Applications to Data Science

Ernesto Jiménez-Ruiz
Lecturer in Artificial Intelligence

Before we start...

Where are we?

- ✓ Introduction.
- ✓ RDF-based knowledge graphs.
- ✓ SPARQL 1.0
- ✓ RDFS Semantics and RDF(S)-based knowledge graphs.
- ✓ OWL (2) ontology language. Focus on modelling.

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– **Application to Data Science (today).**

– SPARQL 1.1, OWL 2 profiles and entailment regimes.

– Ontology Alignment.

– Machine Learning and Knowledge Graphs.

The Knowledge Scientist

Tasks of a Data Scientist

– Understand the data and its context

– Reliability of the data (shared with Data Engineers)

– Data wrangling

– Data analytics

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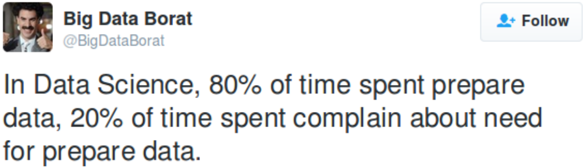
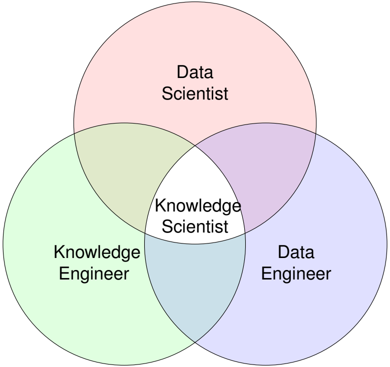


The Knowledge Scientist (i)

- **Data Engineer:** harnesses and collects data.
- **Data Scientist:** draws value from data.
- **Knowledge Engineer:** encodes domain expertise.
- **Knowledge Scientist:** adds context to the data to make it more useful, clean, reliable and ready to be used.

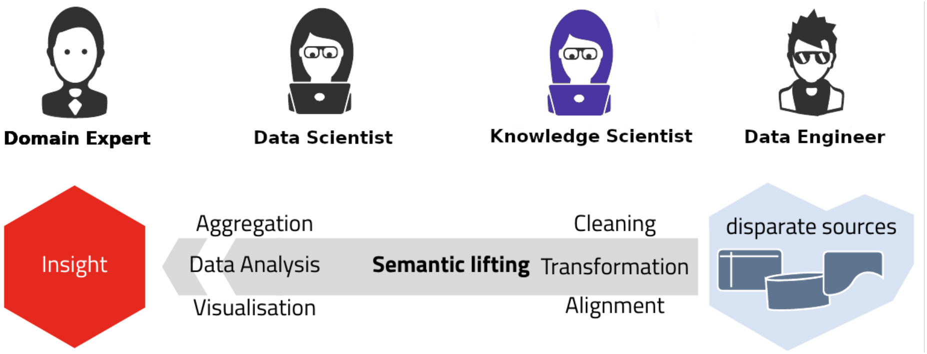


The Knowledge Scientist (ii)

- Bridges the data and the business requirements/questions.
- Outputs a data model (*i.e.*, **knowledge graph**): how business users see the world.
- Drives a semantic-lifting of the data (from Data Engineers to Data Scientists)
- Relies on Semantic Web technology and skills (*e.g.*, ontology modelling, data integration)

George Fletcher and others. **Knowledge Scientists: Unlocking the data-driven organization**. 2020

The Knowledge Scientist (iii)



Adapted from: SIRIUS Centre for Scalable Data Access, `https://sirius-labs.no/`

Why Ontologies and Graphs of Knowledge?

Graph(s) of Knowledge / Knowledge Graphs

- Semantic Web in more **controlled scenarios**, *e.g.*,
  - **Integrate and orchestrate** data within an organisation
  - Enterprise data as a knowledge graph to **drive products** and make them more "**intelligent**"

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  - Graph data models extensively studied in AI…
  - …but Google has relaunched the interest on **KGs in industry**

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- **Not new**:
  - Graph data models extensively studied in AI. . .
  - . . . but Google has relaunched the interest on **KGs in industry**
- Availability of **mature** Semantic Web **technology**
  - Query engines
  - Modelling languages
  - Reasoning

Ontologies and Knowledge Graphs

- Core idea of knowledge graphs is the enhancement of the graph data model with...
  - "...an **abstract symbolic representations** of a domain expressed in a formal language"

- In this module: **OWL-layered RDF-based knowledge graphs**

Aidan Hogan and others. **Knowledge Graphs**. CoRR abs/2003.02320, 2020.
Pim Borst, Hans Akkermans, and Jan Top. **Engineering ontologies**, 1999.

