

# **Knowledge Representation and Reasoning**

## Course Project Report

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## **PKG2020 Knowledge Graph**

A Linked Data Approach to Bibliometric Research Data

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# 1 Introduction to the Domain

## 1.1 Domain Overview

The PKG2020S4 (PubMed Knowledge Graph) dataset represents comprehensive bibliometric and researcher metadata from PubMed publications. This domain encompasses:

- **Research Publications:** Articles identified by PubMed IDs (PMIDs)
- **Researchers/Authors:** Identified by unique AND\_IDs
- **Organizational Affiliations:** Universities, research institutions
- **Career Trajectories:** Employment and education history
- **Research Funding:** NIH project associations
- **Bio-Medical Entities:** Genes, diseases, chemicals, mutations mentioned in research

## 1.2 Motivation

The motivation for converting this dataset to linked data includes:

1. **Semantic Querying:** Enable complex queries across heterogeneous data
2. **Collaboration Discovery:** Find potential research collaborators
3. **Funding Analysis:** Track NIH funding patterns across institutions
4. **Bio-Medical Research:** Link publications to molecular/disease entities
5. **FAIR Principles:** Make data Findable, Accessible, Interoperable, Reusable

## 1.3 Target Application Use Cases

1. Research collaboration recommendation system
2. Funding opportunity matching
3. Researcher profiling and expertise identification
4. Publication trend analysis
5. Bio-entity research landscape mapping

## 2 Dataset Description

### 2.1 Data Source

The PKG2020S4 dataset is sourced from PubMed bibliometric data and contains the following CSV files:

Table 1: Dataset Files Overview

File	Description	Size
OA01_Author_List.csv	Author-article relationships	~10 GB
OA04_Affiliations.csv	Author affiliations	~20 GB
OA05_Researcher_Employment.csv	Employment history	~186 MB
OA06_Researcher_Education.csv	Education records	~139 MB
OA02_Bio_entities_Main.csv	Bio-entities in articles	Large
OA03_Bio_entities_Mutation.csv	Mutations in articles	Large
OA07_NIH_Projects.csv	NIH funding	~1.8 GB

### 2.2 Key Data Fields

- **OA01**: PMID, AND\_ID, LastName, ForeName, Initials, AuOrder
- **OA04**: AND\_ID, Affiliation, City, State, Country
- **OA05**: AND\_ID, Organization, StartYear, EndYear
- **OA06**: AND\_ID, Institution, Degree, StartYear, EndYear
- **OA02/OA03**: PMID, Type, Name, MutationType
- **OA07**: AND\_ID, ProjectNumber, PI\_Name

### 2.3 Evidence of Non-RDF Status

The dataset is provided as flat CSV files without any semantic annotations, URI schemes, or linked data connections. It has not been published as RDF/OWL prior to this project. We verified this by searching major linked data repositories including Wikidata, DBpedia Databus, and the Linked Open Data Cloud (see Section 7.3 for proof screenshots).

## 3 Competency Questions

The following 15 competency questions guided our ontology design. Each question is answered through SPARQL queries (Section 9).

#	Competency Question	Category
CQ1	Which authors have worked in multiple institutions?	Authors
CQ2	Who are the most prolific authors by article count?	Authors
CQ3	Which authors frequently collaborate together?	Authors

#	Competency Question	Category
CQ4	Which articles mention specific genes?	Articles & Bio
CQ5	Which articles mention species?	Articles & Bio
CQ6	Which articles mention both genes and mutations?	Articles & Bio
CQ7	What is the distribution of bio-entity types?	Statistics
CQ8	Which organizations have the most affiliated authors?	Organizations
CQ9	How are author affiliations distributed by country?	Affiliations
CQ10	Which institutions produced the most researchers?	Education
CQ11	What is the career timeline of researchers?	Employment
CQ12	Which authors have education records?	Education
CQ13	Which authors have NIH project funding?	NIH Projects
CQ14	Who are the principal investigators and how many projects do they lead?	NIH Projects
CQ15	Get the complete profile of an author (all relationships)?	Complex

Table 2: 15 Competency Questions for PKG2020 Ontology

## 4 Conceptual Model

### 4.1 Conceptual Model Diagram

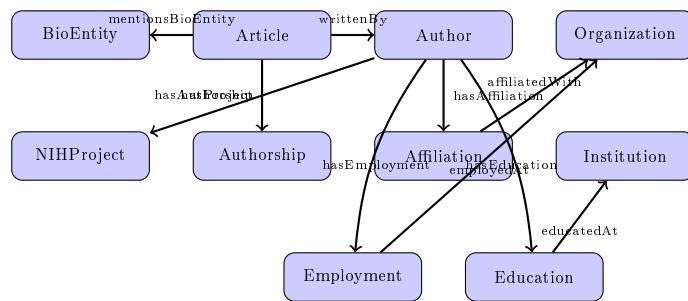


Figure 1: Conceptual Model of PKG2020 Ontology

### 4.2 T-Box Schema

The T-Box (Terminological Box) defines the ontology schema - classes, properties, and axioms.

