CITY
UNIVERSITY OF LONDON
EST 1894

Applications to Data Science

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Lecturer in Artificial Intelligence

Before we start...

Some important information

- Course work submission reminder:
  - Sunday, 6 March 2022, 5:00 PM.
  - Submit files individually as mentioned in the instructions (*i.e.*, *myOnto.ttl, myOnto.owl, myVideo.mp4 and myOntoCode.pdf*).
  - If video is $> 200Mb$ then upload it into Google/One drive and upload in moodle a text file with the link to the video (*i.e.*, *myVideoLink.txt*).
- Drop-in sessions during reading week.
  - Tuesday: 1-2:30pm (online). Using wonder.me: `https://bit.ly/in3067-inm713-online-lab`
  - Thursday: 3-4pm (as usual in Zoom) - Coursework Part 2 discussion

Where are we? Module organization (tentative)

✓ Introduction.
✓ OWL (2) ontology language. Focus on modelling.
✓ RDF-based knowledge graphs.
✓ SPARQL 1.0 Query Language.

5. **Applications to Data Science**. From tabular data to KG. (Today)
6. RDFS Semantics and OWL 2 profiles.
7. SPARQL 1.1 and Graph Database solutions.
8. Ontology Alignment.
9. Ontology Embeddings and Machine Learning.
10. Other topics. *Possibly RML mappings, SHACL constraint language...*

Data Science Bottleneck

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Big Data Borat
@BigDataBorat

Follow

In Data Science, 80% of time spent prepare data, 20% of time spent complain about need for prepare data.

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One of the main problems is the lack of understanding of the data and the domain.

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`

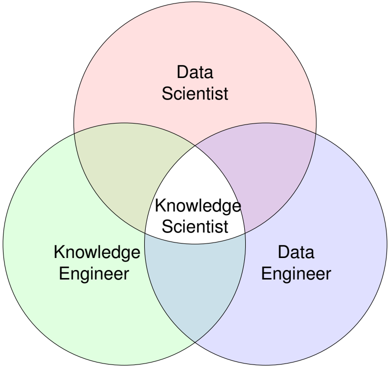
Semantic Understanding of Tabular Data

- **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.

The Knowledge Scientist

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/knowledge integration, graph databases)

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

The Knowledge Scientist: DS perspective

- Domain understanding.
- Designing & developing ontologies and KGs together with domain experts.
- Developing data processing pipelines to drive the semantic shifting of the data.
- Application of data analytics and ML with KGs.

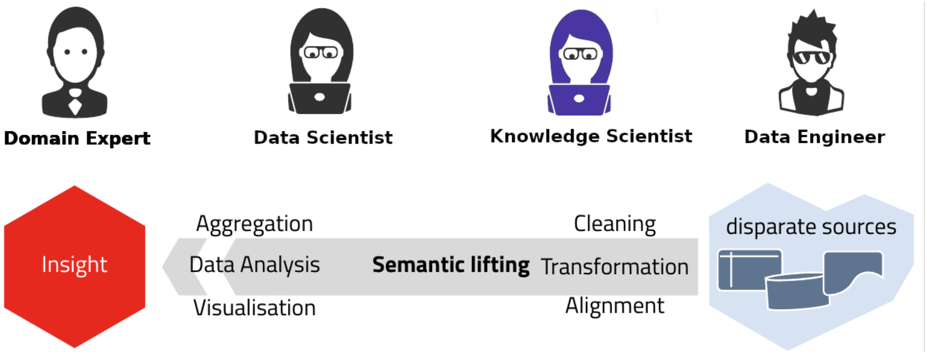
George Fletcher and others. **Knowledge Scientists: Unlocking the data-driven organization**. 2020
Stratos Kontopoulos. **Semantic AI & the Role of the Knowledge Scientist**. 2021

The Knowledge Scientist: SE/CS perspective

- Domain understanding.
- Deploying the semantic infrastructure (*e.g.*, triplestores, reasoning, query formulation, required APIs).
- Integration with other components.

George Fletcher and others. **Knowledge Scientists: Unlocking the data-driven organization**. 2020
Stratos Kontopoulos. **Semantic AI & the Role of the Knowledge Scientist**. 2021

The Knowledge Scientist: overview



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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- **Not new**:
  - Graph data models extensively studied in AI…
  - …but Google has relaunched the interest on **KGs in industry**

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  - Enterprise data as a knowledge graph to **drive products** and make them more "**intelligent**"
- **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**. 2021 `https://kgbook.org/`.
Pim Borst, Hans Akkermans, and Jan Top. **Engineering ontologies**, 1999.

