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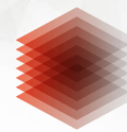
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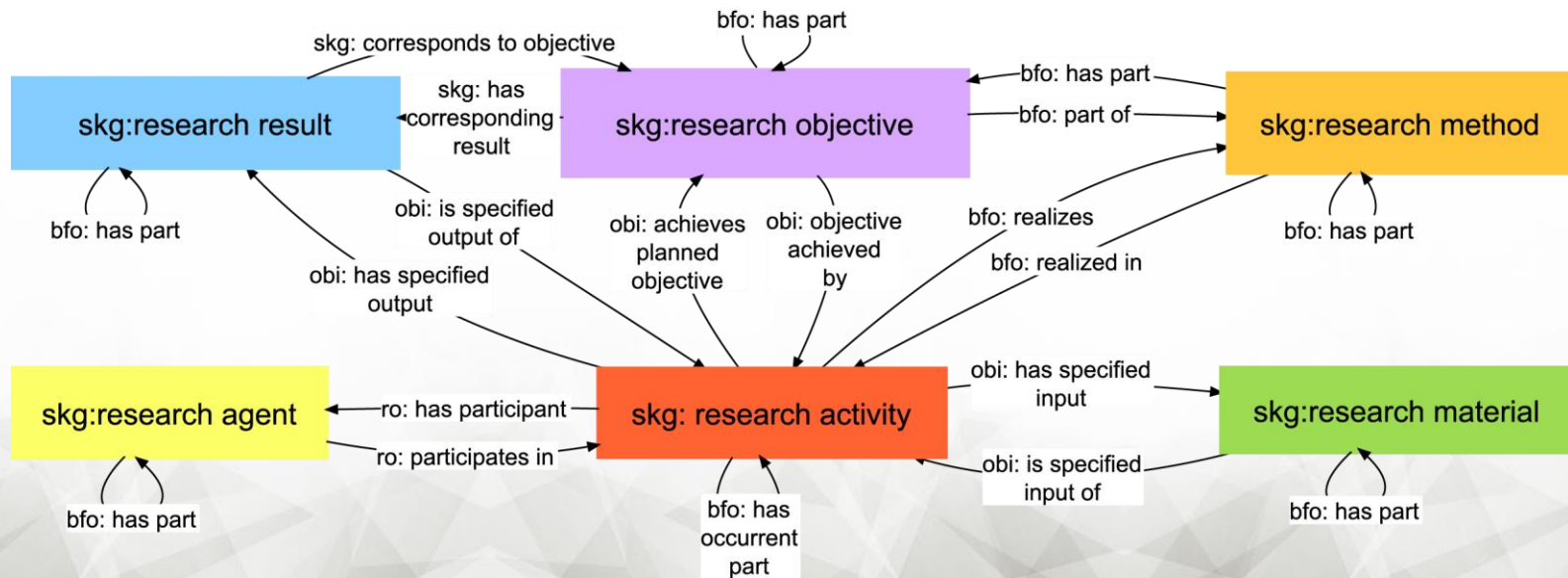


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Towards Representing Research Contributions in Scholarly Knowledge Graphs Using Knowledge Graph Cells

L. Vogt, J. D'Souza, M. Stocker, S. Auer



Scholarly Communication

The Problem

Research is predominantly communicated using **unstructured text**. And the contents of scholarly publications are **not machine-actionable**.



Scholarly Communication

The Problem

The number of publications is **increasing exponentially**, with more than **2.5 million** new publications being issued **each year**.

[Jinha \(2010\) Article 50 million: an estimate of the number of scholarly articles in existence. *Learned Publishing* 23\(3\), 258–263.](#)

Scholarly Communication

The Problem

As a result, researchers often have to search the contents of **potentially relevant** publications themselves to find those that are actually relevant to them. This becomes increasingly **impossible** with an exponentially increasing number of publications.

[Landhuis \(2016\) Scientific literature: information overload. *Nature* 535\(7612\), 457–458.](#)

Scholarly Communication

The Solution

A promising **solution** to this knowledge management problem is to make these contents machine-actionable.

Scholarly Communication

The Context – The FAIR Guiding Principles

Research communities and public stake holders have identified an increasing demand for the Findability, Accessibility, Interoperability, and Reusability of data and metadata (FAIR Guiding Principles).

[Wilkinson et al. \(2016\) The FAIR Guiding Principles for scientific data management and stewardship. *Scientific Data* 3\(1\): 160018.](#)

Scholarly Communication

The Context – The FAIR Guiding Principles

The use of ontologies, knowledge graphs, the Resource Description Framework (RDF), and the Web Ontology Language (OWL) have proven to provide the **semantic technologies** required for implementing the FAIR Guiding Principles.

Jacobsen et al. (2019) FAIR principles: interpretations and implementation considerations. *Data Intelligence* 2(1-2), 10–29.

Vogt et al. (2019) SOCCOMAS: a FAIR web content management system that uses knowledge graphs and that is based on semantic programming. *Database* 2019: baz067.

Scholarly Communication

The Goal – A knowledge graph of scholarly publications

Our goal is to develop a **knowledge graph** of **scholarly publications** that makes available the **contents** of the publications in a form that complies with the **FAIR** Principles.

Challenges

Machine-actionability requires common data model

In order to build a FAIR knowledge graph of scholarly publications, some challenges have to be overcome. First, **machine-actionability** and **FAIRness** requires data to be **formalized** and **standardized** to some degree. This requires the development of a basic **data model** for integrating scholarly contents within the graph (**Research Contribution Model**).

Challenges

Machine-actionable graphs are often too complex for human readers

Another challenge results from the discrepancy between the requirements for machine-actionability as opposed to human-readability of data, with the former usually resulting in overly complex graphs with lots of information that is irrelevant for a human reader. We developed the idea of Knowledge Graphs Cells to tackle this problem.

The Research Contribution Model (RCM)

The Research Contribution Model (RCM)

Challenge

Modelling the contents of scholarly publications is very challenging, as they cover **multiple domains**, each with its own set of **established standards** and **terminological conventions**.

The Research Contribution Model (RCM)

Scholarly publications contain assertions

Scholarly publications contain assertions. An **assertion** is a proposition which is asserted or denied to be **true**. Independent of a particular domain, we can distinguish different basic types of assertions.

The Research Contribution Model (RCM)

Types of assertions

- **empirical data** (descriptive, phenomenon, observation, measurement)
- **activity of producing data** (process of observing, measuring, etc.)
- **method of producing data** (plan for a data production activity)

The Research Contribution Model (RCM)

Types of assertions

- **result** (ontological, hypothesis, theory, test-result value, explanation, etc.)
- **activity of analyzing data** (process of analyzing, testing, etc.)
- **method of analyzing data** (plan for a data analysis activity)

The Research Contribution Model (RCM)

Types of assertions

- Data (phenomena), results
- (theories), and methods (plans for
- research activities) are the key elements of scholarly discourse.

Szostak (2007) Interdisciplinarity and the Classification of Scholarly Documents by Phenomena, Theories, and Methods. *Interdisciplinarity and transdisciplinarity in the organization of scientific knowledge: Actas del VIII Congreso ISKO-España*, 469–477.

The Research Contribution Model (RCM)

Types of assertions

- For each **type** of a
- scholarly assertion, we specify a
- **graph pattern/template.**

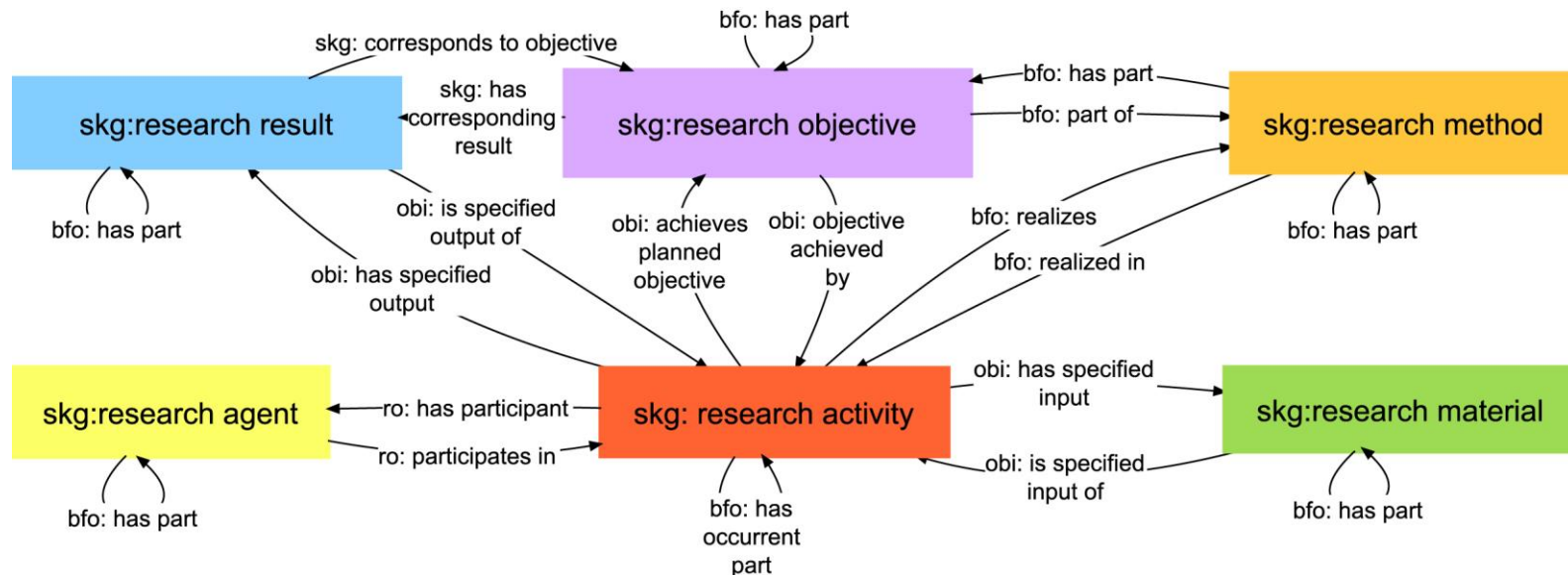
The Research Contribution Model (RCM)

Types of assertions

- **result** (ontological, hypothesis, theory, test-result value, ex
 - **ad**
an
 - **m**
analysis activity)
- And the **RCM** relates them to one another.