Why Ontologies and Knowledge Graphs?

- Independence of logical/physical schema: **domain model**
- Vocabulary closer to domain experts: **more user-friendly**
- Incomplete and semi-structured data: **flexibility**
- Integration of heterogeneous sources: **unified view**

♠ They can complement tabular data not necessarily substitute.

Why Ontologies and Knowledge Graphs? (5-star data)

- ⋆ **OL**: make your data available on the Web (in any format) under an open license.

Tim Berners-Lee. **5 ⋆ data:** `https://5stardata.info/en/`

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♠ This also applies within a company (intranet), not only for the Web. Ideally with an OL, but at least data accessible by everyone in the company.

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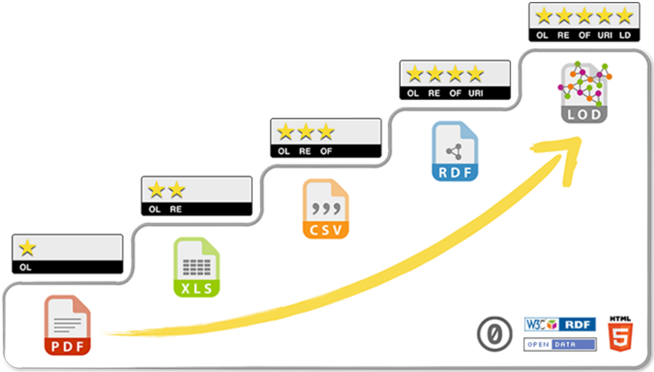
Why Ontologies and Knowledge Graphs? (5-star data)



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Challenges:

- How to **expose** data (*e.g.*, databases, csv files) as knowledge graphs?
- How to **create** (or reuse) and use (abstract) **knowledge** (*i.e.*, *Ontologies*)?
- How to **align** different knowledge graphs? ♠
- How to check **consistency and trust** of the data and knowledge? ♠

♠ Better with things than with strings

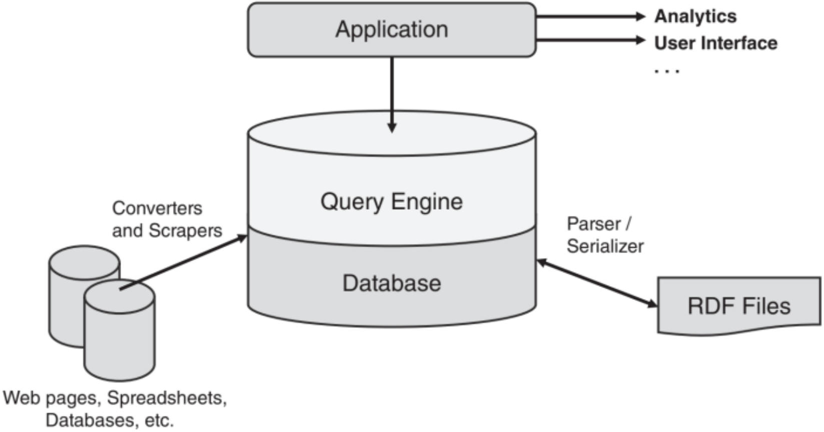
Challenges:

- How to **expose** data (*e.g.*, databases, csv files) as knowledge graphs?
  - *RDF and Today's session (4-5 $\star$ data)*
- How to **create** (or reuse) and use (abstract) **knowledge** (*i.e.*, *Ontologies*)?
  - *RDFS and OWL*
- How to **align** different knowledge graphs? ♠
  - *Ontology Alignment: In two weeks time (5 $\star$ data)*
- How to check **consistency and trust** of the data and knowledge? ♠
  - *Reasoning: Next week.*

♠ Better with things than with strings

From (Tabular) Data to Knowledge Graphs:
Towards 5 $\star$ data

General Semantic Web Architecture



Exposing data as an RDF-based Knowledge Graph

- ✓ **End-users' friendly access** to "unfriendly" tabular data.
- ✓ **Pay as you go** (modular) data integration via mappings.

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– **Option 1**: **Virtual exposure of data** (OBDA)

✓ Data remains in its original format.

✗ Typically only over relational databases.