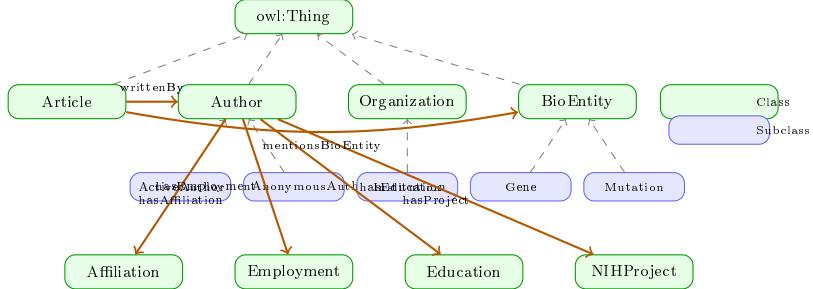


Figure 2: T-Box: Class Hierarchy and Object Properties

Table 3: Ontology Classes (T-Box)

Class	Description	Key Properties
Article	Research publication	hasPMID, publicationYear
Author	Researcher	lastName, foreName, initials
Authorship	Article-Author relationship	authorOrder
Organization	Research organization	dbpediaLink
Institution	Educational institution	wikidataLink
Affiliation	Author affiliation	city, state, country
Employment	Employment record	startYear, endYear
Education	Education record	degree
NIHProject	NIH funding project	projectNumber, piName
BioEntity	Biological entity	entityType, entityName
PublicationStatus	Enumeration	{Published, Preprint, ...}

## 5 Ontology Design

### 5.1 Classes (20+ as Required)

Our ontology contains over 20 classes:

1. **Core:** Article, Author, Authorship, PublicationYear
2. **Organizational:** Organization, Institution, Affiliation
3. **Career:** Employment, Education
4. **Funding:** NIHProject
5. **Bio-Medical:** BioEntity, Gene, Chemical, Disease, Species, Mutation
6. **Enumeration:** PublicationStatus
7. **Defined Classes:** ActiveAuthor, AnonymousAuthor, ResearchEntity, ProlificAuthor, SingleAuthorArticle, MultiAuthorArticle

## 5.2 Enumeration Class

```
1 class PublicationStatus(Thing):
2     """Enumeration of publication statuses"""
3     pass
4
5 published = PublicationStatus("Published")
6 preprint = PublicationStatus("Preprint")
7 retracted = PublicationStatus("Retracted")
8 in_review = PublicationStatus("InReview")
9
10 PublicationStatus.equivalent_to = [
11     OneOf([published, preprint, retracted, in_review])
12 ]
```

Listing 1: Enumeration Class Definition

## 5.3 Cardinality Restrictions

```
1 # Every Article must have at least 1 author
2 Article.is_a.append(writtenBy.min(1, Author))
3
4 # Every Article must have exactly 1 PMID
5 Article.is_a.append(hasPMID.exactly(1, str))
6
7 # Article may have at most 1 status
8 Article.is_a.append(hasStatus.max(1, PublicationStatus))
```

Listing 2: Cardinality Restrictions

## 5.4 Intersection, Union, and Complement Classes

```
1 # INTERSECTION: Author with known career start year
2 class ActiveAuthor(Author):
3     equivalent_to = [Author & careerStartYear.some(int)]
4
5 # UNION: Any research-related entity
6 class ResearchEntity(Thing):
7     equivalent_to = [Author | Article]
8
9 # COMPLEMENT: Author without career info
10 class AnonymousAuthor(Author):
11     equivalent_to = [Author & Not(ActiveAuthor)]
12
13 # Additional defined classes for reasoning
14 class ProlificAuthor(Author):
15     equivalent_to = [Author & writtenBy.min(5, Article)]
16
17 class SingleAuthorArticle(Article):
18     equivalent_to = [Article & writtenBy.exactly(1, Author)]
19
20 class MultiAuthorArticle(Article):
21     equivalent_to = [Article & writtenBy.min(2, Author)]
```