The Research Contribution Model (RCM)

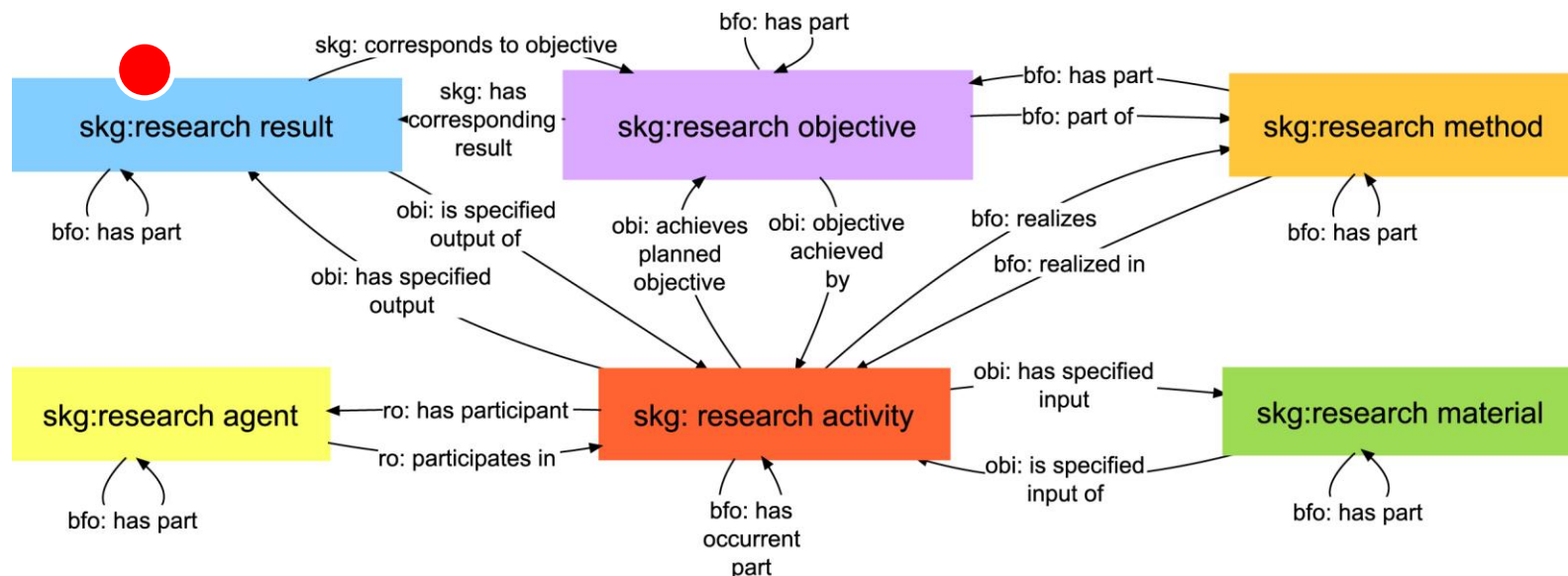
Integrating different types of assertions



The Research Contribution Model (RCM)

Integrating different types of assertions

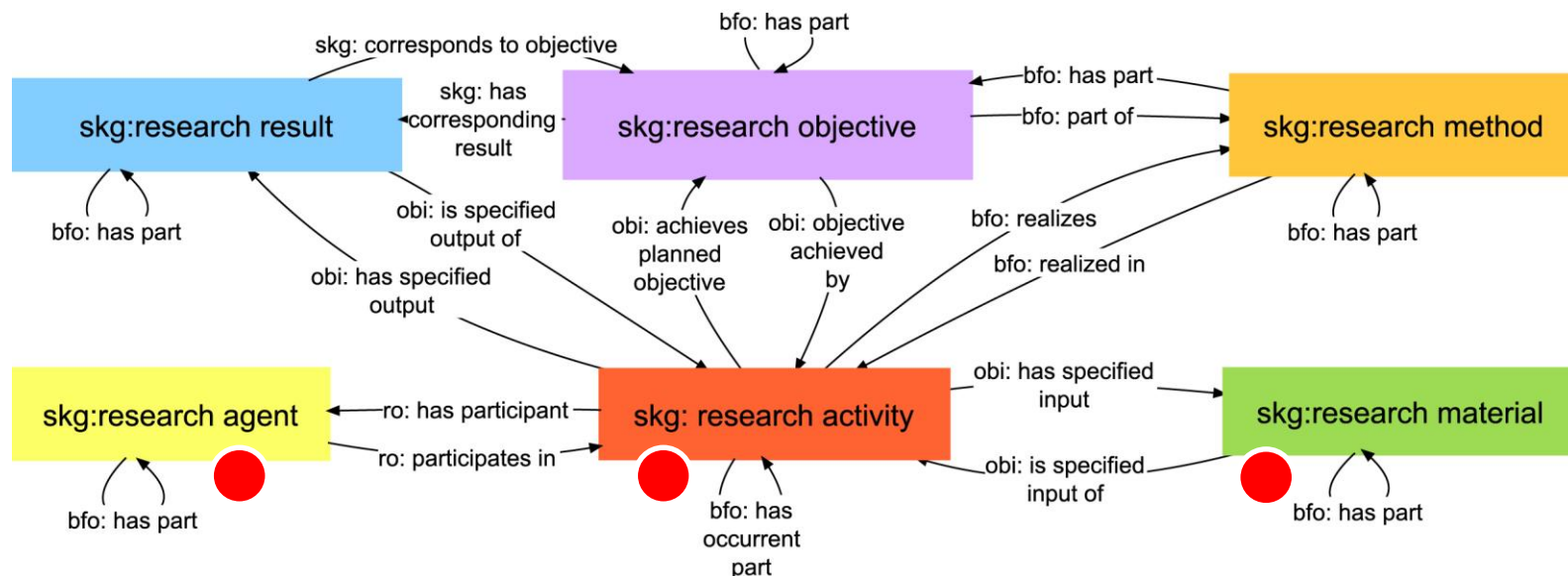
empirical data



The Research Contribution Model (RCM)

Integrating different types of assertions

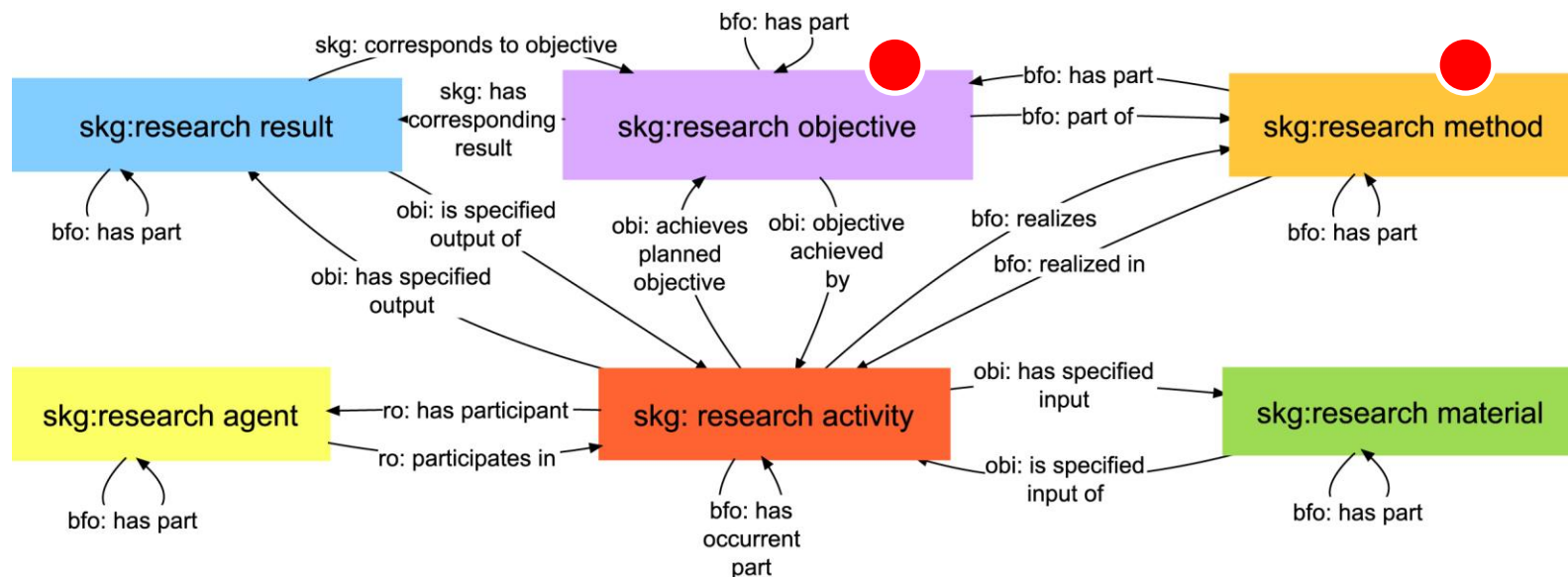
activity of producing data



The Research Contribution Model (RCM)

Integrating different types of assertions

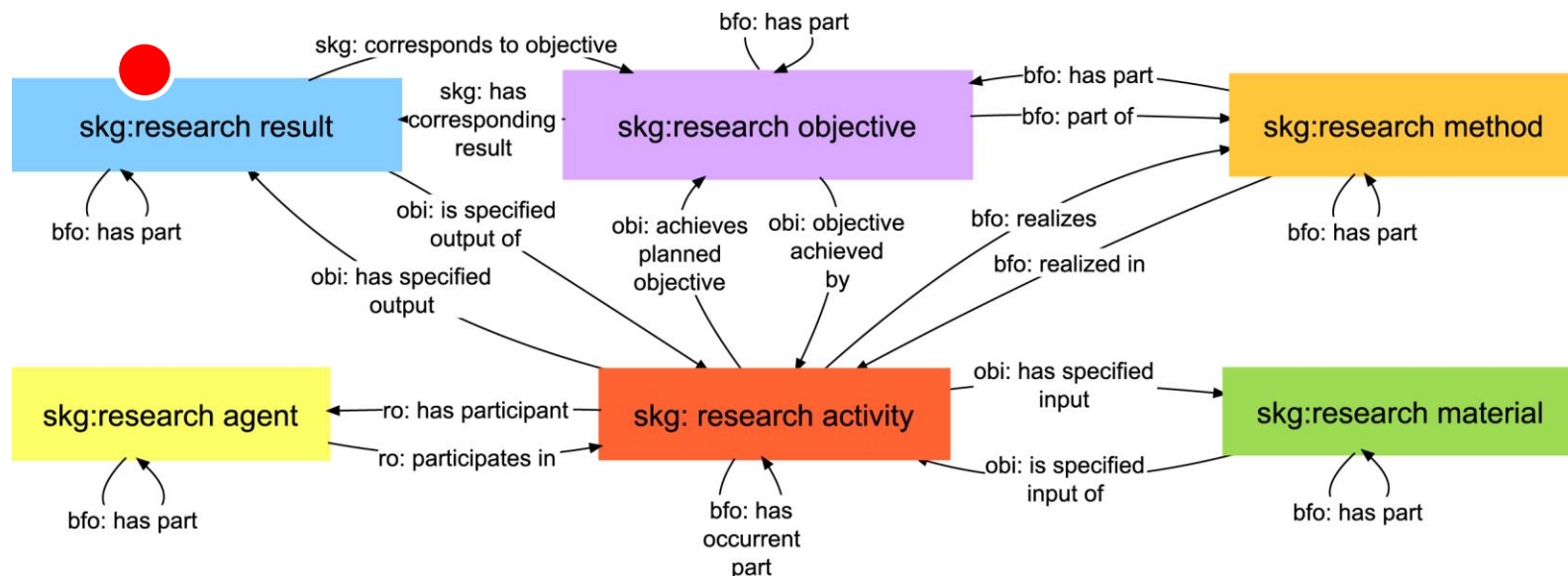
method of producing data



The Research Contribution Model (RCM)

