jchen, foaf:knows, ex:npaton) }

abbreviate: ex: for http://www.cs.man.ac.uk/ foaf: for <u>http://xmlns.com/foaf/0.1/</u>



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## **RDF** syntaxes

 "serialisation formats" – for ExtRep of RDF graphs – graphs are IntReps!

• there are several: **–Turtle** -N-Triples **–JSON-LD –N3** -RDF/XML

. . .



{(ex:jchen, foaf:knows, ex:sattler), (ex:jchen, rdf:type, foaf:Person), (ex:jchen, rdf:type, foaf:Agent), (ex:sattler, foaf:title, "Dr."), (ex:sattler, foaf:lastName, "Sattler"), (ex:jchen, foaf:title, "Dr."), (ex:sattler, foaf:knows, ex:npaton), (ex:jchen, foaf:knows, ex:npaton)





## RDF syntaxes

• "serialisation formats" – for ExtRep of RDF graphs – graphs are IntReps!

• there are several: **–Turtle** -N-Triples **–JSON-LD –N3** -RDF/XML

. . .

7 triples in **Turtle**:







## RDF syntaxes

—

• "serialisation formats" – for ExtRep of RDF graphs – graphs are IntReps! • there are several: -Turtle -N-Triples **–JSON-LD –N3** -RDF/XML

Triples in **JSON-LD**:

{"@context": { }, "@graph": [{ "@type": "Person", "title": "Dr.", }, { "@type": "Person", "title": "Dr.",







# Parsing/serialising RDF graphs



- See eg <u>https://json-ld.org/</u>
- See eg <u>https://github.com/RDFLib/rdflib</u>
  - for Python parsers/serialisers/libraries
  - for RDF/XML, N3, NTriples, N-Quads, Turtle, ...
  - with support for SPARQL for querying

### <u>FLib/rdflib</u> s/libraries N-Quads, Turtle, ... <sup>r</sup> querying





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# Day 1: SPARQL a query language for RDF

### **Uli Sattler**

Professor in Computer Science University of Manchester ESSAI 2024 Athens
### SPARQL

- We have
  - a data structure/internal representation: graphs!
  - schema languages (later: RDF, SHACL)
    - plus various external representions (Turtle, N3, N-triples, JSON-LD,..)
- For manipulating RDF graphs: you can use
  - libraries for your favourite programming language:
    - rdflib in Python
    - Jena, RDF4J, CommonsRDF, ... in Java
    - •

- a query language
  - SPARQL, a W3C standardised QL
  - Cypher, supported by Neo4j
    - <u>http://neo4j.com/developer/cypher/</u>
    - has "graph structural" features like "shortest path"
    - lacks "regular path" queries



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## **SPARQL: Basic Graph Patterns**

- are at the core of SPARQL queries:
  - a BGP is a list/set of triple patterns
    - -e.g.,
    - with abbreviations for shared subjects or predicates
    - separated by .
  - a *triple pattern* is a triple where *variables* can be used as subject, predicate, or object - e.g., {?x rdf:type foaf:Person}





## SPARQL: Clauses (1)

- We combine a BGP with a query type – ASK
  - e.g., ASK WHERE {ex:sattler rdf:type foaf:Person}
  - returns true or false (only)
  - SELECT
    - e.g., SELECT ?p WHERE {?p rdf:type foaf:Person}
    - very much like SQL SELECT
  - Careful:
    - ASK returns a Boolean (not an RDF graph!)
    - SELECT returns a table (not an RDF graph!)
    - SPARQL is *not* closed over graphs!
      - unusual: compare to SQL or XQuery!