Exposing data as an RDF-based Knowledge Graph

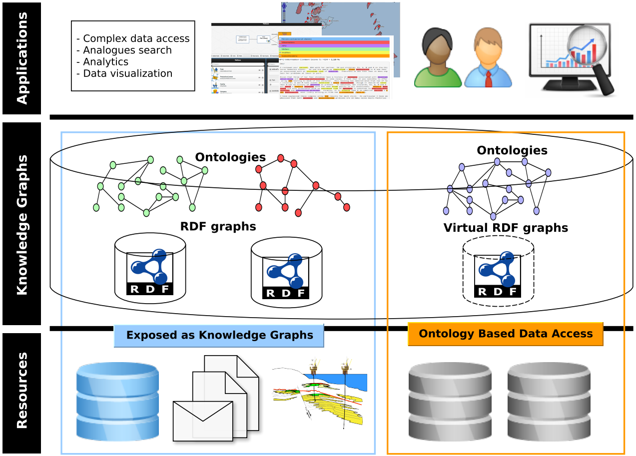
✓ **End-users' friendly access** to "unfriendly" tabular data.

✓ **Pay as you go** (modular) data integration via mappings.

– **Option 1**: **Virtual exposure of data** (OBDA)
  - ✓ Data remains in its original format.
  - ✗ Typically only over relational databases.

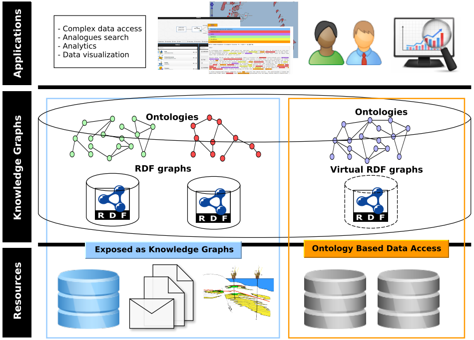
– **Option 2**: **Data Export/Materialization**
  - ✓ Easy to exchange data (RDF).
  - ✓ Integration of data in disparate formats.
  - ✗ Data replication.
  - – Due to size or privacy it may not be possible to export the data.

Exposing data as RDF: Architecture



Exposing data as RDF: Ingredients

- **Ontology vocabulary**. Custom and/or given by a public KG.
- **Mappings**. Define a transformation from the tabular data to RDF data.
- **Ontology Axioms** (optional)



Exposing data as RDF: W3C Mapping Standards

- **Relational Database to RDF**:
  - A Direct Mapping of Relational Data to RDF: `https://www.w3.org/TR/rdb-direct-mapping/`
  - R2RML: RDB to RDF Mapping Language: `https://www.w3.org/TR/r2rml/`
  - Each mapping involves the creation of a **SQL query** and the transformation of the results to RDF triples.

- **CSV to RDF**:
  - Generating RDF from Tabular Data on the Web (CSV2RDF): `https://www.w3.org/TR/csv2rdf/`
  - Each mapping is a **(small) script** that creates specific RDF triples from the CSV file (*e.g.*, data frame).

Exposing data as RDF: Direct Mapping Example

Automatic triples:

```
ex:row1 ex:col1 ‘‘China’’
ex:row1 ex:col2 ‘‘Beijing’’
ex:row2 ex:col1 ‘‘Indonesia’’
ex:row2 ex:col2 ‘‘Jakarta’’
...
```

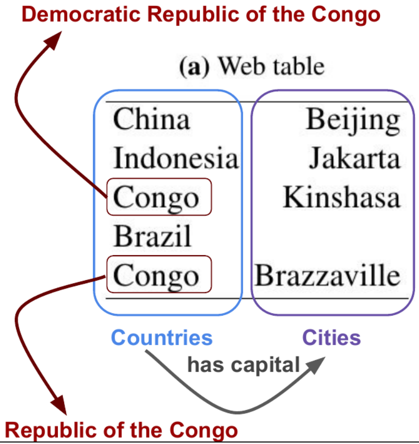
China	Beijing
Indonesia	Jakarta
Congo	Kinshasa
Brazil	
Congo	Brazzaville

Exposing data as RDF: Enhanced Mapping/Transformation (i)

– We know the **semantics** of the data.