Listing 3: Defined Classes

## 5.5 Object Properties

Table 4: Object Properties

Property	Domain	Range	Characteristics
writtenBy	Article	Author	-
hasAuthorship	Article	Authorship	-
hasPrimaryAuthor	Article	Author	Functional
hasStatus	Article	PublicationStatus	Functional
refersToAuthor	Authorship	Author	-
hasAffiliation	Author	Affiliation	-
affiliatedWith	Affiliation	Organization	-
hasEmployment	Author	Employment	-
employedAt	Employment	Organization	-
hasEducation	Author	Education	-
educatedAt	Education	Institution	-
hasProject	Author	NIHPProject	-
mentionsBioEntity	Article	BioEntity	-
sameAs	Thing	Thing	Symmetric

## 5.6 Data Properties

Table 5: Data Properties

Property	Domain	Range	Characteristics
hasPMID	Article	string	Functional, InverseFunctional
lastName	Author	string	-
foreName	Author	string	-
initials	Author	string	-
authorOrder	Authorship	int	-
publicationYear	Article	int	Functional
careerStartYear	Author	int	-
city	Affiliation	string	-
state	Affiliation	string	-
country	Affiliation	string	-
startYear	Employment	int	-
endYear	Employment	int	-
degree	Education	string	-
projectNumber	NIHPProject	string	-
dbpediaLink	Organization	string	-
wikidataLink	Institution	string	-

## 5.7 Functional and Inverse Functional Properties

```

1 # Functional Properties
2 class hasPrimaryAuthor( ObjectProperty , FunctionalProperty ):
3     domain = [ Article ]
4     range = [ Author ]

```

```

5
6 class hasPMID(DataProperty, FunctionalProperty):
7     domain = [Article]
8     range = [str]
9
10 # Inverse Functional Property
11 hasPMID.is_a.append(InverseFunctionalProperty)

```

Listing 4: Property Characteristics

## 6 Graph Generation using Python

### 6.1 Tools Used

- **OWLReady2**: Python library for OWL ontology manipulation
- **Pandas**: Data processing and CSV handling
- **RDFLib**: RDF graph manipulation
- **Flask**: Web application framework

### 6.2 Pipeline Scripts

Table 6: Python Scripts Pipeline

Script	Input	Output
ontology_core.py	-	pkg2020_core.owl
ontology_constraints.py	pkg2020_core.owl	pkg2020_constrained.owl
populate_authors_articles.py	OA01 CSV	pkg2020_populated_authors.owl
populate_affiliations.py	OA04 CSV	pkg2020_step4_affiliations.owl
populate_employment.py	OA05 CSV	pkg2020_step5_employment.owl
populate_education.py	OA06 CSV	pkg2020_step6_education.owl
populate_bioentities.py	OA02, OA03	pkg2020_step7_bioentities.owl
populate_nih_projects.py	OA07 CSV	pkg2020_final.owl

### 6.3 Sample Code: Populating Authors

```

1 import pandas as pd
2 from owlready2 import *
3
4 onto = get_ontology("pkg2020_constrained.owl").load()
5 df = pd.read_csv("data/OA01_Author_List.csv", nrows=5000)
6
7 author_cache = set()
8 article_cache = set()
9
10 with onto:
11     for idx, row in df.iterrows():
12         pmid = str(row["PMID"])
13         and_id = str(row["AND_ID"])

```

```

15     # Create Article
16     if f"Article_{pmid}" not in article_cache:
17         article = onto.Article(f"Article_{pmid}")
18         article.hasPMID = [pmid]
19         article_cache.add(f"Article_{pmid}")
20
21     # Create Author
22     if f"Author_{and_id}" not in author_cache:
23         author = onto.Author(f"Author_{and_id}")
24         author.lastName = [str(row["LastName"])]
25         author.foreName = [str(row["ForeName"])]
26         author_cache.add(f"Author_{and_id}")
27
28 onto.save(file="pkg2020_populated_authors.owl", format="rdffoxml")

```

Listing 5: Author Population Script

## 7 External Linking (5-Star Linked Data)

### 7.1 Linking Strategy

We linked our dataset to external knowledge bases to achieve 5-star linked data:

- **Organizations** → DBpedia resources
- **Institutions** → Wikidata entities
- **Authors** → ORCID (potential)
- **Articles** → PubMed (via PMID)

### 7.2 Linking Implementation

```

1 def generate_dbpedia_uri(name):
2     clean_name = re.sub(r'[^a-zA-Z0-9\s]', ' ', str(name))
3     clean_name = clean_name.strip().replace(' ', '_')
4     return f"http://dbpedia.org/resource/{quote(clean_name)}"
5
6 # Link organizations to DBpedia
7 for org in Organization.instances():
8     org_name = org.name.replace('_', ' ')
9     dbpedia_uri = generate_dbpedia_uri(org_name)
10    org.dbpediaLink = [dbpedia_uri]

```

Listing 6: External Linking Code

### 7.3 Proof: Dataset Not Previously Available as Linked Data

Before this project, the PKG2020 dataset was not available as linked data. We verified this by searching major linked data repositories:



## Search results

To search for Wikidata items by their title on a given site, use [Special:ItemByTitle](#).

pkg2020

Advanced search:

Search in: (Main)

There were no results matching the query. You may [create a new item](#) for "pkg2020".