Why Ontologies and KGSs?

– 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 KGs? (Experiences from Industry)

- Knowledge graphs are **not complex**: they are the simplest way to layer human expertise onto stored data.
- Investing in knowledge graphs is **resilient**: an initial investment that pays off by allowing companies to pre-prepare for unanticipated and unfolding use cases
- **Unifying logical representation** for data an semantics to get out the data science enterprise mess.

Juan Sequeda and Ora Lassila. **Designing and Building Enterprise Knowledge Graphs**. 2021
Ora Lassila. **On the broad applicability of Semantic Web technologies**. (COST DKG Talk Series. 2021
https://www.youtube.com/watch?v=f9wautaqWUs
Juan Sequeda and Ora Lassila. https://watch.knowledgegraph.tech/knowledge-espresso/videos/knowledge-espresso-with-ora-lassila-and-juan-sequeda

FAIR principles and 5-star data

Why Ontologies and KGs?

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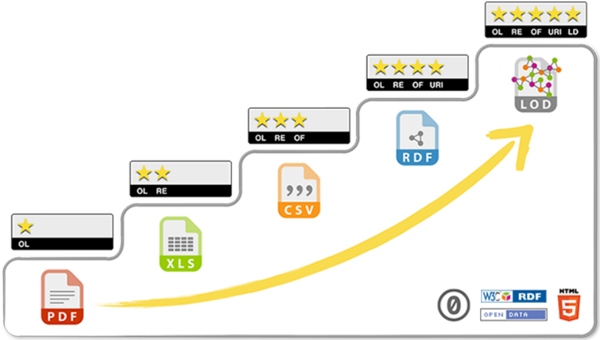
♠ This also applies within a company (intranet), not only for the Web. Ideally with an OL, but at least data accessible by everyone in the company.

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

5-star Data



♠ **LOD**: Linked Open Data.

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

5-star Data: Technical 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

5-star Data: Technical challenges:

- How to **expose** data (*e.g.*, databases, csv files) as knowledge graphs?
  - *RDF (Week 3) and Today's session - 4-5 ⋆ data*
- How to **create** (or reuse) and use (abstract) **knowledge** (*i.e.*, *Ontologies*)?
  - *OWL (Week 2)*
- How to **align** different knowledge graphs? ♠
  - *Ontology Alignment (Week 8) - 5 ⋆ data*
- How to check **consistency and trust** of the data and knowledge? ♠
  - *Reasoning with RDFS and OWL (Week 7) - 6 ⋆ data?*

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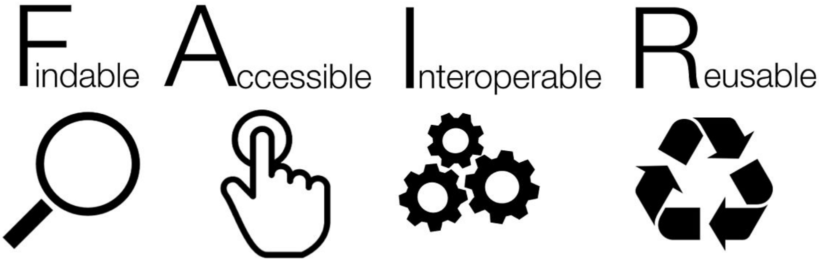
FAIR Data Principles (i)



♠ For for machines and people.

The FAIR Guiding Principles for scientific data management and stewardship. Nature Scientific Data 2016.
`https://www.go-fair.org/fair-principles/`

FAIR Data Principles (ii)

- **Findable**: (meta)data is assigned an unique identifier and data is described with rich metadata.
- **Accessible**: (meta)data can be accessed via a known protocol. ($\star$)
- **Interoperable**: meta(data) uses a formal (knowledge representation) language.
- **Reusable**: well described (meta)data with rich provenance.