– **Potential automatic triples:**

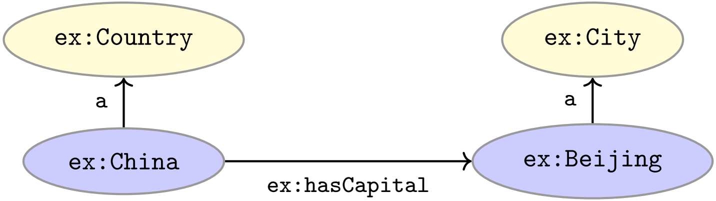
```
ex:China rdf:type ex:Country
ex:Beijing rdf:type ex:City
ex:China ex:hasCapital ex:Beijing
...
```



Exposing data as RDF: Enhanced Mapping/Transformation (ii)

Return capital of China (for $\mathcal{G}$ below):

```
PREFIX ex:  <http://example.org/>
SELECT DISTINCT ?capital WHERE {
    ex:China ex:hasCapital ?capital .
}
```



Exposing data as RDF: Enhanced Mapping/Transformation (ii)

Return capital of China (for $\mathcal{G}$ below): Query Result= {ex:Beijing}

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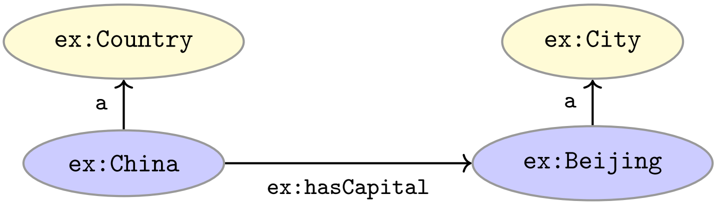

Exposing data as RDF: Mappings

Mapping or Transformation $\varphi \rightsquigarrow \psi$

- φ: query over database or CSV extraction

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- RDB to RDF mapping:
  `SELECT col1 FROM TABLE` $\rightsquigarrow$ `ex:{col1} rdf:type ex:Country`

Exposing data as RDF: Mappings

Mapping or Transformation $\varphi \rightsquigarrow \psi$

– φ: query over database or CSV extraction

– ψ: RDF triple template

– RDB to RDF mapping:

SELECT col1 FROM TABLE $\rightsquigarrow$ ex:{col1} rdf:type ex:Country

– CSV to RDF mapping:

```
for value in data_frame[col1]:                           (φ)
    subject = "ex:" + value   #e.g., ex:China
    create_triple(subject rdf:type ex:Country)  (ψ)
```

Exposing data as RDF: Mappings

Mapping or Transformation $\varphi \rightsquigarrow \psi$

- φ: query over database or CSV extraction
- ψ: RDF triple template
- RDB to RDF mapping:
  `SELECT col1 FROM TABLE` $\rightsquigarrow$ `ex:{col1} rdf:type ex:Country`
- **CSV to RDF mapping:** (in this module)

```
for value in data_frame[col1]:                              (φ)
    subject = ‘‘ex:’’ + value   #e.g., ex:China
    create_triple(subject rdf:type ex:Country)   (ψ)
```

Semantic Understanding of Tabular Data

Semantic enrichment or augmentation

- **Semi-automatic** process.
- Key for an **enhanced transformation** to RDF triples.
- But also for other tasks with independence of a final KG creation.
  - Tabular data in the form of CSV files is the common input format in a **data analytics pipeline**.
  - The **lack of semantics and context in datasets** hinders their usability.
  - Gaining **semantic understanding** will be very valuable for data integration, data cleaning, data mining, machine learning and knowledge discovery tasks.

Contribution of Semantics in Data Wrangling Challenges

- *Data parsing*, e.g. converting csv's or tables.
- (+++)*Data dictionary*: basic types and semantic types.
- (++)*Data integration* from multiple sources (foreign key discovery).
- (++)*Entity resolution*: duplication and record linkage.
- (+)*Format variability*: e.g. for dates and names.
- (+)*Structural variability* in the data.
- (++)Identifying and repairing *missing data*.
- (+)*Anomaly detection* and repair.
- (+++)**Metadata/contextual information**. (Semantic) data governance.

AIDA Project: `https://www.turing.ac.uk/research/research-projects/artificial-intelligence-data-analytics-aida`

Adding Semantics to Tabular Data: Basic Tasks

– Matching a cell to a KG entity (**CEA task** - Cell-Entity Annotation)
– Assigning a semantic type (*e.g.*, a KG class) to an (entity) column (**CTA task** - Column-Type Annotation)
– Assigning a KG property to the relationship between two columns (**CPA task** - Columns-Property Annotation)

Ernesto Jiménez-Ruiz and others. **SemTab 2019: Resources to Benchmark Tabular Data to Knowledge Graph Matching Systems**. ESWC 2020