Integrating different types of assertions

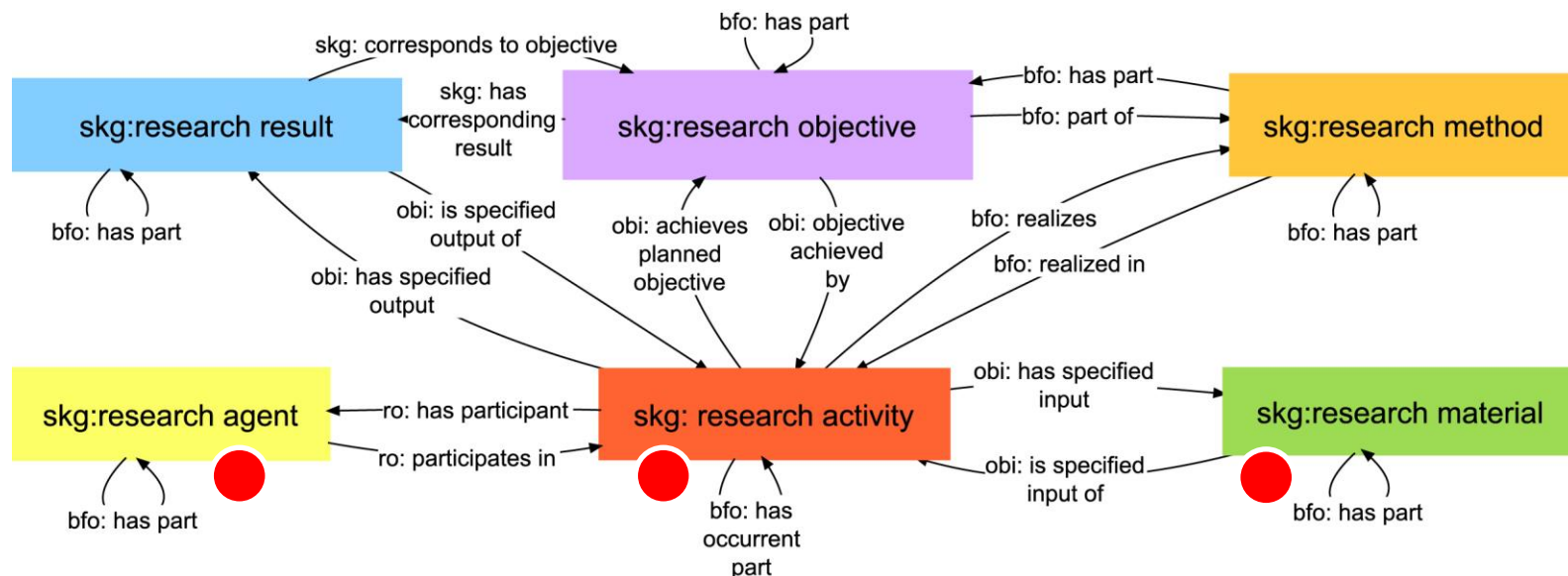
result



The Research Contribution Model (RCM)

Integrating different types of assertions

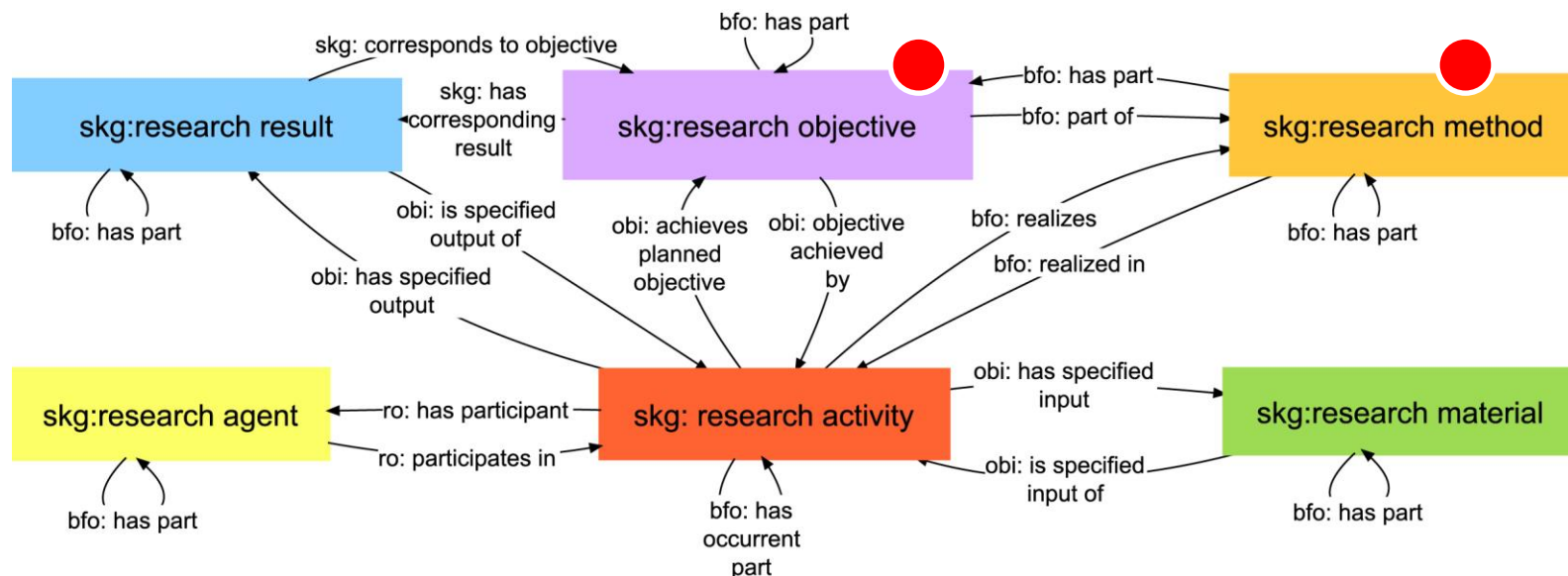
activity of analyzing data



The Research Contribution Model (RCM)

Integrating different types of assertions

method of analyzing data



The Research Contribution Model (RCM)

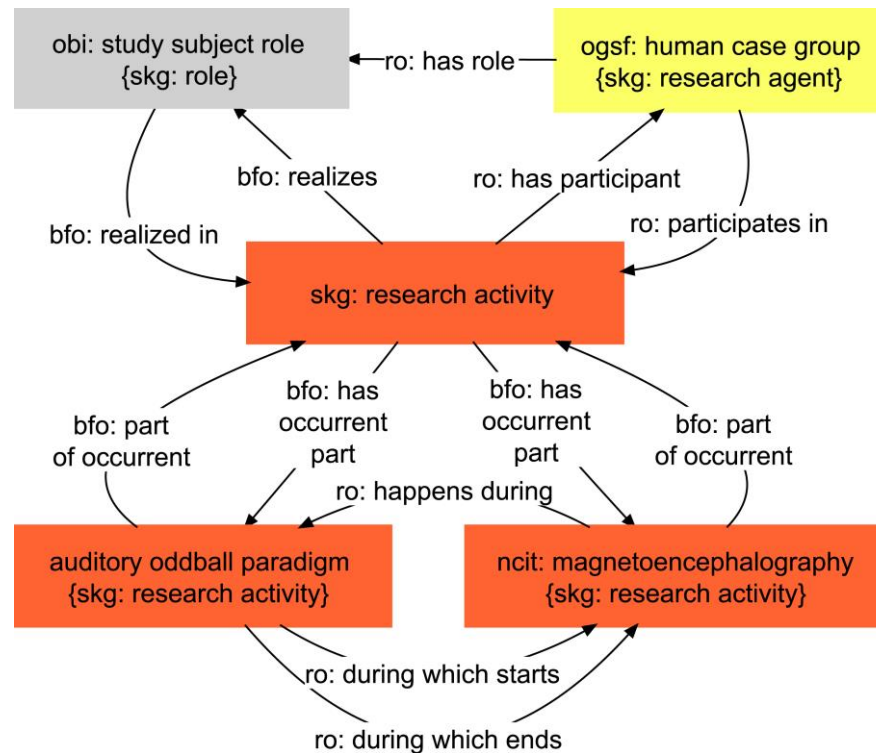
Inherent nested hierarchy

Because **the world is granular** and because every whole can be **partitioned** into finer grains—a research result consists of sets of results, a method of sets of steps, an activity of sets of events and material entities of sets of parts—the RCM can be applied like a **Matryoshka**.



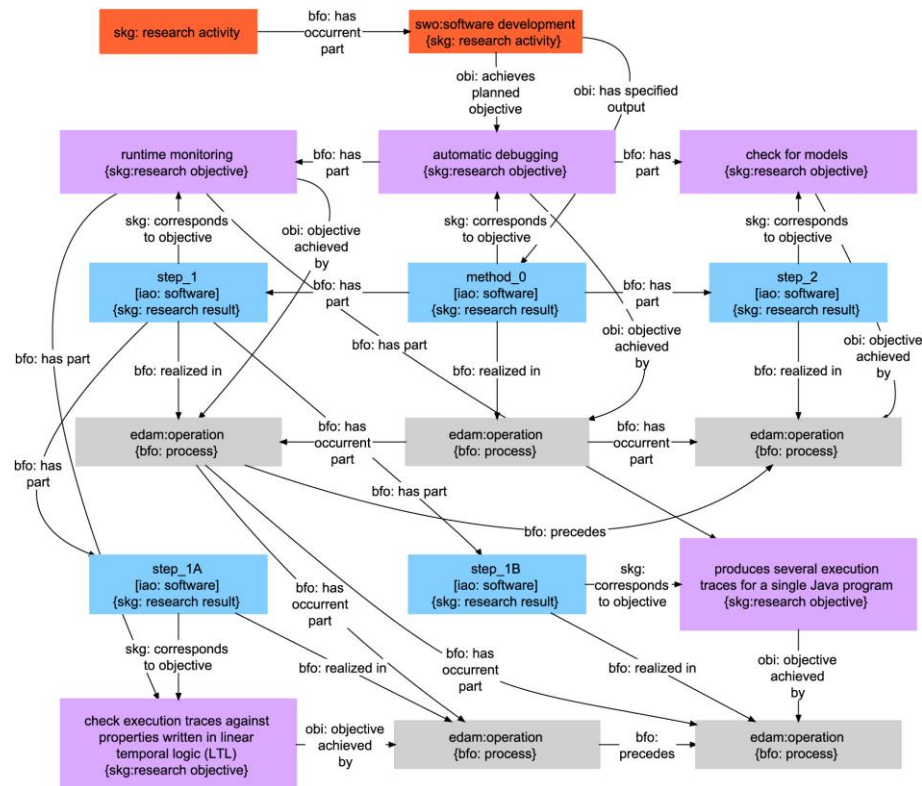
The Research Contribution Model (RCM)

Magnetoencephalography during auditory oddball paradigm



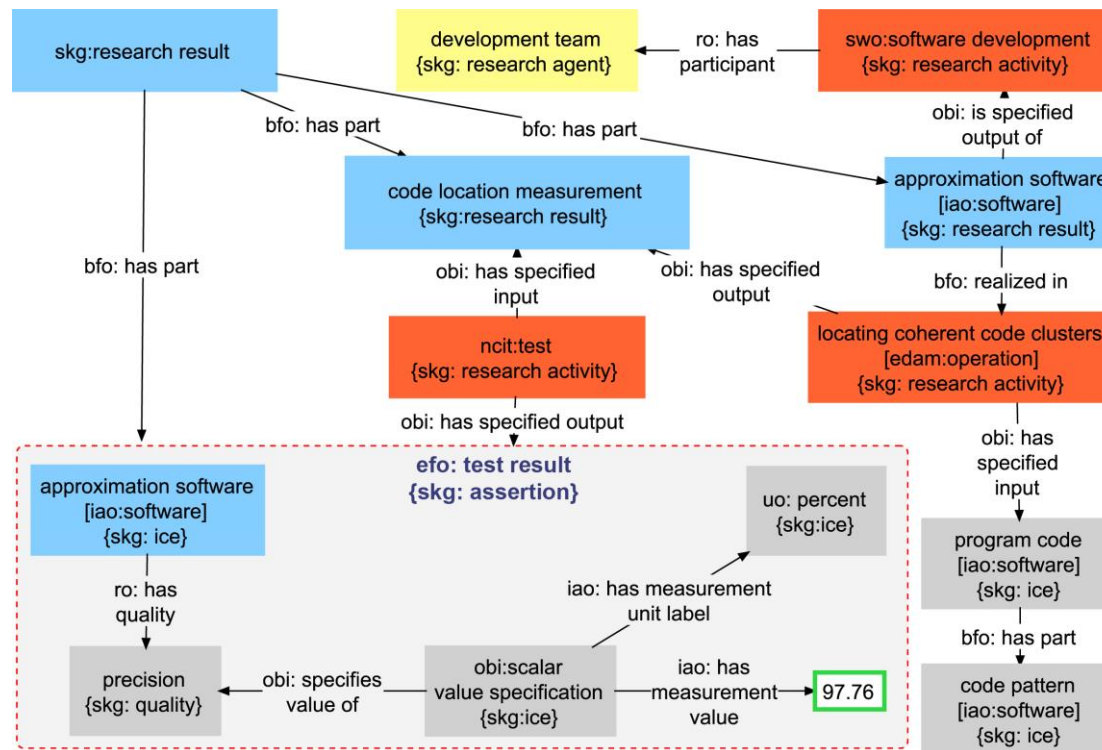
The Research Contribution Model (RCM)