($\star$) Not necessarily open. (FAIR $\neq$ OPEN)

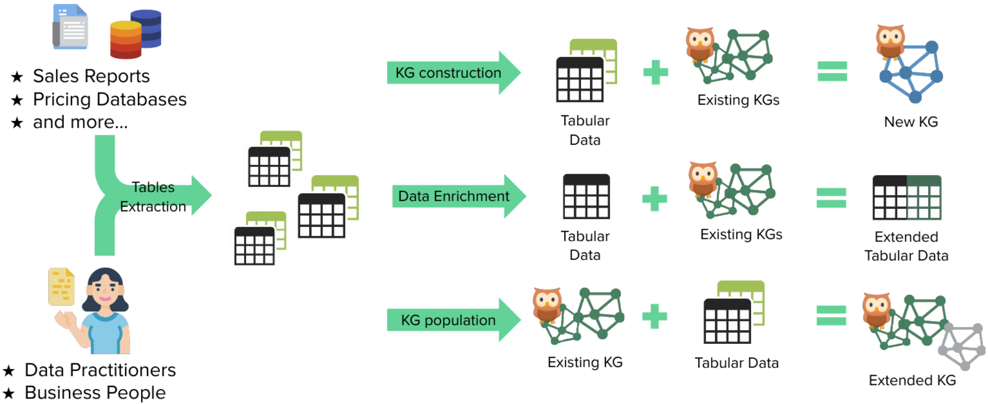
FAIR Data Principles (iii)

- FAIR data is more valuable, easier to find and combine thanks to unique identifiers and a formal shared knowledge representation.
- “KGs must be in want of FAIR data. And FAIR data is in want of KGs”.

Carole Golbe. FAIRy stories: the FAIR Data principles in theory and in practice.
`https://www.slideshare.net/carolegoble/fairy-stories-the-fair-data-principles-in-theory-and-in-practice`

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

Semantic Table Understanding/Interpretation



Vincenzo Cutrona. **Why Table Understanding Matters**. See last year invited speakers.

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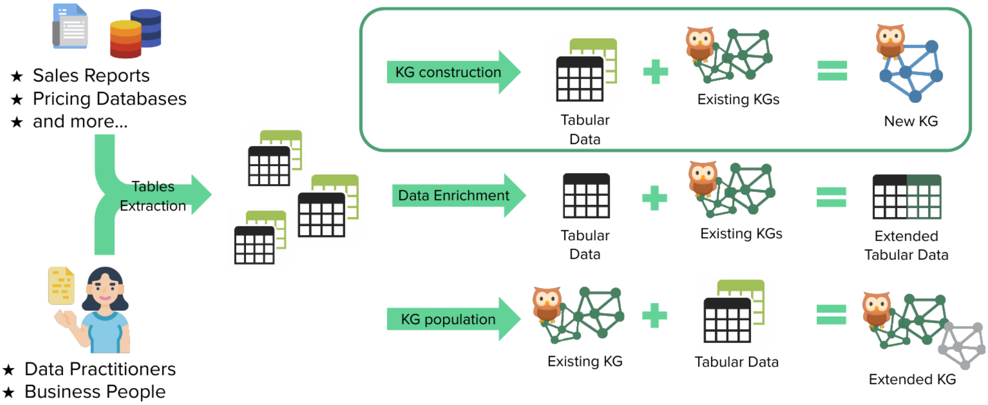

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Exposing data as an RDF-based Knowledge Graph

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

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  ✓ Data remains in its original format.

  ✗ Typically only over relational databases.

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– **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.

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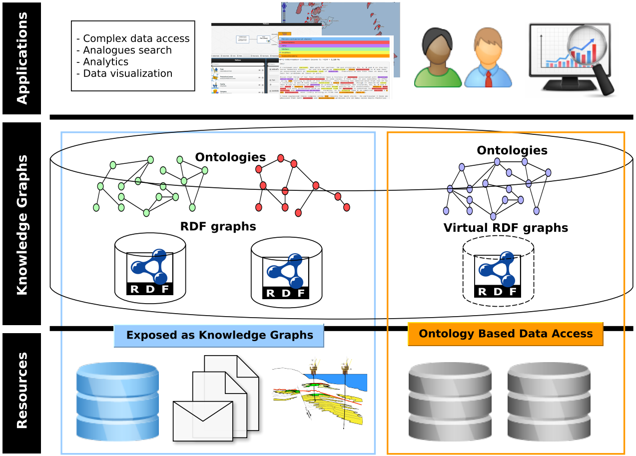
  - – Due to size or privacy it may not be possible to export the data.