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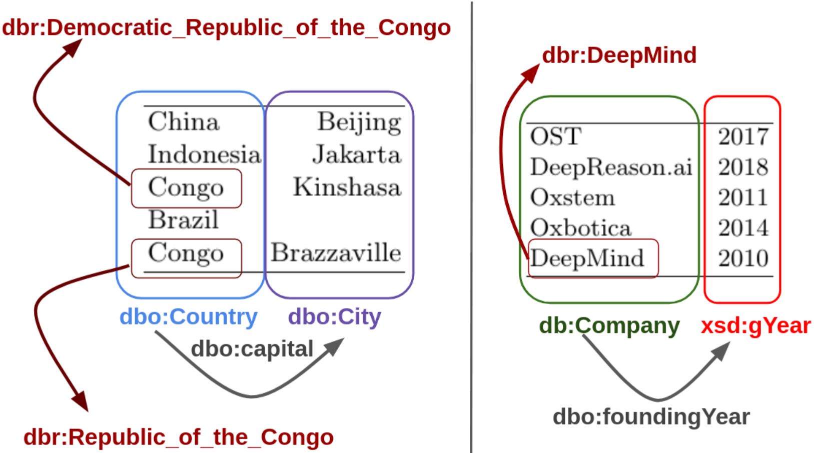
† *For a semi-automatic process, we assume the existence of a (possibly incomplete)* ***Knowledge Graph (KG)*** *relevant to the domain.*
‡ *When transforming to RDF, if no KG matching then create a fresh entity URI.*

Ernesto Jiménez-Ruiz and others. **SemTab 2019: Resources to Benchmark Tabular Data to Knowledge Graph Matching Systems**. ESWC 2020

Adding Semantics to Tabular Data: Basic Tasks (with DBPedia)



Semantic Understanding of Tabular Data:
SemTab Challenge

SemTab Challenge

– Provides a **systematic evaluation** framework of Tabular Data to KG matching systems.

– Evaluates the **three basic tasks**: CTA, CEA and CPA.

– Relies on:
  – an **automatic** dataset generator, and
  – **manually** curated datasets.

– **Target KGs**: DBPedia (2019) and Wikidata (2020)

– Co-organised an sponsored by **IBM Research**.

SemTab: Semantic Web Challenge on Tabular Data to Knowledge Graph Matching:
`http://www.cs.ox.ac.uk/isg/challenges/sem-tab/`

SemTab Rounds and Datasets

Stats	Automatically Generated				Tough Tables
	Round 1	Round 2	Round 3	Round 4 (AG)	Round 4 (2T)
Tables	34,295	12,173	62,614	22,207	180
Avg. rows	7.3	6.9	6.3	21	1,080
Avg. cols	4.9	4.6	3.6	3.5	4.5

- Tables and ground truth: `http://www.cs.ox.ac.uk/isg/challenges/sem-tab/`
- SemTab 2019: Resources to Benchmark Tabular Data to Knowledge Graph Matching Systems. Extended Semantic Web Conference (ESWC). 2020.
- Tough Tables: Carefully Evaluating Entity Linking for Tabular Data. International Semantic Web Conference (ISWC). 2020
- Results of SemTab 2020. ISWC 2020

SemTab Participation

– The community is active and growing

Participants	Round 1	Round 2	Round 3	Round 4
2019	*17*	*11*	*9*	*8*
2020*	18	16	18	10
CEA	10	10	9	10§
CTA	15	13†	16‡	9§
CPA	9	11	8	7

$\star$ One system from a MSc student at City

Outliers:

† 3 systems with F-score < 0.3

‡ 8 systems with F-score < 0.3

§ 1 system with F-score < 0.3

SemTab Results Overview: Average F1-score†

- Noise in synthetic datasets not challenging enough.
- The 2T dataset brings additional complexity.

Task	Automatically Generated				Tough Tables
	Round 1	Round 2	Round 3	Round 4 (AG)	Round 4 (2T)
CEA	0.93	0.95	0.94	0.92	0.54
CTA	0.83	0.93	0.94	0.92	0.59
CPA	0.93	0.97	0.93	0.96	-

† *Averages of top-10 systems without outliers*

Semantic Understanding of Tabular Data: Techniques

Common Techniques

– **Pre-processing**: spelling error, stopwords, unicode fixing, etc.

– **Regular expressions** to identify data formats (*e.g.*, numbers, phones, dates, names).