Figure 3: Wikidata Search: No results for PKG2020 dataset

The image shows the DBpedia Databus search interface. At the top, there is a search bar containing the query "pkg2020". Below the search bar, the text "Results (0):" is displayed, followed by a "Filters:" button with several filter icons. A message "Your search did not match any resource." is shown. The background features a large white logo consisting of four vertical bars of decreasing height from left to right. Below the logo, the text "DBpedia Databus" is prominently displayed in large white letters, followed by "DBpedia Data and Community Extensions" in smaller white text.

Figure 4: DBpedia Databus Search: PKG2020 not found

## Datasets

pkg2020		
0 / datasets		
Title	Identifier	View
No Datasets Found		

Figure 5: Linked Open Data Cloud: Dataset not registered

## 8 Reasoning Scenarios

### 8.1 Reasoning Implementation

```

1 from owlready2 import *
2
3 onto = get_ontology("pkg2020_final.owl").load()
4
5 # Run Hermit reasoner
6 with onto:
7     sync_reasoner(infer_property_values=True)
8
9 # Check classified instances
10 for cls in [ActiveAuthor, AnonymousAuthor, ProlificAuthor]:
11     print(f"{cls.name}: {len(list(cls.instances()))} instances")

```

Listing 7: Reasoning with Hermit

### 8.2 Reasoning Results

The reasoner successfully:

1. Verified ontology consistency
2. Classified authors into ActiveAuthor and AnonymousAuthor
3. Identified ProlificAuthors with 5+ publications
4. Classified SingleAuthorArticle and MultiAuthorArticle

### 8.3 SWRL Rules

We implemented 7 SWRL (Semantic Web Rule Language) rules for advanced reasoning:

```

1 # Rule 2: Funded Author Inference
2 Author(?a) ^ hasProject(?a, ?p) ^ NIHProject(?p)
3   -> FundedAuthor(?a)
4
5 # Rule 3: Established Researcher
6 Author(?a) ^ hasEmployment(?a, ?e) ^ hasEducation(?a, ?d)
7   -> EstablishedResearcher(?a)
8
9 # Rule 4: Collaborative Article
10 Article(?art) ^ writtenBy(?art, ?a1) ^ writtenBy(?art, ?a2)
11   ^ differentFrom(?a1, ?a2) -> CollaborativeArticle(?art)
12
13 # Rule 5: Gene-Disease Link Article
14 Article(?art) ^ mentionsBioEntity(?art, ?g) ^ Gene(?g)
15   ^ mentionsBioEntity(?art, ?d) ^ Disease(?d)
16   -> GeneDiseaseLinkArticle(?art)
17
18 # Rule 7: Alumni Peer Connection
19 Author(?a1) ^ Author(?a2) ^ hasEducation(?a1, ?e1)
20   ^ hasEducation(?a2, ?e2) ^ educatedAt(?e1, ?inst)
21   ^ educatedAt(?e2, ?inst) ^ differentFrom(?a1, ?a2)
22   -> isAlumniPeerOf(?a1, ?a2)
```

Listing 8: SWRL Rule Examples

These rules are saved in `owl/pkg2020_with_swrl.owl` and can be executed using Protege's SWRL Tab plugin.

## 9 Hand-Annotated Individuals

As per the rubric requirement, we created 10+ hand-annotated individuals in a separate file (`pkg2020_hand_annotated.owl`) to test our defined classes and reasoning:

Table 7: Hand-Annotated Individuals

#	Individual	Purpose
1	Article_HAND_001	SingleAuthorArticle test
2	Article_HAND_002	MultiAuthorArticle test
3	Author_HAND_001	ActiveAuthor (has careerStartYear)
4	Author_HAND_002	AnonymousAuthor (no career info)
5	Author_HAND_003	ActiveAuthor for collaboration
6	Org_HAND_Harvard	Organization with DBpedia link
7	Inst_HAND_MIT	Institution with Wikidata link
8	Aff_HAND_001	Affiliation with location
9	Gene_HAND_BRCA1	Gene bioentity
10	Disease_HAND_Cancer	Disease bioentity