Exposing data as RDF: Architecture

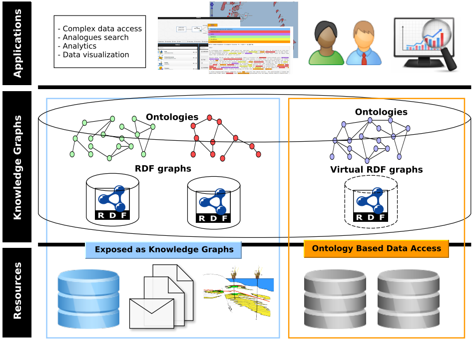


Exposing data as RDF: Ingredients

– **Ontology vocabulary**. Custom and/or given by a public KG.

– **Mappings**. Define a transformation from the tabular data to RDF data.

– **Ontology Axioms** (optional) - ♠



♠ Ernesto Jimenez-Ruiz and others. **BootOX: Practical Mapping of RDBs to OWL 2**. ISWC 2015

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.

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- **CSV to RDF**:
  - Direct mapping from CSV to RDF (CSV2RDF): `https://www.w3.org/TR/csv2rdf/`
  - General (declarative) RDF Mapping Language (RML): `https://rml.io/specs/rml/`
  - A mapping can also be seen as a **(small) script** that creates specific RDF triples from the CSV file (*e.g.*, data frame).

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  - A mapping can also be seen as a **(small) script** that creates specific RDF triples from the CSV file (*e.g.*, data frame). In this module.

Exposing data as RDF: Direct Mapping Example

Automatic triples:

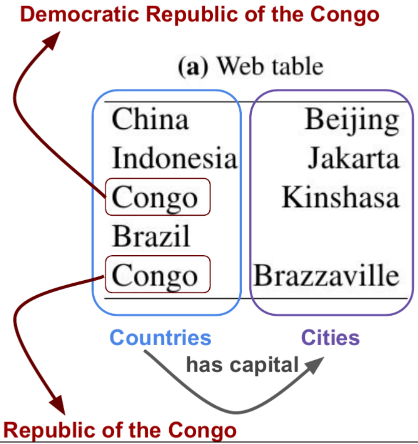
```
ex:row1 ex:col1 ''China''
ex:row1 ex:col2 ''Beijing''
ex:row2 ex:col1 ''Indonesia''
ex:row2 ex:col2 ''Jakarta''
...
```

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:**

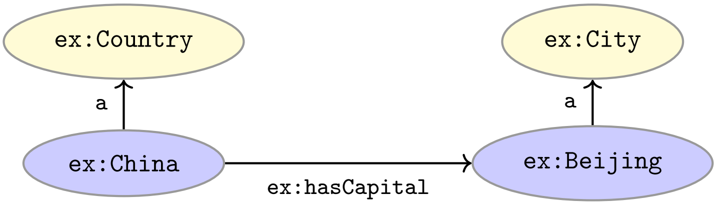
```
ex:China rdf:type ex:Country
ex:Beijing rdf:type ex:City
ex:China ex:hasCapital ex:Beijing
...
```



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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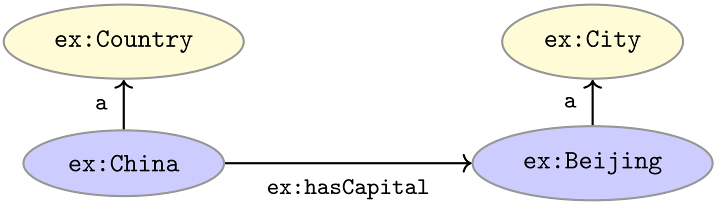

Exposing data as RDF: Mappings

Mapping or Transformation $\varphi \rightsquigarrow \psi$

- φ: query over database or CSV extraction
- ψ: RDF triple template

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  `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
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- **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)
```

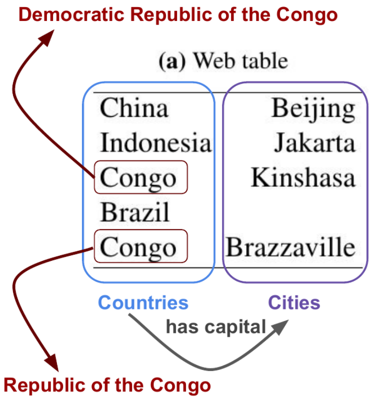
Exposing data as RDF: (Manually defined) Mappings

– Column 1 is composed by Countries.

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

– Column 2 entities are the capitals of column 1 entities.