## SPARQL Clauses (2)

- There are two query types that return graphs:
   CONSTRUCT
  - e.g., CONSTRUCT {?p rdf:type :Befriended} WHERE {?p foaf:knows ?q}
  - like XQuery element and attribute constructors
  - DESCRIBE
    - e.g., DESCRIBE ?p WHERE {?p rdf:type foaf:Person}
    - implementation dependent!
    - returns a"description"
      - -as a graph
      - -whatever the service deems helpful!
      - -similar to querying system tables in SQL
- <sup>:</sup>ul! in SQL



### Examples: Data

@prefix rdf: <<u>http://www.w3.org/1999/02/22-rdf-syntax-ns#</u>> .
@prefix foaf: <<u>http://xmlns.com/foaf/0.1/</u>> .
@prefix ex: <<u>http://www.cs.man.ac.uk/</u>> .

ex:bobthebuilder

foaf:firstName "Bob"; foaf:lastName "Builder"; foaf:knows ex:wendy ; foaf:knows ex:farmerpickles; foaf:knows ex:billbibs.

ex:wendy

foaf:firstName "wendy"; foaf:knows ex:farmerpickles.

ex:farmerpickles

foaf:firstName "Farmer"; foaf:lastName "Pickles"; foaf:knows ex:bobthebuilder.

ex:billbibs

foaf:firstName "Bill";
foaf:lastName "Bibby".





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## Example: Count Friends!

How many friends does Bob Builder have?

SELECT DISTINCT COUNT(?friend) WHERE {ex:bobthebuilder foaf:firstName "Bob"; foaf:lastName "Builder"; foaf:knows ?friend };

Quite similar to a SQL query:





### SELECT COUNT(DISTINCT k.Whom) FROM Persons P, knows k WHERE (P.PersonID = k.Who AND P.FirstName = "Bob" AND P.LastName = "Builder");





## Example: Find Friends' Friends?

Give me Bob Builder's friends' friends' names? SELECT ?first, ?last WHERE {ex:bobthebuilder foaf:firstName "Bob"; foaf:lastName "Builder"; foaf:knows ?x. ?x foaf:knows ?y. ?y foaf:firstName ?first; foaf:lastName ?last}







### Friends network?

Give me everybody in Bob Builder's friends' friends...?

SELECT ?first, ?last WHERE {ex:bobthebuilder foaf:firstName "Bob"; foaf:lastName "Builder"; foaf:knows+ ?friend. ?friend foaf:firstName ?first; foaf:lastName ?last}

SPARQL supports full regular expressions in path queries!





# Working with RDF graphs through SPARQL endpoints

- by hand
  - eg Wikidata
- programmatically
  - eg through REST APIs



```
Wikidata Query Service
                                           O Help
                             Examples
                                                         More tools
                                                                      -
1 #Brightest stars, with image
2 #defaultView:ImageGrid
3 # Brightest celestial bodies
4 SELECT ?star ?starLabel ?images ?apparent_magnitude
5 WHERE {
    SERVICE wikibase:label { bd:serviceParam wikibase:language "en". }
    { SELECT ?star ?apparent_magnitude ?images
      WHERE {
         ?star wdt:P31 wd:Q523;
               wdt:P1215 ?apparent_magnitude;
               wdt:P18 ?images .
        FILTER(?apparent_magnitude < 1)</pre>
      } LIMIT 10
15 } ORDER BY (?apparent_magnitude)
```







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# Day 1: RDFS a schema language for RDF

### **Uli Sattler**

Professor in Computer Science University of Manchester ESSAI 2024 Athens

## RDF

- in RDF, we can state *factual* knowledge:
  - how 2 nodes relate
    - e.g. (ex:sattler, foaf:knows, foaf:npaton)
  - how a node relates to a literal
    - e.g. (ex:jchen, foaf:title, "Dr.")
  - what type a node has via rdf:**type** 
    - e.g. (ex:sattler, rdf:type, foaf:Person)
- but we can't say anything about
  - classes
    - e.g., foaf:Person implies foaf:Agent
  - properties
    - e.g., worksWith implies knows





# RDFS: a schema language for RDF

- 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)



## Reasoning: Default Values++

- RDFS does not describe/constrain structure
  - that is, unlike in other schema languages,
    - in RDFS, we don't describe what has to be the case
      - we don't write integrity constraints
    - RDFS can't be used to "validate" documents/graphs
- RDFS allows us to provide extra information
  - •...a bit like default values!
  - •...rather than requesting information, we infer it!