Description of a software development



The Research Contribution Model (RCM)

Measurement of precision



Employing the RCM in a knowledge graph

Bottom-up data entry—at the level of individual assertions

Europe PMC Funders Group
 Author Manuscript
***J Neurol.* Author manuscript; available in PMC 2019 June 11.**

Published in final edited form as:
J Neurol. 2015 October 1; 262(10): 2232–2240. doi:10.1007/s00415-015-7832-2.

Voxel based analysis in neuroferritinopathy expands the phenotype and determines radiological correlates of disease severity

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⁵Medical Toxicology Centre, Wolfson Building, Claremont Place, Newcastle University, Newcastle upon Tyne, NE2 4AA

Europe PMC Funders Group Author Manuscripts

Example taken from:

Udell (2015) Annotating to extract findings from scientific papers. *hypothesis.is*, <https://web.hypothesis.is/blog/annotating-to-...>

Employing the RCM in a knowledge graph

Bottom-up data entry—at the level of individual assertions

PDF Viewer

doi:10.1007/s00415-015-7832-2

Annotation

Neuroferritinopathy is an autosomal dominant adult-onset movement disorder which occurs due to mutations in the ferritin light chain gene (FTL). Extensive iron deposition and cavitation are observed post-mortem in the basal ganglia, but whether more widespread pathological changes occur, and whether they correlate with disease severity is unknown.

3D-T1w and quantitative T2 whole brain MRI scans were performed in 10 clinically symptomatic patients with the 460InsA FTL mutation and 10 age-matched controls. **Voxel-based morphometry (VBM) and voxel-based relaxometry (VBR) were subsequently performed.** Clinical assessment using the Unified Dystonia Rating Scale (UDRS) and Unified Huntington's Disease Rating Scale (UHDRS) was undertaken in all patients.

VBM detected significant tissue changes within the substantia nigra, midbrain and dentate together with significant cerebellar atrophy in patients (FWE, $p < 0.05$). Iron deposition in the caudate head and cavitation in the lateral globus pallidus correlated with UDRS score ($p < 0.001$). There were no differences between groups with VBR.

Our data show that progressive iron accumulation in the caudate nucleus, and cavitation of the globus pallidus correlate with disease severity in neuroferritinopathy. We also confirm sub-clinical

Text: “Voxel-based morphometry (VBM) and voxel-based relaxometry (VBR) were subsequently performed.”

mark assertion
in text

Example taken from:

Udell (2015) Annotating to extract findings from scientific papers. *hypothesis.is*, <https://web.hypothesis.is/blog/annotating-to-...>

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Data Analysis Method ▼

Text: *"Voxel-based morphometry (VBM) and voxel-based relaxometry (VBR) were subsequently performed."*

classify the
assertion

Example taken from:

Udell (2015) Annotating to extract findings from scientific papers. *hypothesis.is*, <https://web.hypothesis.is/blog/annotating-to-...>

Employing the RCM in a knowledge graph

Bottom-up data entry—at the level of individual assertions

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Data Analysis Method ▼

Text: “Voxel-based morphometry (VBM) and voxel-based relaxometry (VBR) were subsequently performed.”

x ero:morphometry

x chmo:relaxometry

semantic
enrichment

Example taken from:

Udell (2015) Annotating to extract findings from scientific papers. *hypothesis.is*, <https://web.hypothesis.is/blog/annotating-to-...>

Employing the RCM in a knowledge graph

Bottom-up data entry—at the level of individual assertions

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Data Analysis Method ▼

Text: “Voxel-based morphometry (VBM) and voxel-based relaxometry (VBR) were subsequently performed.”

x ero:morphometry

x chmo:relaxometry

has part:

x ero:voxel-based morphometry

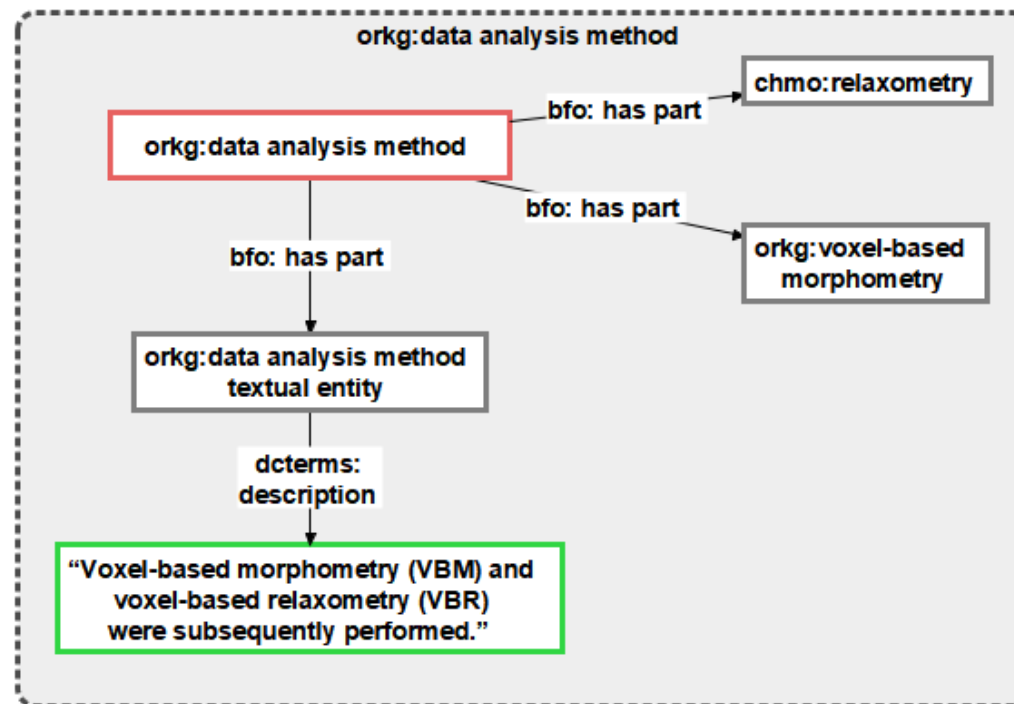
drag & drop or automated

using **templates** for
semantifying the
assertion

ic papers. [hypothesis.is](https://web.hypothesis.is/blog/annotating-to-...), <https://web.hypothesis.is/blog/annotating-to-...>

Employing the RCM in a knowledge graph

Bottom-up data entry—at the level of individual assertions



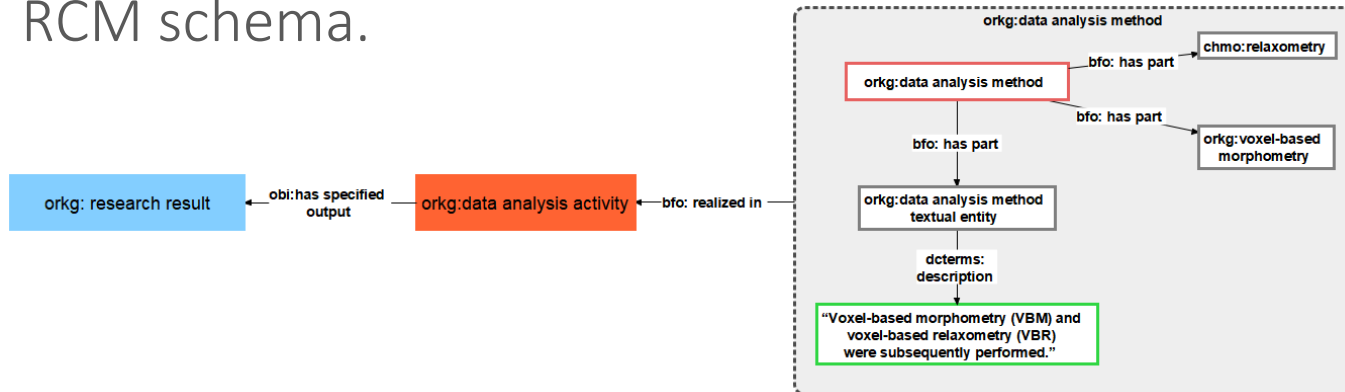
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Employing the RCM in a knowledge graph

Bottom-up data entry—at the level of individual assertions

This semantified scholarly assertion can be **automatically linked** to and **integrated** with the general RCM schema.



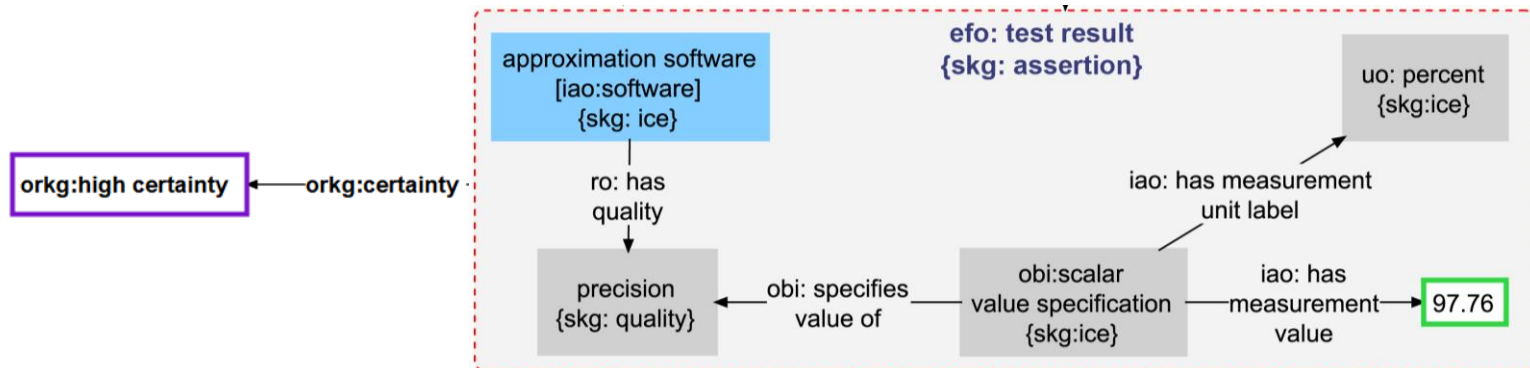
Example taken from:

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Employing the RCM in a knowledge graph

Use of named graphs allows statements about statements

Because each assertion is organized in its own **named graph**, we can e.g. specify its **degree of certainty**, ...