```
for row in data_frame:
    subj = "ex:"  + row[col1]   #e.g., ex:China
    obj = "ex:"  + row[col2]   #e.g., ex:Beijing
    create_triple(subj ex:hasCapital obj)
```



Semantic Understanding of Tabular Data:
Automating the Process

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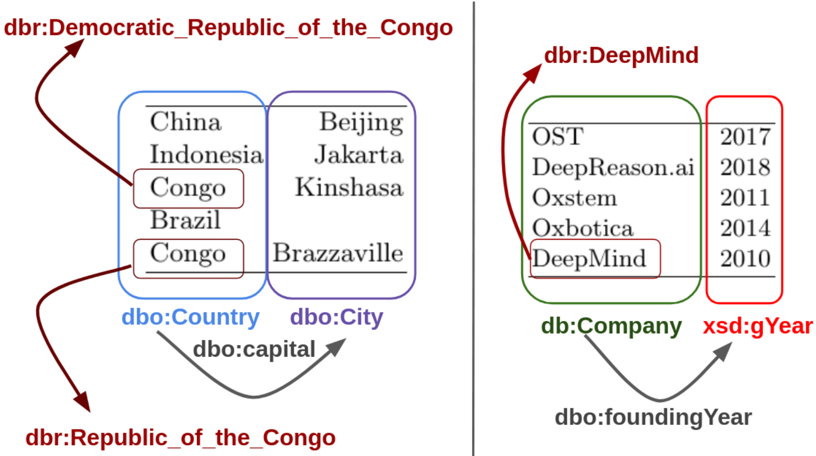
† *For a semi-automatic process, we assume the existence of a (possibly incomplete)* ***Knowledge Graph (KG)*** *relevant to the domain.*
‡ *When transforming to RDF, if no KG matching then create a fresh entity URI.*

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)



SemTab Challenge

- **Systematic evaluation** 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, Wikidata and Schema.org.
- Co-organised and 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/`

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).
- **NLP techniques** to process textually-rich fields.

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- **Fuzzy search** over a KG
  - Via online look-up services
  - Or local indexes
- 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 (*e.g.*, `dbr:London rdf:type dbo:City`)
  - Relationships (*e.g.*, `dbr:London dbo:country dbr:United_Kingdom`)
  - 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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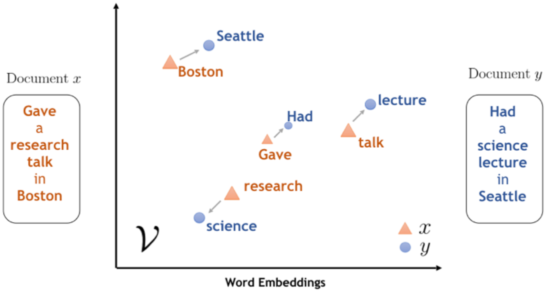
- Comparison among vectors via **Cosine similarity** (*e.g.*, between vectors for 'Congo' and 'Republic of Congo')
- **Precomputed word embeddings:**
  - `https://wikipedia2vec.github.io/wikipedia2vec/pretrained/`