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- Access to the **KG's SPARQL Endpoint** (local or online)

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- Access to the **KG's SPARQL Endpoint** (local or online)
- **Lexical similarity** (*e.g.*, Levenshtein)
- Word and KG **embeddings**

Common Knowledge Graphs

Wikidata: `https://www.wikidata.org/`

- $>$90 million entities
- Free and public (anyone can edit)

DBPedia: `https://dbpedia.org/`

- $>$900 million triples
- Extracted from Wikipedia

Google KG: `https://developers.google.com/knowledge-graph`

- Private, only accessible via look-up
- $>$1,000 million entities

Fuzzy Search: KG look-up Services

- Given a string (*e.g.*, “Congo”)
- Return a set of candidate KG entities, *e.g.*,
  `http://dbpedia.org/resource/Republic_of_the_Congo`
  `http://dbpedia.org/resource/Congo_River`
- Typical starting point for CEA and CTA tasks
- DBPedia, Wikidata and Google KG provide look-up services via a REST API.
- Some systems have built their own local index for fuzzy search.

GitHub repositories: `https://github.com/city-knowledge-graphs`

Lexical Processing and Similarity

- **Datatype prediction**, *e.g.*, ptype:
  `https://github.com/alan-turing-institute/ptype`
- **Spelling corrector:** `https://norvig.com/spell-correct.html`

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- **Spelling corrector:** `https://norvig.com/spell-correct.html`
- **Lexical similarity:**
  - Levenshtein distance:
    `levenshtein('Congo', 'Republic of Congo')=12`
  - Jaro Winkler:
    `jaro_winkle('Congo', 'Republic of Congo')=0.0`
    `jaro_winkle('Congo', 'Congo Republic')=0.893`
  - **I-Sub**:
    `isub('Congo', 'Republic of Congo')=0.727`

Access to KG SPARQL Endpoint

- Get additional **contextual information**:
  - Additional type information
  - Entity Relationships
  - Members of a type

- Access via **SPARQL queries** (no fuzzy search)

- Typically required for:
  - the **CPA task**
  - **disambiguation** in CTA and CEA tasks

GitHub repositories: `https://github.com/city-knowledge-graphs`

Word and KG Embeddings: Capturing Context

- **Embeddings**: representation in the form of a real-valued vector.
- Very useful to **capture the meaning/semantics** of a word (or a KG entity).
- Comparison among vectors via **Cosine similarity** (*e.g.*, between vectors for ‘Congo’ and ‘Republic of Congo’)

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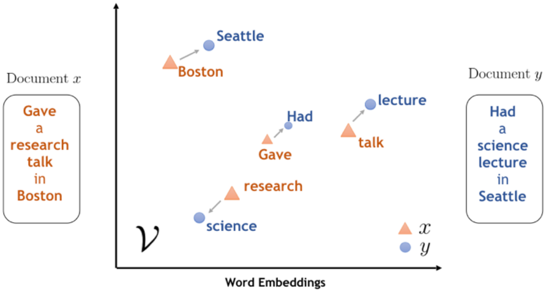
- Comparison among vectors via **Cosine similarity** (*e.g.*, between vectors for ‘Congo’ and ‘Republic of Congo’)
- **Precomputed word embeddings:**
  - `https://wikipedia2vec.github.io/wikipedia2vec/pretrained/`
  - `https://fasttext.cc/docs/en/pretrained-vectors.html`
- **Precomputed KG embeddings:**
  - Wikidata: `http://139.129.163.161/index/toolkits#pretrained-embeddings`
  - DBPedia: `http://www.kgvec2go.org/`

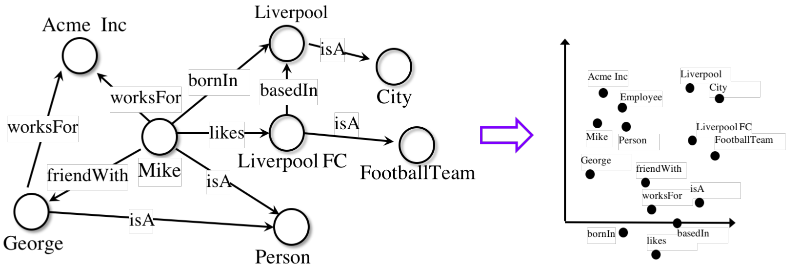
Word Embeddings: Example



Systems like `Word2Vec` require a corpus of documents as training.

Example from: `https://dsgiitr.com/blogs/word_embeddings/`

Knowledge Graph Embeddings: Example



KG Embedding Systems exploit the neighbourhood of an entity to calculate its vector.

Example from: `https://docs.ampligraph.org/en/1.0.3/`

OWL2Vec*: Embedding of OWL Ontologies. `https://arxiv.org/pdf/2009.14654.pdf`

Semantic Understanding of Tabular Data: User Interfaces

OpenRefine

- `https://openrefine.org/`
- Previously known as *Google Refine*.
- **Interface to support** the cleaning and transformation of messy data.
- Includes a **reconciliation service** to link the data with a KG (*e.g.*, Wikidata is default installation).
- In this module we will not use OpenRefine, but perform our own reconciliation programmatically.