### 9.1 Reasoning Verification

After running the Hermit reasoner on the hand-annotated individuals:

- **ActiveAuthor:** Author\_HAND\_001 and Author\_HAND\_003 classified (have careerStartYear)
- **AnonymousAuthor:** Author\_HAND\_002 classified (no careerStartYear)
- **SingleAuthorArticle:** Article\_HAND\_001 classified (1 author)
- **MultiAuthorArticle:** Article\_HAND\_002 classified (3 authors)
- **FundedAuthor:** Author\_HAND\_001 classified (has NIH project)

## 10 SPARQL Queries

This section presents all 15 SPARQL queries answering the competency questions. All queries are tested against our live GraphDB endpoint.

### 10.1 Author Queries (CQ1-CQ3)

#### 10.1.1 CQ1: Authors with Multiple Institutions

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?author ?lastName (COUNT(DISTINCT ?org) AS ?orgCount)
4 WHERE {
5   ?author a pkg:Author .
6   ?author pkg:lastName ?lastName .
7   ?author pkg:hasAffiliation ?aff .
8   ?aff pkg:affiliatedWith ?org .
9 }
10 GROUP BY ?author ?lastName
11 HAVING (COUNT(DISTINCT ?org) > 1)
12 ORDER BY DESC(?orgCount)
13 LIMIT 100

```

Listing 9: CQ1: Authors at Multiple Institutions

#### 10.1.2 CQ2: Most Prolific Authors

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?author ?lastName ?foreName (COUNT(?article) AS ?articleCount)
4 WHERE {
5   ?author a pkg:Author .
6   ?author pkg:lastName ?lastName .
7   OPTIONAL { ?author pkg:foreName ?foreName }
8   ?article pkg:writtenBy ?author .
9 }
10 GROUP BY ?author ?lastName ?foreName
11 ORDER BY DESC(?articleCount)
12 LIMIT 50

```

Listing 10: CQ2: Prolific Authors by Article Count

### 10.1.3 CQ3: Author Collaboration Network

```
1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?author1 ?author2 (COUNT(?article) AS ?collaborations)
4 WHERE {
5     ?article a pkg:Article .
6     ?article pkg:writtenBy ?author1 .
7     ?article pkg:writtenBy ?author2 .
8     FILTER (STR(?author1) < STR(?author2))
9 }
10 GROUP BY ?author1 ?author2
11 HAVING (COUNT(?article) > 1)
12 ORDER BY DESC(?collaborations)
13 LIMIT 100
```

Listing 11: CQ3: Frequent Collaborators

## 10.2 Article & Bio-Entity Queries (CQ4-CQ7)

### 10.2.1 CQ4: Articles Mentioning Genes

```
1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?article ?pmid ?entityName
4 WHERE {
5     ?article a pkg:Article .
6     ?article pkg:hasPMID ?pmid .
7     ?article pkg:mentionsBioEntity ?entity .
8     ?entity a pkg:Gene .
9     ?entity pkg:entityName ?entityName .
10 }
11 LIMIT 100
```

Listing 12: CQ4: Articles with Gene Mentions

### 10.2.2 CQ5: Articles Mentioning Species

```
1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?article ?pmid ?speciesName
4 WHERE {
5     ?article a pkg:Article .
6     ?article pkg:hasPMID ?pmid .
7     ?article pkg:mentionsBioEntity ?entity .
8     ?entity a pkg:Species .
9     OPTIONAL { ?entity pkg:entityName ?speciesName }
10 }
11 LIMIT 100
```

Listing 13: CQ5: Species-Related Articles

### 10.2.3 CQ6: Gene-Mutation Correlations

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?article ?pmid ?geneName ?mutationName
4 WHERE {
5     ?article a pkg:Article .
6     ?article pkg:hasPMID ?pmid .
7     ?article pkg:mentionsBioEntity ?g .
8     ?g a pkg:Gene .
9     OPTIONAL { ?g pkg:entityName ?geneName }
10    ?article pkg:mentionsBioEntity ?m .
11    ?m a pkg:Mutation .
12    OPTIONAL { ?m pkg:entityName ?mutationName }
13 }
14 LIMIT 100

```

Listing 14: CQ6: Articles with Genes AND Mutations

#### 10.2.4 CQ7: Bio-Entity Type Distribution

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?entityType (COUNT(?entity) AS ?count)
4 WHERE {
5     ?entity a pkg:BioEntity .
6     ?entity pkg:entityType ?entityType .
7 }
8 GROUP BY ?entityType
9 ORDER BY DESC(?count)