  - `https://fasttext.cc/docs/en/pretrained-vectors.html`
  - `https://www.analyticsvidhya.com/blog/2020/03/pretrained-word-embeddings-nlp/`
- **Precomputed KG embeddings:**
  - Wikidata: `http://139.129.163.161/index/toolkits#pretrained-embeddings`
  - DBpedia: `http://www.kgvec2go.org/`

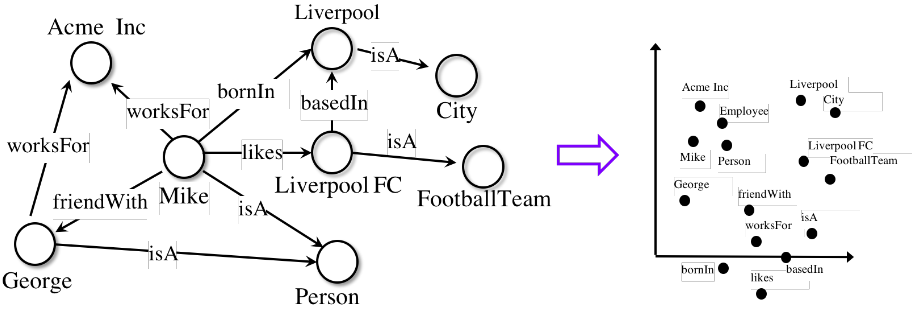
Word Embeddings: Example



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

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

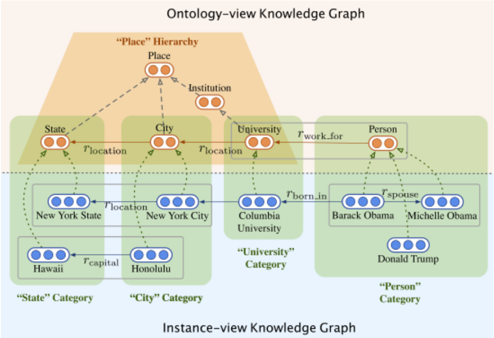
Knowledge Graph Embeddings: Example (i)

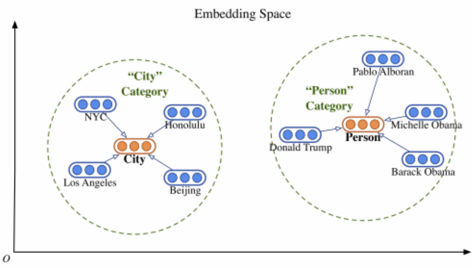


KG Embedding Systems exploit the neighbourhood of an entity to calculate its vector.

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

Knowledge Graph Embeddings: Example (ii)





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Example from: Universal Representation Learning of Knowledge Bases by Jointly Embedding Instances and Ontological Concepts. KDD 2019.

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 the default installation).
- In this module we will not use OpenRefine, but perform our own reconciliation programmatically.

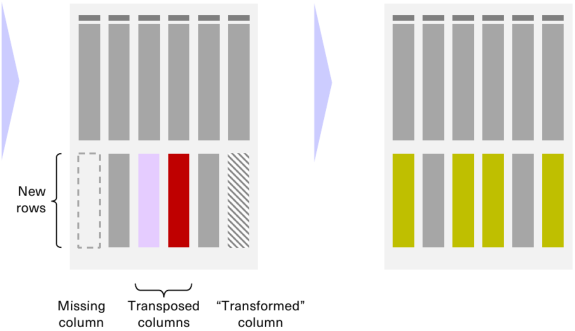
Applications

Examples of Applications of KGs and Semantics

- Data Wrangling (Alan Turing Institute)
- Data Access in Oil & Gas Industry
- Data Access and Prediction in Ecotoxicology
- Semantic Reasoning and Ontologies for Autonomous Vehicles
- FAIR Implementation for Life Science
- Amazon Product Graph

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/`

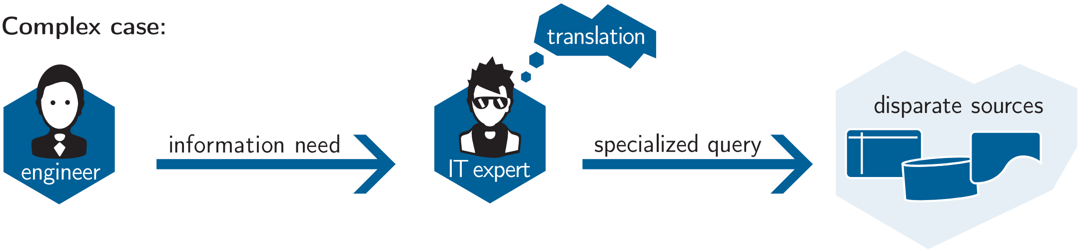