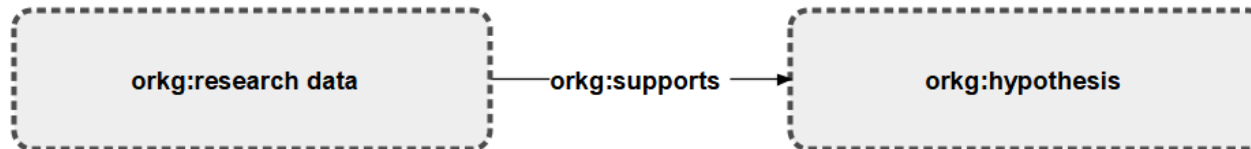


Prieto et al. (2019) Data-driven classification of the certainty of scholarly assertions. *PeerJ* 8, e8871.

Employing the RCM in a knowledge graph

Use of named graphs allows statements about statements

...or **relate** it to another assertion
(supporting, contradicting, neutral), ...



Prieto *et al.* (2019) Data-driven classification of the certainty of scholarly assertions. *PeerJ* 8, e8871.

● Employing the RCM in a knowledge graph

● Use of named graphs allows statements about statements

... or provide **personal opinions** about it,
for instance the data provider wants to
point out that they conceived a **logical
inconsistency**, or a **wrong statistical
method** being applied.

[Prieto et al. \(2019\) Data-driven classification of the certainty of scholarly assertions. PeerJ 8, e8871.](#)

Knowledge Graph Cell (KGC)

Knowledge Graph Cell (KGC)

Goal

Provide a means to have the contents of scholarly publications in a **machine-actionable** format but at the same time present the contents in **human-readable UI-pages**.

Knowledge Graph Cell (KGC)

Basic idea

The representation of the contents of a scholarly publication in a knowledge graph usually comprises several UI-pages.

Knowledge Graph Cell (KGC)

Basic idea

We **partition** the overall data graph into **integrated sub-graphs**, with each sub-graph comprising information that should be represented on **one such UI-page**.

Knowledge Graph Cell (KGC)

Basic idea

We specify a KGC for each sub-graph so that **each UI-page** of a scholarly knowledge graph **has a specific KGC** assigned to it.

Knowledge Graph Cell (KGC)

Basic idea

A KGC can be **instantiated** through **user input**, resulting in the generation of

- 1) a sub-graph that is based on the **graph-template** specified in its KGCs and
- 2) a corresponding **UI-page**.

Knowledge Graph Cell (KGC)

Basic idea

The user input for a given KGC can **trigger the instantiation** of another KGC. This way, KGCs can relate to one another and we can specify the entire organization of the data of a knowledge graph application as **a set of interlinked KGCs**.

Knowledge Graph Cell (KGC)

Basic idea

A **middleware** reads the information contained in the KGCs and in the overall data graph and **executes it**, thereby generating the knowledge graph application.

Knowledge Graph Cell (KGC)

Organization of an RDF-based KGC into sets of Quad Templates

An RDF-based KGC is organized into Quads:

Subject (URI) Property (URI) Object (URI/Literal) :NG(URI),

with each Quad being described in a KGC as a Quad Template (QT).

Knowledge Graph Cell (KGC)

Organization of an RDF-based KGC into sets of Quad Templates

An RDF-k

Subject (U

described in the
forthcoming paper

al) :NG(URI),

with each

Template

Quad

Knowledge Graph Cell (KGC)

Organization of a Neo4j-based KGC

Currently, we are developing a
Neo4j-based implementation of
the KGC idea.

Case Study: COVID-19 Data

Case description

We want to model information about a **population** that has been infected with the **SARS-CoV-2 Coronavirus**. We want to cover **Basic Reproduction Number (R0)** and **Case Fatality Rate (CFR)** **measurements**, each with **95% Confidence Intervals**. All this information should be represented **on a single UI-page**.

Case Study: COVID-19 Data

Infectious Agent Population KGC

We want to model this information with a general **Infectious Agent Population KGC**, which can be reused for other types of infections.