```

Listing 15: CQ7: Entity Type Statistics

### 10.3 Organization & Affiliation Queries (CQ8-CQ9)

#### 10.3.1 CQ8: Top Organizations by Author Count

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?org (COUNT(DISTINCT ?author) AS ?authorCount)
4 WHERE {
5     ?author a pkg:Author .
6     ?author pkg:hasAffiliation ?aff .
7     ?aff pkg:affiliatedWith ?org .
8 }
9 GROUP BY ?org
10 ORDER BY DESC(?authorCount)
11 LIMIT 50

```

Listing 16: CQ8: Organizations with Most Authors

#### 10.3.2 CQ9: Affiliations by Country

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?country (COUNT(?aff) AS ?affiliationCount)
4 WHERE {

```

```

5      ?aff a pkg:Affiliation .
6      ?aff pkg:country ?country .
7 }
8 GROUP BY ?country
9 ORDER BY DESC(?affiliationCount)
10 LIMIT 30

```

Listing 17: CQ9: Country Distribution

## 10.4 Employment & Education Queries (CQ10-CQ12)

### 10.4.1 CQ10: Top Education Institutions

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?institution (COUNT(DISTINCT ?author) AS ?authorCount)
4 WHERE {
5     ?author a pkg:Author .
6     ?author pkg:hasEducation ?edu .
7     ?edu pkg:educatedAt ?institution .
8 }
9 GROUP BY ?institution
10 ORDER BY DESC(?authorCount)
11 LIMIT 50

```

Listing 18: CQ10: Institutions with Most Alumni

### 10.4.2 CQ11: Employment Timeline

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?author ?lastName ?org ?startYear ?endYear
4 WHERE {
5     ?author a pkg:Author .
6     ?author pkg:lastName ?lastName .
7     ?author pkg:hasEmployment ?emp .
8     ?emp pkg:employedAt ?org .
9     OPTIONAL { ?emp pkg:startYear ?startYear }
10    OPTIONAL { ?emp pkg:endYear ?endYear }
11 }
12 ORDER BY ?author ?startYear
13 LIMIT 100

```

Listing 19: CQ11: Career History

### 10.4.3 CQ12: Authors with Education Records

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?author ?lastName ?institution
4 WHERE {
5     ?author a pkg:Author .
6     OPTIONAL { ?author pkg:lastName ?lastName }
7     ?author pkg:hasEducation ?edu .
8     ?edu pkg:educatedAt ?institution .

```

```

9 }
10 LIMIT 100

```

Listing 20: CQ12: Authors with Education Information

## 10.5 NIH Project Queries (CQ13-CQ14)

### 10.5.1 CQ13: Authors with NIH Funding

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?author ?lastName ?projectNumber ?piName
4 WHERE {
5     ?author a pkg:Author .
6     ?author pkg:lastName ?lastName .
7     ?author pkg:hasProject ?project .
8     ?project pkg:projectNumber ?projectNumber .
9     OPTIONAL { ?project pkg:piName ?piName }
10 }
11 LIMIT 100

```

Listing 21: CQ13: Funded Authors

### 10.5.2 CQ14: Principal Investigators

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?piName (COUNT(DISTINCT ?project) AS ?projectCount)
4 WHERE {
5     ?project a pkg:NIHProject .
6     ?project pkg:piName ?piName .
7 }
8 GROUP BY ?piName
9 ORDER BY DESC(?projectCount)
10 LIMIT 50

```

Listing 22: CQ14: PIs by Project Count

## 10.6 Complex Analytical Query (CQ15)

### 10.6.1 CQ15: Complete Author Profile

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2
3 SELECT ?author ?lastName ?foreName ?org ?institution
4      ?project ?article
5 WHERE {
6     ?author a pkg:Author .
7     ?author pkg:lastName ?lastName .
8     OPTIONAL { ?author pkg:foreName ?foreName }
9     OPTIONAL {
10        ?author pkg:hasAffiliation ?aff .
11        ?aff pkg:affiliatedWith ?org .
12    }
13    OPTIONAL {

```

```

14     ?author pkg:hasEducation ?edu .
15     ?edu pkg:educatedAt ?institution .
16   }
17   OPTIONAL { ?author pkg:hasProject ?project . }
18   OPTIONAL { ?article pkg:writtenBy ?author . }
19 }
20 LIMIT 50