## Reasoning: Default Values++

- RDFS does **not** describe/constrain structure
- RDFS allows us to provide *extra information*

@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>. @prefix foaf: <http://xmlns.com/foaf/0.1/> . @prefix ex: <http://www.cs.man.ac.uk/>.

```
ex:sattler
 foaf:title "Dr.";
 foaf:knows ex:jiaoyanchen ;
 foaf:knows
  foaf:title "Count";
```

```
foaf:lastName "Dracula"
```



Facts



## Reasoning: Default Values++

- RDFS does **not** describe/constrain structure
- RDFS allows us to provide *extra information*

@prefix rdfs: <<u>http://www.w3.org/2000/01/rdf-</u> <u>schema#</u>>. @prefix foaf: <http://xmlns.com/foaf/0.1/> . foaf:knows rdfs:domain foaf:Person. foaf:knows rdfs:range foaf:Person. foaf:Person rdfs:subClassOf foaf:Agent









### What do schemas usually do again?

- In other schema languages, we usually describe ExtReps:
  - what's allowed
  - what's required
  - what's assumed
    - default values
  - what's expected
  - what's forbidden (e.g., in Schematron)
- In RDFS, we can only state
  - what's assumed/known, and thus
  - what can be inferred
    - ex:jchen rdf:type foaf:Person. here: ex:sattler rdf:type foaf:Person.

foaf:knows rdfs:domain foaf:Person. foaf:knows rdfs:range foaf:Person







# SPARQL, RDFS, and Reasoning

Inferences can be materialised

- add reasoning results to your KG
  - make background knowledge explicit in KG
  - harmonise your KG





## SPARQL, RDFS, and Reasoning

- SPARQL queries are sensitive to RDF(S) inference
  - the way XPath is sensitive to default values!
  - also sensitive to more expressive language inferences
    - like OWL tomorrow!
- Inference has a cost
  - results may be surprising
  - query answering may be (!) computationally expensive!



### Solves all problems?

### • No!

- RDFS can't express complex conceptual knowledge
  - see OWL tomorrow
- we need to decide *which* additional information to make explicit in KG
  - too much: KG size may increase dramatically
  - too little: missing knowledge
- No validation!
  - this is a formalism specific quirk
  - there is SHACL





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# Day 1: SHACL another schema language for RDF

### **Uli Sattler**

Professor in Computer Science University of Manchester ESSAI 2024 Athens

### SHACL: another schema language for RDF

### • in SHACL, we have shapes

- to describe constraints on nodes and edges:
- eg in our KG, each Person has to have a first name or a last name

```
ex:PersonInstanceShape
    a sh:NodeShape ;
    sh:targetNode ex:Person ;
    sh:property [
        sh:path [ sh:alternativePath
                 (foaf:firstName)
                 foaf:lastName)] ;
        sh:minCount 1 ;
    •
```

• eg our KG must have at least 1 instance of Person

```
ex:PersonInstanceShape
    a sh:NodeShape ;
    sh:targetNode ex:Person ;
    sh:property [
        sh:path [ sh:inversePath
                          rdf:type ]
        sh:minCount 1 ;
```





### **SHACL:** validation

 given a KG and shapes, we can ask a validator to test whether KG satisfies constraints in shapes:



KG











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# Day 1: RDFS & SHACL an interesting relation

### **Uli Sattler**

Professor in Computer Science University of Manchester ESSAI 2024 Athens

can affect each other:





can affect each other: it may be that









### SHACL shape







can affect each other: it may also be that







### SHACL shape



### "our KG must have at least 1 instance of Person"





## Summary of today

- KGs can contain factual and conceptual knowledge
  - eg in RDF and RDFS
- Reasoning makes implicit knowledge explicit
- Materialisation of reasoning results can
  - harmonise a factual knowledge graph
  - prevent us from validating invalid documents
  - ensure that *implicitly* valid documents are validated





Any questions?





### The End of Today's session

### Tomorrow: more on reasoning & OWL



### 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

model te vs. MySQL e conceptual mode

utinte ferme aliense limplementatione



## 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
- formalism
- core data model
- data model
- database

— ...

– external repr.

- domain mo
- schema
- schema lai
- application
- system

— ...

- internal rep

odel	– robust
	<ul> <li>– extensible</li> </ul>
nguage	<ul> <li>scalable</li> </ul>
	<ul> <li>self-describing</li> </ul>
	– valid
or.	<ul> <li>– expressive</li> </ul>
	– 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 Al