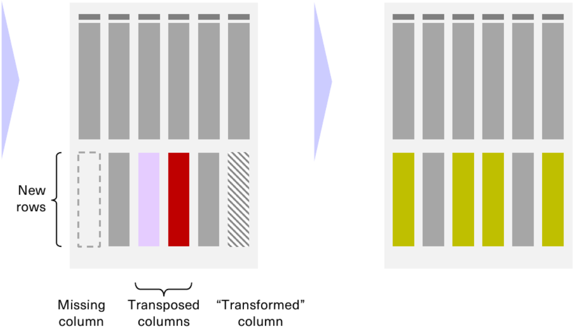
Applications

Examples of Applications of KGs and Semantics

- Data Wrangling (Alan Turing Institute)
- Data Access in Oil & Gas Industry
- Data Access and Prediction in Ecotoxicology
- Data Access of Geological Images

AIDA project: Data Wrangling with DataDiff

- The structure of a dataset may change after an update
- Changes may break the analytical pipeline.
- ✓ Datadiff **identifies and patches** these changes.
- ✗ Limitation: **exhaustive comparison** of columns.
- ✓ Semantic table understanding **may limit the comparison**.



Data Diff: Interpretable, Executable Summaries of Changes in Distributions for Data Wrangling. C. Sutton, T. Hobson, J. Geddes and R. Caruana. In KDD 2018.

Data Access in Oil & Gas Industry

- Data access currently takes **30-70%** of the engineers' time.
- Data cannot be moved from the original sources.
- The EU project Optique advocated for an **Ontology-Based Data Access** (OBDA) process. Requirements:
  - Domain ontology.
  - Mappings to create a virtual KG.

Ontology Based Data Access in Statoil. Journal of Web Semantics, 44, pp. 3-36
`https://openaccess.city.ac.uk/id/eprint/22959/`

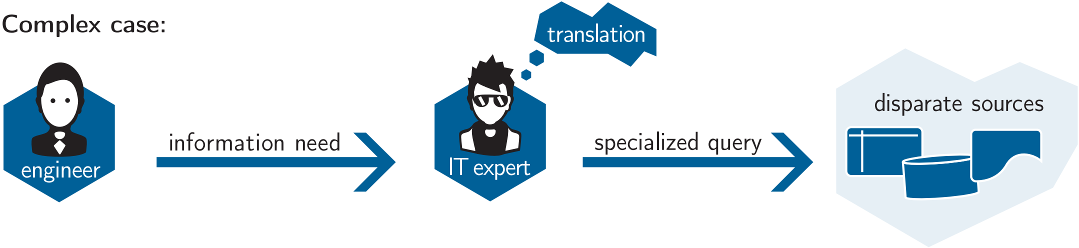
Data Access in Oil & Gas Industry: Limitations

Simple case:

Problem when the information needs fall outside predefined-queries

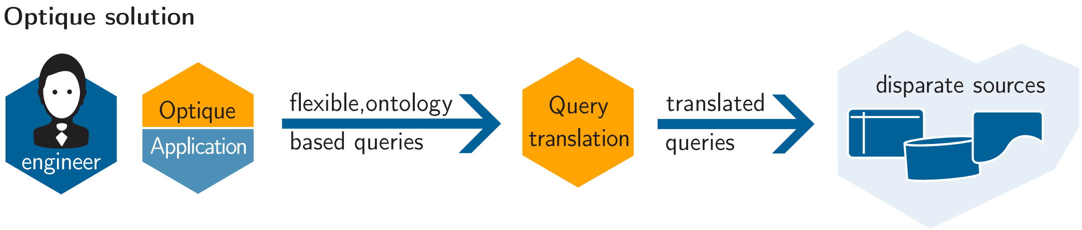
Data Access in Oil & Gas Industry: Limitations

Complex case:



The process may take several days

Data Access in Oil & Gas Industry: Optique Solution

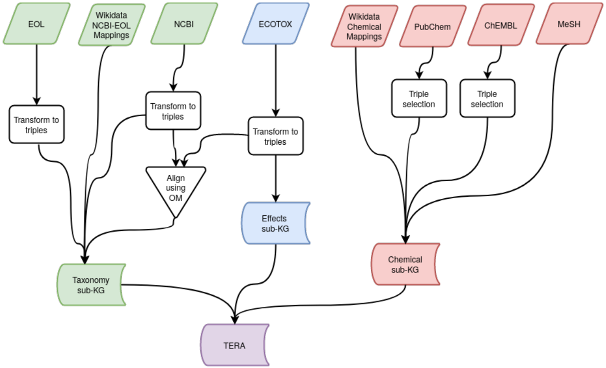


Optique Solution

1. Mediator to create ontology-driven queries (SPARQL).
2. Mediator to translate SPARQL queries into SQL queries.
3. Effort required to create the ontology and maintain the mappings (modular approach).