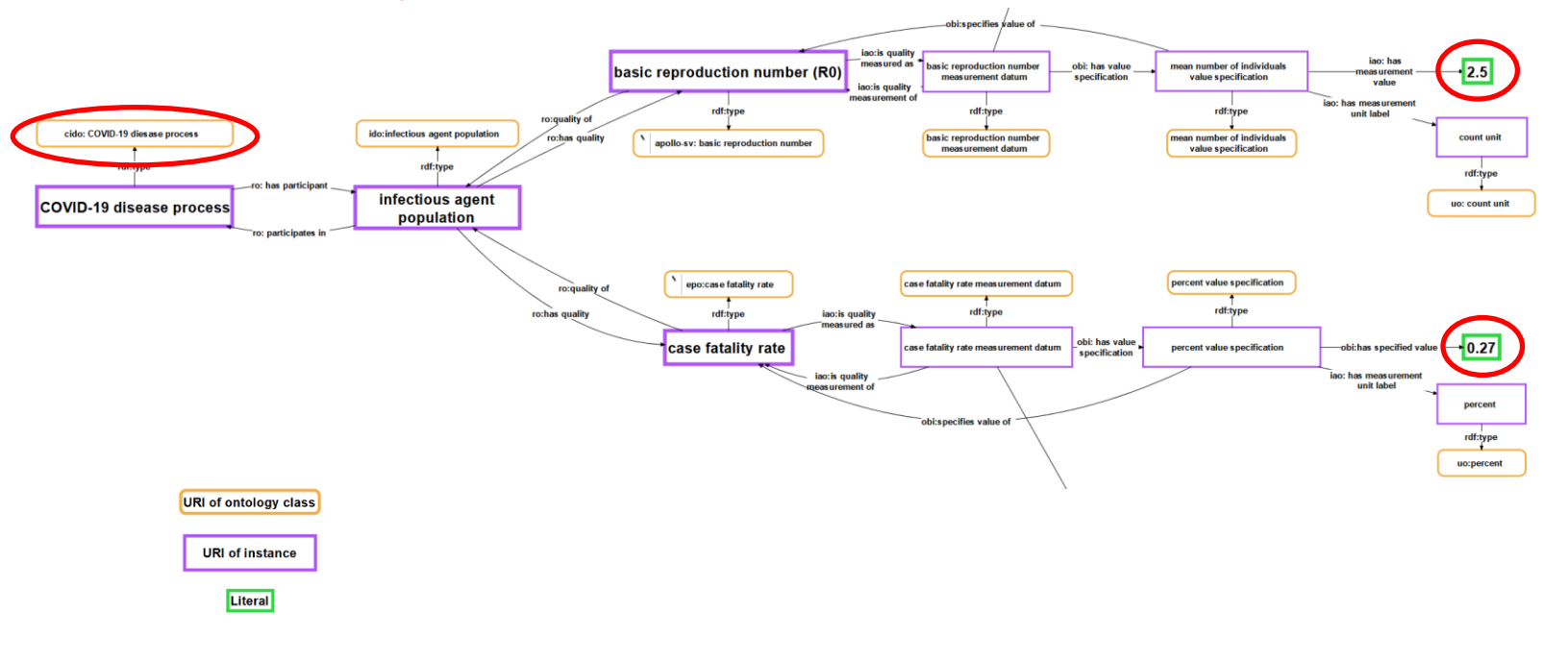
Underlying OWL graph pattern



Case Study: COVID-19 Data

Infectious Agent Population KGC

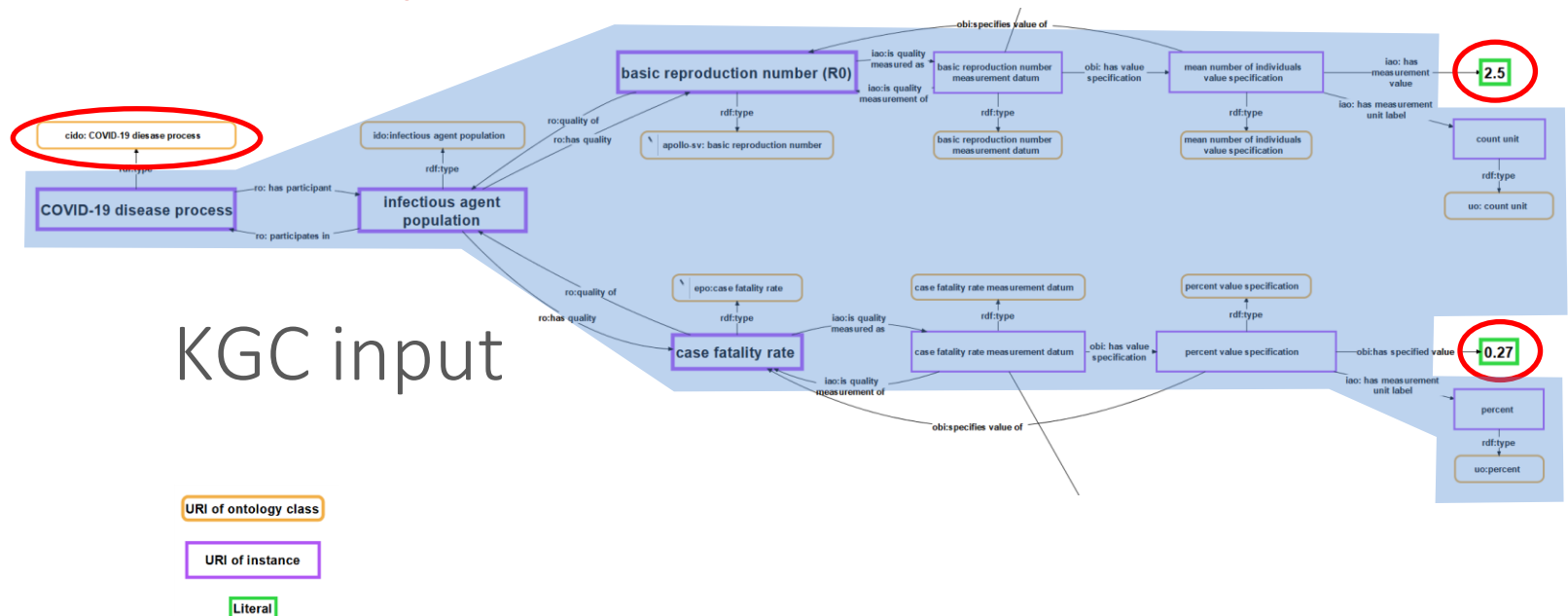
user input



Case Study: COVID-19 Data

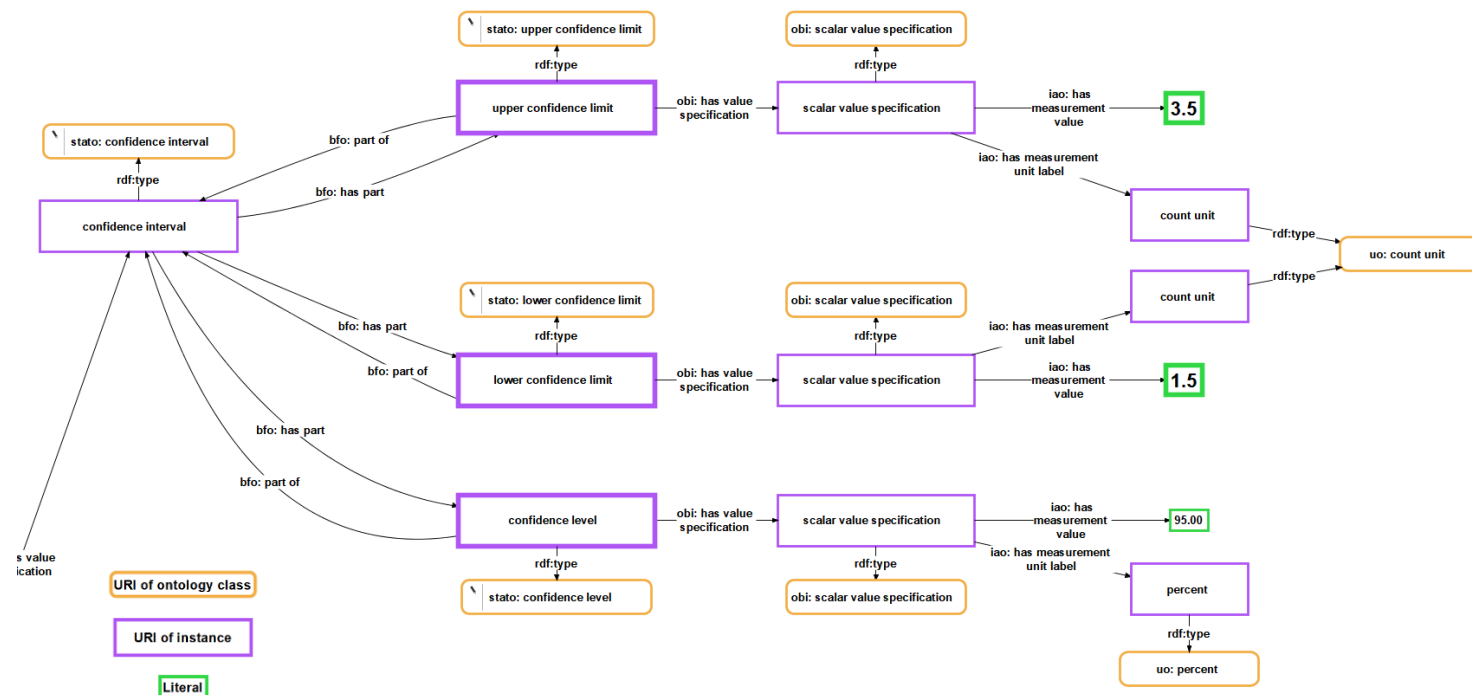
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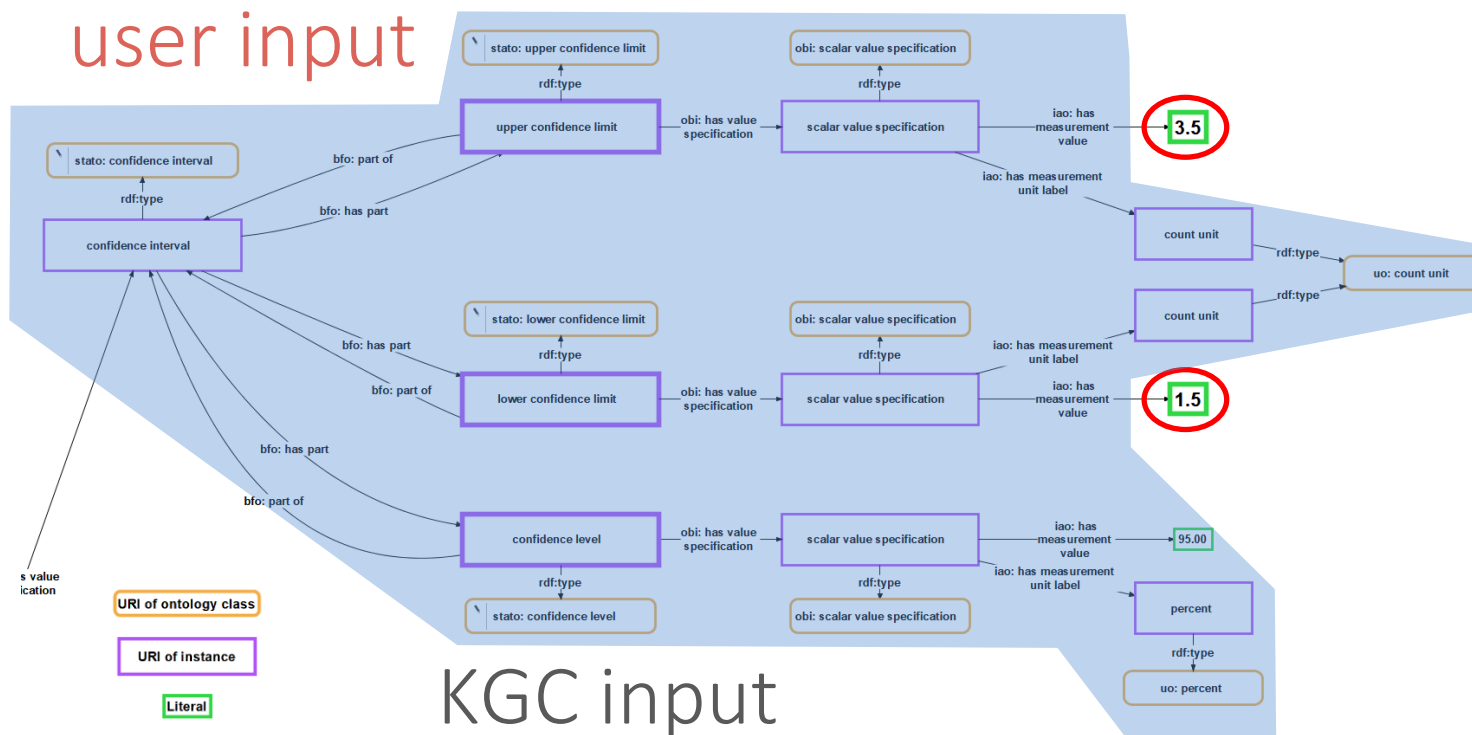


Case Study: COVID-19 Data

Underlying OWL graph pattern



Infectious Agent Population KGC



Case Study: COVID-19 Data

Infectious Agent Population KGC

Next, we described the Infectious Agent Population KGC as a set of **Cypher scripts**.

Case Study: COVID-19 Data

Infectious Agent Population KGC

Instantiation Cypher script

```

1. INITIALIZE SCHEMA AND DATA
2. LOAD DATA FROM CSV FILES
3. CREATE INDEXES FOR PERFORMANCE
4. CREATE VIEWS FOR ANALYSIS
5. RUN ANALYTICAL QUERIES
6. VISUALIZE RESULTS
7. EXPORT RESULTS TO OTHER FORMATS
8. CLEANUP AND MAINTENANCE
9. MONITORING AND LOGGING
10. SECURITY AND ACCESS CONTROL
11. BACKUP AND RECOVERY
12. SCALING AND DISTRIBUTION
13. OPTIMIZATION
14. TESTING
15. DEPLOYMENT
16. SUPPORT
17. DOCUMENTATION
18. TRAINING
19. EVALUATION
20. IMPROVEMENT
21. MAINTENANCE
22. MONITORING
23. LOGGING
24. SECURITY
25. ACCESS CONTROL
26. BACKUP
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```


Case Study: COVID-19 Data

Infectious Agent Population KGC

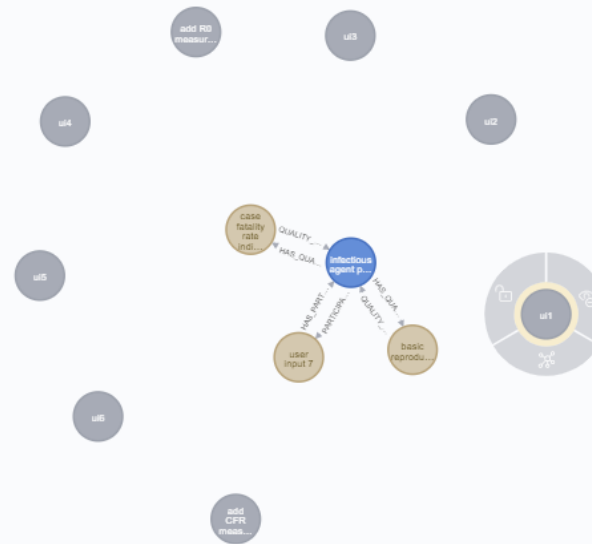
UI-page Cypher script

// search for all nodes belonging to ORKG entry1 kgc data graph data_graph_entry1_kgc_1 that contain gui information