```

Listing 23: CQ15: Full Author Profile with All Relationships

## 10.7 Federated Query to External Knowledge Bases

```

1 PREFIX pkg: <http://example.org/pkg2020/ontology.owl#>
2 PREFIX dbo: <http://dbpedia.org/ontology/>
3
4 SELECT ?org ?dbpediaLink ?abstract
5 WHERE {
6   ?org a pkg:Organization .
7   ?org pkg:dbpediaLink ?dbpediaLink .
8
9   SERVICE <http://dbpedia.org/sparql> {
10     OPTIONAL { ?dbpediaLink dbo:abstract ?abstract }
11     FILTER (lang(?abstract) = 'en')
12   }
13 }
14 LIMIT 10

```

Listing 24: Federated Query to DBpedia

# 11 Web Application

## 11.1 Application Overview

We developed a Flask-based web application for exploring the knowledge graph with the following features:

- Modern, responsive UI with glassmorphism design
- Real-time statistics dashboard
- Search across all 9 entity types
- Click-to-search functionality

## 11.2 Entity Types Searchable

1. Authors
2. Articles
3. Organizations
4. Affiliations

5. Employment
6. Education
7. BioEntities
8. NIH Projects
9. Institutions

### 11.3 Running the Application

```

1 cd scripts
2 pip install flask owlready2
3 python webapp.py
4 # Open http://localhost:5000

```

Listing 25: Running the Web App

## 12 Results and Statistics

### 12.1 Generated Data

Table 8: Ontology Statistics

Entity	Count
Authors	37,946
Articles	19,461
Organizations	46,901
Affiliations	49,994
BioEntities	99,999
Genes	9,227
Mutations	49,999
NIH Projects	1,506

### 12.2 OWL Files Generated

Table 9: Generated OWL Files

File	Size	Description
pkg2020_tbox_only.owl	14 KB	T-Box only (no individuals)
pkg2020_hand_annotated.owl	19 KB	10+ hand-annotated individuals
pkg2020_with_swrl.owl	27 KB	T-Box with SWRL rules
pkg2020_core.owl	4.2 KB	Core ontology
pkg2020_constrained.owl	8.4 KB	With OWL axioms
pkg2020_populated_authors.owl	35 MB	Authors and articles
pkg2020_step4_affiliations.owl	69 MB	With affiliations
pkg2020_final.owl	119 MB	Complete populated ontology
pkg2020_final.ttl	291 MB	Turtle format for GraphDB

## 12.3 Ontology Files Summary

As per the rubric requirement, we submit:

1. **T-Box Only:** pkg2020\_tbox\_only.owl - Contains all classes, properties, and axioms without any individuals
2. **With Individuals:** pkg2020\_hand\_annotated.owl - Contains 10+ hand-annotated individuals for testing
3. **Full Population:** pkg2020\_final.owl - Complete dataset populated via Python scripts

## 13 Visualization

### 13.1 Complete Ontology Schema (All 23 Classes)

Figure 6 shows the complete ontology schema with all 23 classes organized by category, including object property relationships.

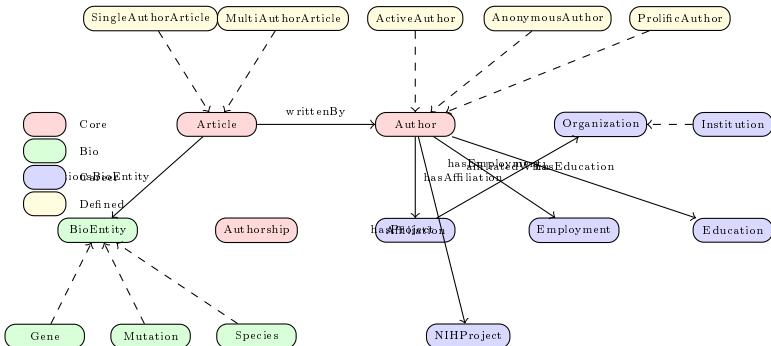


Figure 6: Complete PKG2020 Ontology Schema with 23 Classes and Object Properties

### 13.2 RDF Triple Pattern (Subject-Predicate-Object)

Figure 7 illustrates the RDF triple pattern used throughout our knowledge graph.