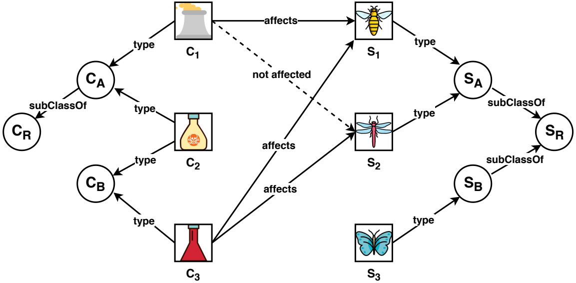
TERA: A KG for Ecotoxicology. Integration and Data Access.

- **Integrates** disparate sources about species, chemicals and effect data.
- Enhances **data access**.



TERA: A KG for Ecotoxicology. Prediction.

– Drives the **prediction of adverse biological effects** of chemicals via KG embeddings.



Resources and publications: `https://github.com/NIVA-Knowledge-Graph/`

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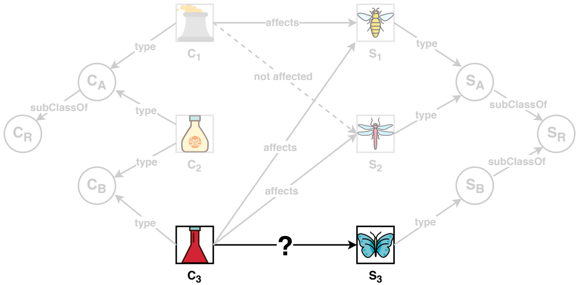
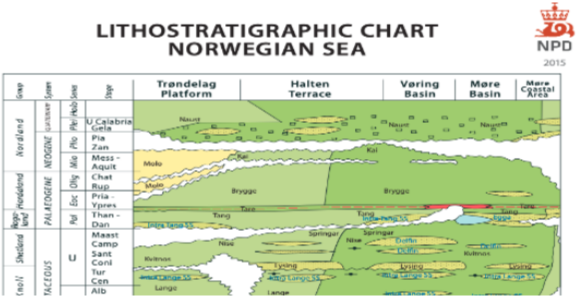


Resources and publications: `https://github.com/NIVA-Knowledge-Graph/`

A KG for Semantic Data Access of Geological Images

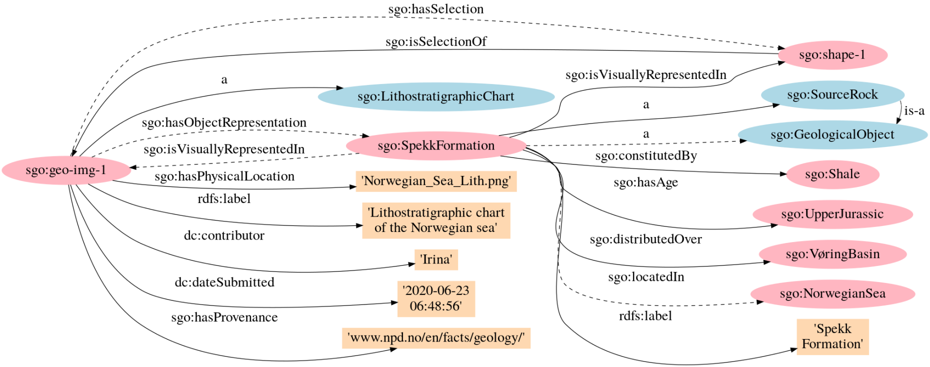
✗ Hard to search for specific images.

✓ Describe the information within the images in a KG.



Resources: `https://sws.ifi.uio.no/project/sirius-geo-annotator/`

A KG for Semantic Data Access of Geological Images



Resources: `https://sws.ifi.uio.no/project/sirius-geo-annotator/`

Laboratory: From CSV to a KG

Support Codes

- `https://github.com/city-knowledge-graphs`
- Lookup
- SPARQL Endpoint
- Lexical similarity
- CSV management