```
MATCH (n)
      WHERE n.data_OrkgEntry="entry1" AND
            n.kgc_kgc_data_graph="data_graph_entry1_kgc_1" AND
            n.gui_information="true"
RETURN n
```

Case Study: COVID-19 Data

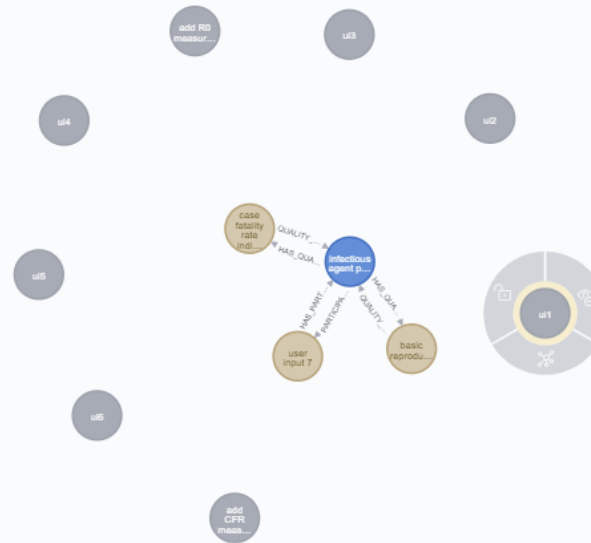
Infectious Agent Population KGC



Literal Value <id>: 36 data_OrkgEntry: entry1 gui_data_type: xsd:float gui_edit_cypher_address: infectiousAgentPopulationKGC_R0_UserInput1_URI gui_element: inputfieldX gui_group_order: 0 gui_information: true
 gui_information_text: mean value gui_label2: key:value gui_order: 1 gui_section_order: 0 gui_tooltip: The mean basic reproduction number kgc_kgc_data_graph: data_graph_entry1_kgc_1 name: user input 1 value: ui1

Case Study: COVID-19 Data

Infectious Agent Population KGC

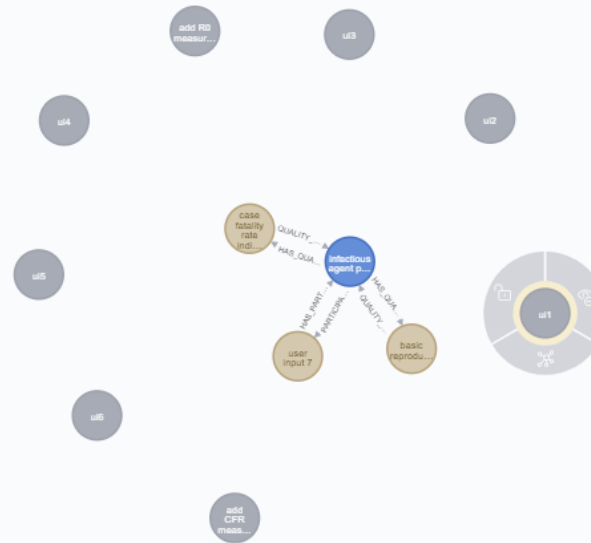


scholarly publication ID

Literal Value <id>: 36 **data_OrkgEntry: entry1** gui_data_type: xsd:float gui_edit_cypher_address: infectiousAgentPopulationKGC_R0_UserInput1_URI gui_element: inputfieldX gui_group_order: 0 gui_information: true
 gui_information_text: mean value gui_label2: Key:value gui_order: 1 gui_section_order: 0 gui_tooltip: The mean basic reproduction number kgc_kgc_data_graph: data_graph_entry1_kgc_1 name: user input 1 value: ui1

Case Study: COVID-19 Data

Infectious Agent Population KGC

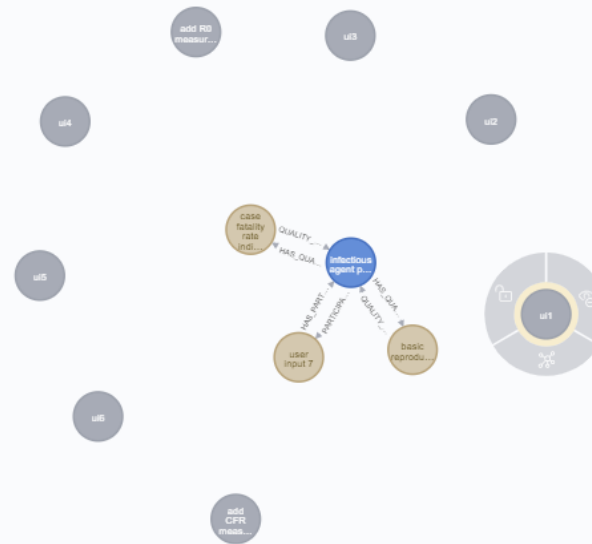


named graph information / UI-page ID

Literal Value <id>: 36 data_OrkgEntry: entry1 gui_data_type: xsd:float gui_edit_cypher_address: infectiousAgentPopulationKGC_R0_UserInput1_URI gui_element: inputfieldX gui_group order: 0 gui_information: true
gui_information_text: mean value gui_label2: key:value gui_order: 1 gui_section_order: 0 gui_tooltip: The mean basic reproduction number **kgc_kgc_data_graph: data_graph_entry1_kgc_1** name: user input 1 value: ui1

Case Study: COVID-19 Data

Infectious Agent Population KGC

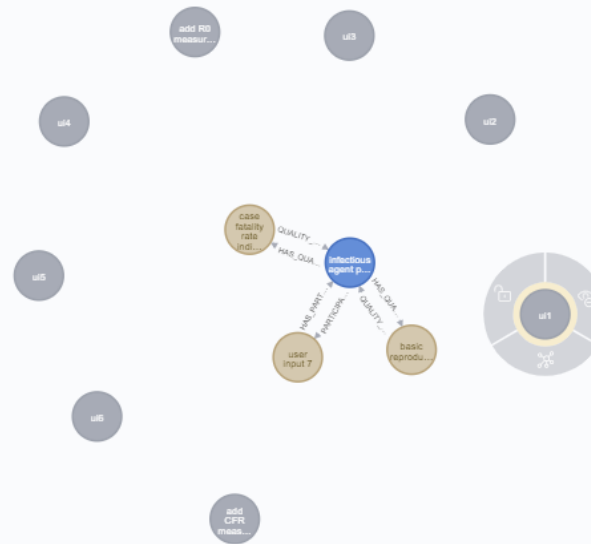


data type specification: float

Literal Value <id>: 36 data_OrkgEntry: entry1 **gui_data_type: xsd:float** gui_edit_cypher_address: infectiousAgentPopulationKGC_R0_UserInput1_URI gui_element: inputfieldX gui_group_order: 0 gui_information: true
gui_information_text: mean value gui_label2: key:value gui_order: 1 gui_section_order: 0 gui_tooltip: The mean basic reproduction number kgc_kgc_data_graph: data_graph_entry1_kgc_1 name: user input 1 value: ui1

Case Study: COVID-19 Data

Infectious Agent Population KGC

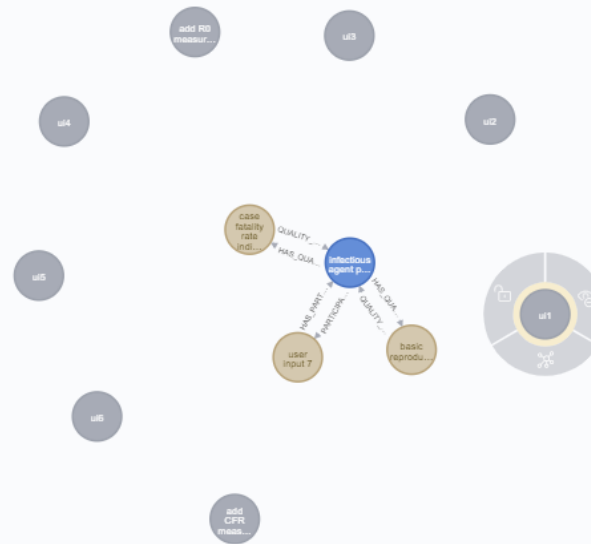


UI-page information

Literal Value <id>: 36 data_OrkgEntry: entry1 gui_data_type: xsd:float gui_edit_cypher address: infectiousAgentPopulationKGC R0 UserInput1_URI gui_element: inputfieldX gui_group_order: 0 gui_information: true
 gui_information_text: mean value gui_label2: key:value gui_order: 1 gui_section_order: 0 gui_tooltip: The mean basic reproduction number kgc_kgc_data_graph: data_graph_entry1_kgc_1 name: user input 1 value: ui1

Case Study: COVID-19 Data

Infectious Agent Population KGC

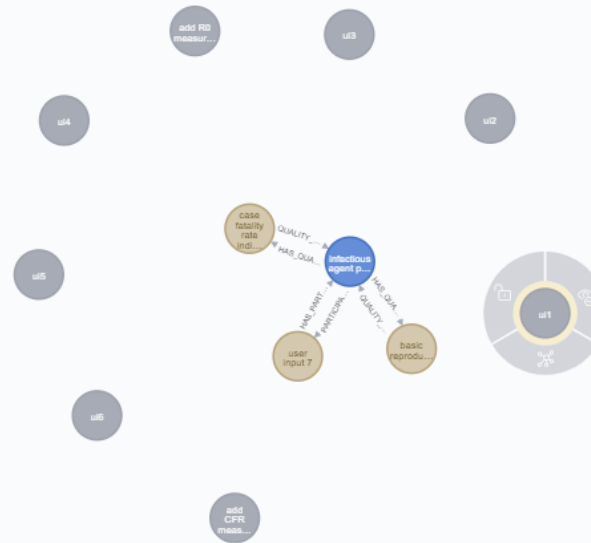


edit Cypher Script

Literal Value <id>: 36 data_OrkgEntry: entry1 gui_data_type: xsd:float **gui_edit_cypher_address: infectiousAgentPopulationKGC_R0_UserInput1_URI** gui_element: inputfieldX gui_group_order: 0 gui_information: true
 gui_information_text: mean value gui_label2: key:value gui_order: 1 gui_section_order: 0 gui_tooltip: The mean basic reproduction number kgc_kgc_data_graph: data_graph_entry1_kgc_1 name: user input 1 value: ui1

Case Study: COVID-19 Data

Infectious Agent Population KGC



value: yet unspecified

Literal Value <id>: 36 data_OrkgEntry: entry1 gui_data_type: xsd:float gui_edit_cypher_address: infectiousAgentPopulationKGC_R0_UserInput1_URI gui_element: inputfieldX gui_group_order: 0 gui_information: true
gui_information_text: mean value gui_label2: key:value gui_order: 1 gui_section_order: 0 gui_tooltip: The mean basic reproduction number kgc_kgc_data_graph: data_graph_entry1_kgc_1 name: user input 1 value: ui1

Case Study: COVID-19 Data

Infectious Agent Population KGC

update Cypher script for R0 mean value

```
// update the values for the R0 mean value [ui1] of entry1 and kgc data graph  
data_graph_entry1_kgc_1
```

```
:param [{entry, dataGraph, guiGroupOrder, guiSectionOrder, ui1, guiOrder1, guiOrder2,  
guiOrder3}] => {RETURN 0 AS guiSectionOrder, "entry1" AS entry, 1 AS guiOrder1, 2 AS  
guiOrder2, 3 AS guiOrder3, "data_graph_entry1_kgc_1" AS dataGraph, 0 AS  
guiGroupOrder, "2.5" AS ui1};
```

```
MATCH (n {data_OrkgEntry:$entry, gui_section_order:$guiSectionOrder,  
gui_group_order:$guiGroupOrder, gui_order:$guiOrder1,  
kgc_kgc_data_graph:$dataGraph})  
SET n.value=$ui1
```

Case Study: COVID-19 Data

Infectious Agent Population KGC

update Cypher script for R0 mean value

```
// update the values for the R0 mean value [ui1] of entry1 and kgc data graph  
data_graph_entry1_kgc_1
```

```
:param [{entry, dataGraph, guiGroupOrder, guiSectionOrder, ui1, guiOrder1, guiOrder2,  
guiOrder3}] => {RETURN 0 AS guiSectionOrder, "entry1" AS entry, 1 AS guiOrder1, 2 AS  
guiOrder2, 3 AS guiOrder3, "data_graph_entry1_kgc_1" AS dataGraph, 0 AS  
guiGroupOrder, "2.5" AS ui1};
```

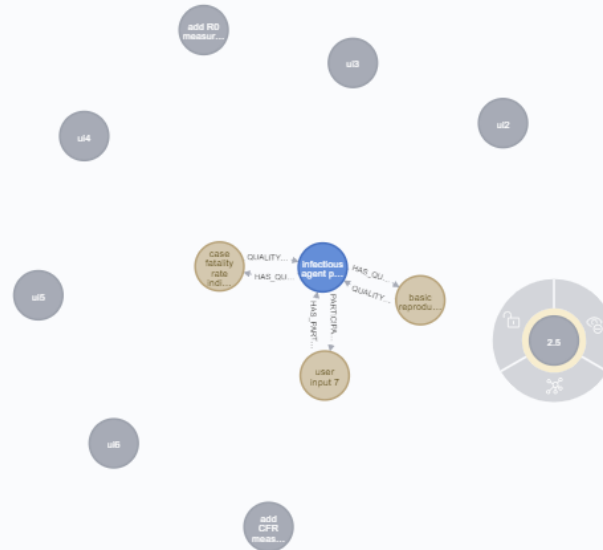
```
MATCH
```

provided by frontend/middleware and user-input