Data Access in Oil & Gas Industry: Limitations

Simple case:

Problem when the information needs fall outside predefined-queries

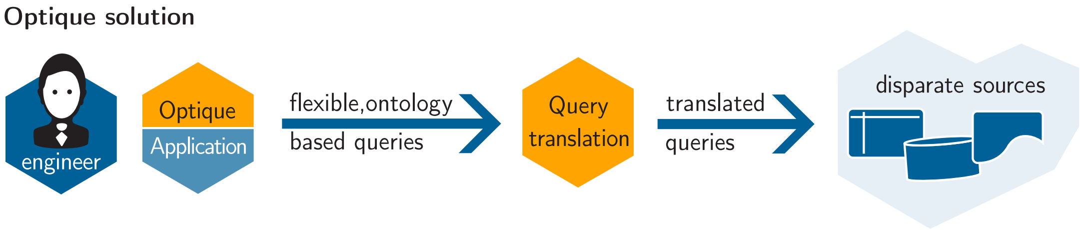
Data Access in Oil & Gas Industry: Limitations

Complex case:



The process may take several days

Data Access in Oil & Gas Industry: Optique Solution

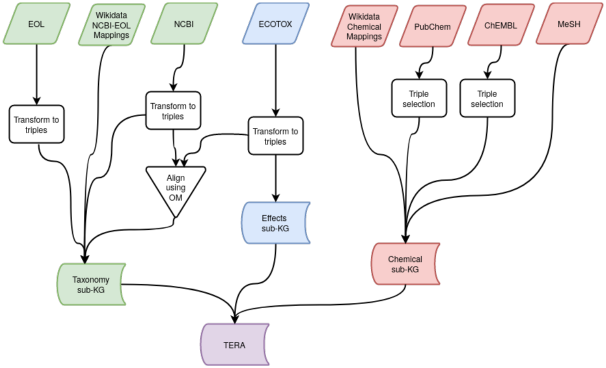


Optique Solution

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).

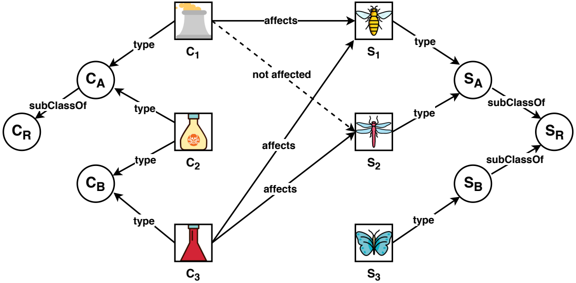
TERA: A KG for Ecotoxicology. Integration and Data Access.

- **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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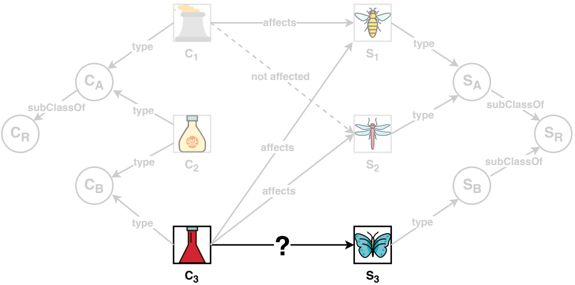

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Semantic Reasoning and Ontologies for Autonomous Vehicles

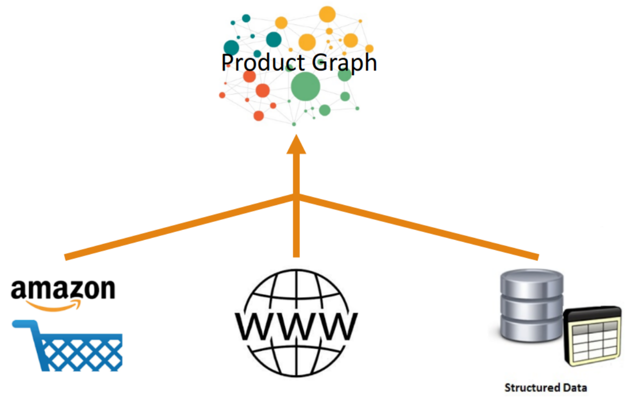
Oxford Semantic Technologies: `https://www.oxfordsemantic.tech/blog/reasonable-vehicles-rule-the-road`

FAIR Implementation for Life Science

Knowledge Graphs play a key role for annotating data.

Pistoia Alliance FAIR Toolkit: `https://fairtoolkit.pistoiaalliance.org/`

Amazon Product (Knowledge) Graph



Challenges and Innovations in Building a Product Knowledge Graph: `http://lunadong.com/talks/PG.pdf`
`https://www.amazon.science/blog/building-product-graphs-automatically`

Laboratory: From CSV to a KG

Support Codes

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

Wonder.me

- Use of **wonder.me**:
  - `https://app.wonder.me/?spaceId=d39fd38d-5cc3-48fd-9952-5990e851b681`
  - Short URL: `https://bit.ly/in3067-inm713-online-lab`