```
SET n.value=gui1
```

Case Study: COVID-19 Data

Infectious Agent Population KGC

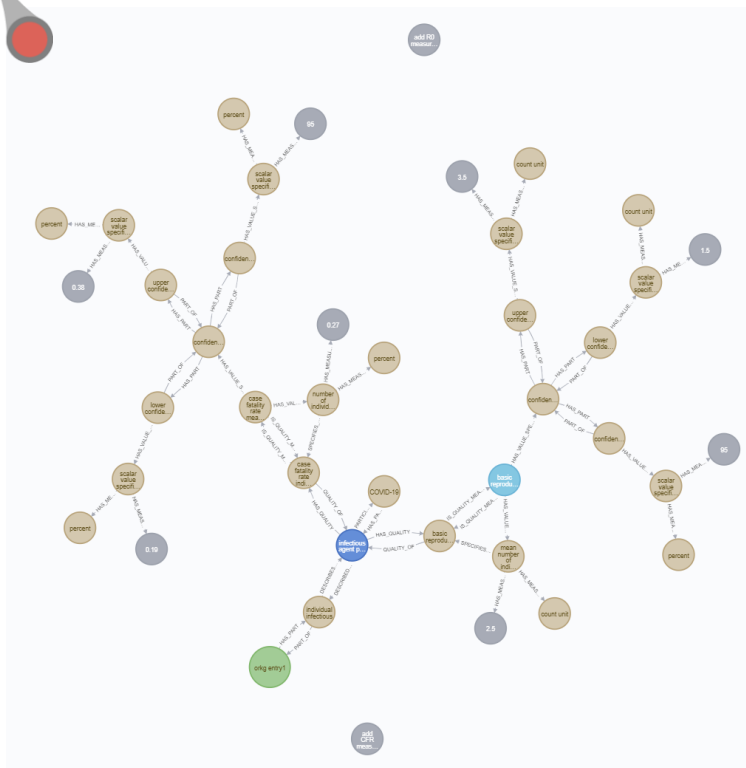


Value: 2.5

Literal Value <id>: 36 data_OrkgEntry: entry1 gui_data_type: xsd.float gui_edit_cypher_address: infectiousAgentPopulationKGC_R0_UserInput1_URI gui_element: inputfieldX gui_group_order: 0 gui_information: true
gui_information_text: mean value gui_label2: key:value gui_order: 1 gui_section_order: 0 gui_tooltip: The mean basic reproduction number kgc_kgc_data_graph: data_graph_entry1_kgc_1 name: user input 1 value: 2.5

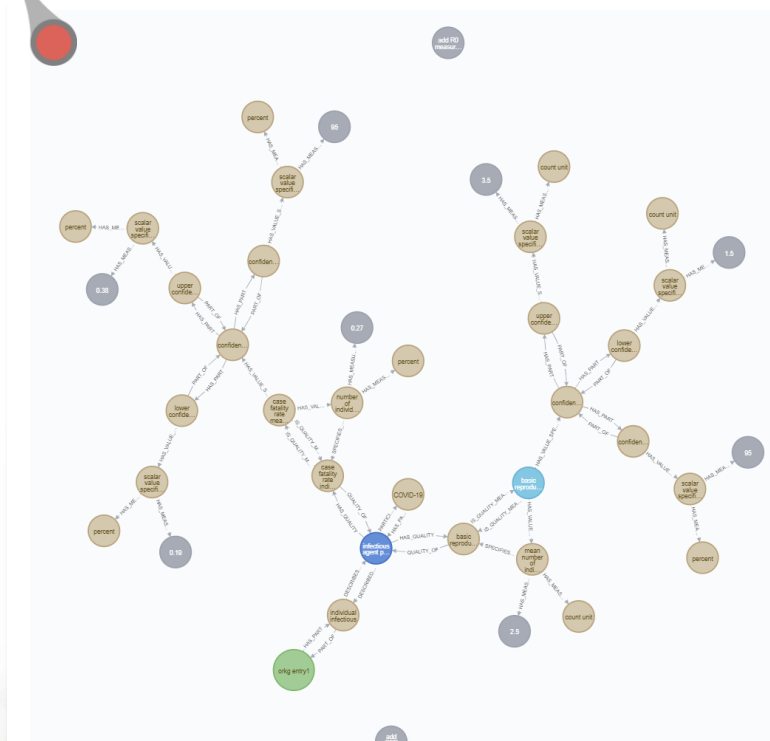
Case Study: COVID-19 Data

Infectious Agent Population KGC

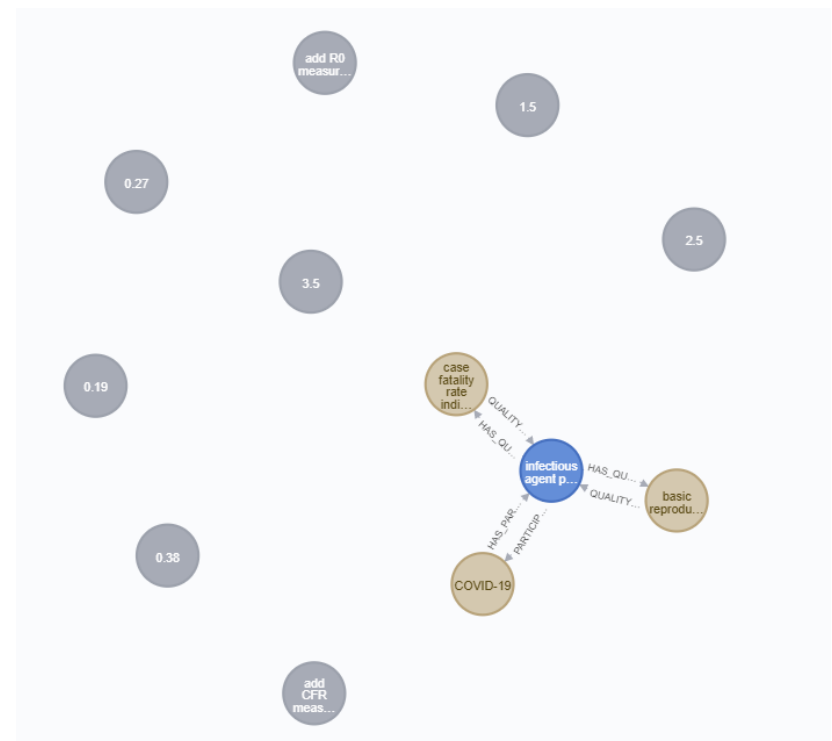


Case Study: COVID-19 Data

Infectious Agent Population KGC



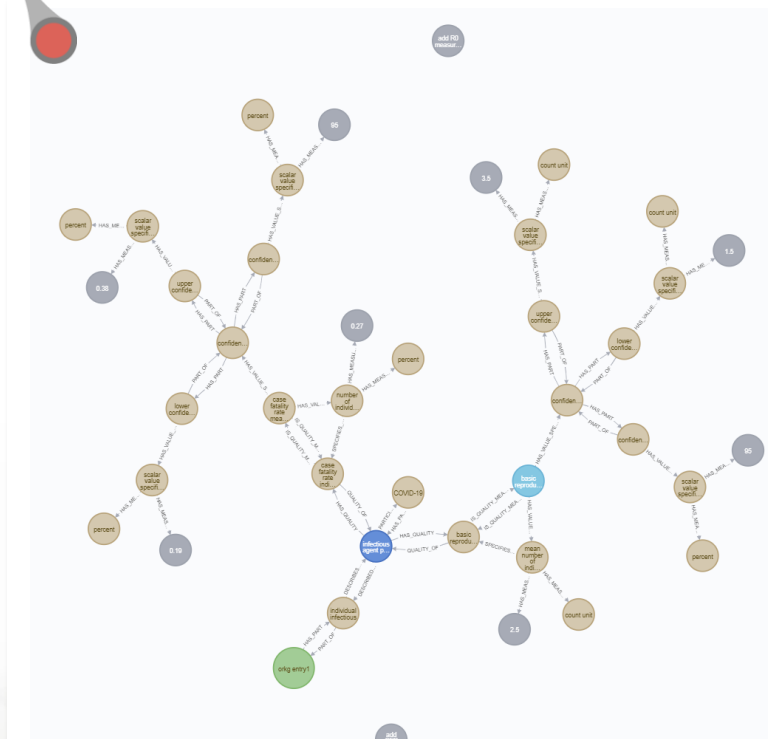
machine-actionable graph



human-readable UI-page

Case Study: COVID-19 Data

Infectious Agent Population KGC



machine-actionable graph

Infectious Agent Population

participates in

[Covid-19 disease process \[cido\]](#)

Basic reproduction number
(95% confidence interval)

2.5

(1.5 - 3.5)

add basic reproduction
number measurement

Case fatality rate
(95% confidence interval)

0.27

%

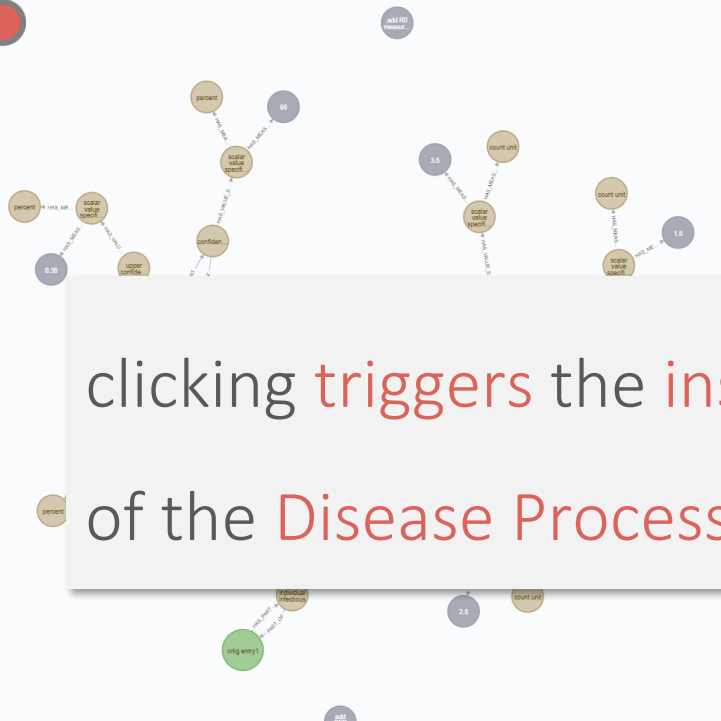
(0.19 - 0.38) %

add case fatality rate
measurement

human-readable UI-page

Case Study: COVID-19 Data

Infectious Agent Population KGC



Infectious Agent Population

participates in

Covid-19 disease process [cido]

Basic reproduction number
(interval)

2.5 (1.5 - 3.5)

on
nt

(interval)

0.27 % (0.19 - 0.38 %)

add case fatality rate
measurement

clicking triggers the instantiation
of the Disease Process KGC

machine-actionable graph

human-readable UI-page

Benefits of using Knowledge Graph Cell (KGC)

Uniform modeling scheme

KGCs can be used for implementing a **uniform modeling scheme** and a specific **data model** (e.g. RCM) in a knowledge graph application, with all user-input being enforced to comply with the model. This results in **semantically consistent and FAIR contents** without the users having to be experts in semantics and understanding graphs.

Benefits of using Knowledge Graph Cell (KGC)

Data consistency

KGCs enforce a certain degree of **data consistency** through

- (i) **input-control** that structures and restricts user input and
- (ii) by employing KGCs in tools and procedures for **checking** the contents of the knowledge graph for consistency without having to rely on DL-based reasoning.

Benefits of using Knowledge Graph Cell (KGC)

Querying

With predefined **SPARQL/Cypher queries**, they provide means to **interact** with the data graph at a fine-grained level without requiring users to understand the query languages.

● Benefits of using Knowledge Graph Cell (KGC)

● Human-readability

KGCs **filters** information contained in the data graph to what is **relevant** to a **human reader** and makes this information available to the frontend.

● Benefits of using Knowledge Graph Cell (KGC)

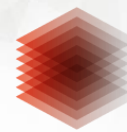
● Agility, flexibility

A knowledge graph application can be developed and specified as a set of interlinked KGCs. The middleware runs the application. New KGCs can be added and existing ones be modified.

RCM and KGCs combined in a Knowledge Graph for Scholarly Publications

FAIRness

When combining the KGC idea with the RCM data model for scholarly publications, we can build a Knowledge Graph for Scholarly Publications that provides data and metadata that are compliant with the **FAIR Guiding Principles**.



Towards Representing Research Contributions in Scholarly Knowledge Graphs Using Knowledge Graph Cells

L. Vogt, J. D'Souza, M. Stocker, S. Auer