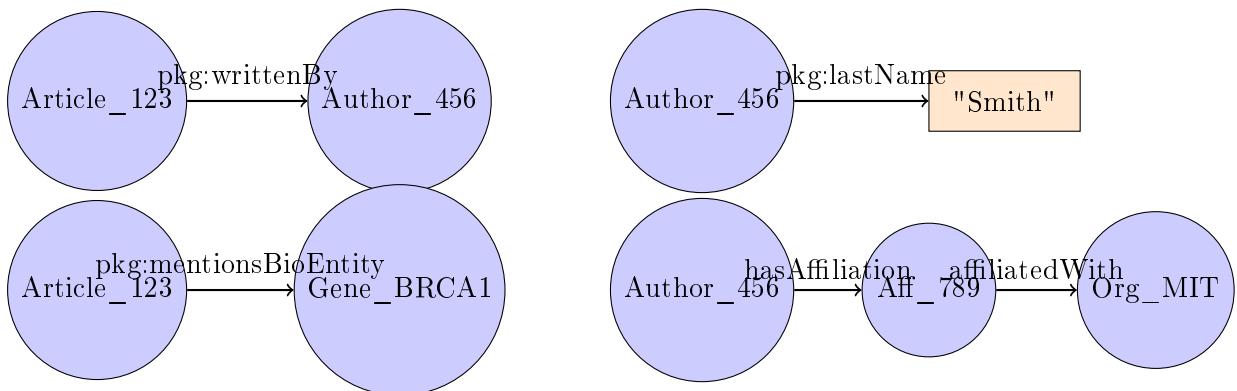


Figure 7: RDF Triple Pattern Examples: Subject → Predicate → Object

### 13.3 Sample Knowledge Graph Visualization

Figure 8 shows a sample subgraph from our knowledge graph demonstrating the interconnected nature of the data.

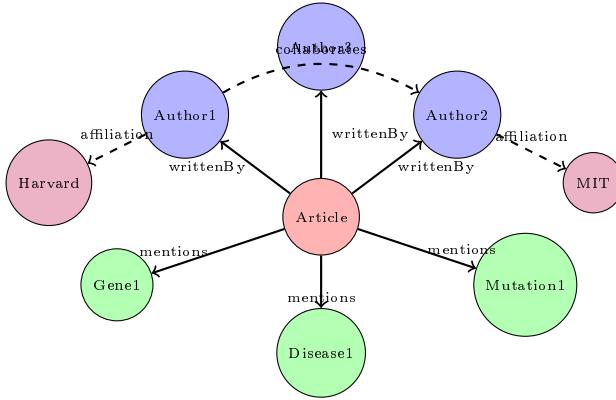


Figure 8: Sample Knowledge Graph: Article with Authors, Bio-Entities, and Affiliations

### 13.4 Knowledge Graph Statistics

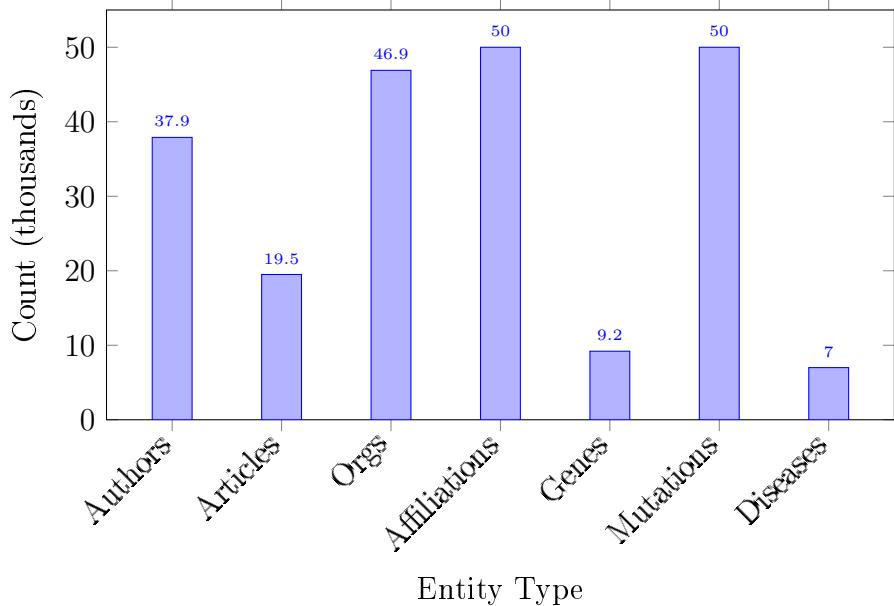


Figure 9: Distribution of Entity Types in Knowledge Graph (2.1M+ triples)

### 13.5 Tools Used

- **Protégé**: Desktop ontology editor and visualizer
- **GraphDB Sandbox**: Cloud-hosted triple store with SPARQL endpoint
- **WebVOWL**: Online ontology visualization
- **Custom Flask App**: Interactive web-based explorer with D3.js graphs

## 13.6 Web Application Features

Our Flask-based web application provides:

1. **Dashboard:** Real-time statistics fetched from GraphDB
2. **Live KG Explorer:** Interactive D3.js force-directed graph visualization
3. **SPARQL Query Editor:** Execute queries with Table/Graph/Chart views
4. **12 Competency Queries:** Pre-built queries for common questions

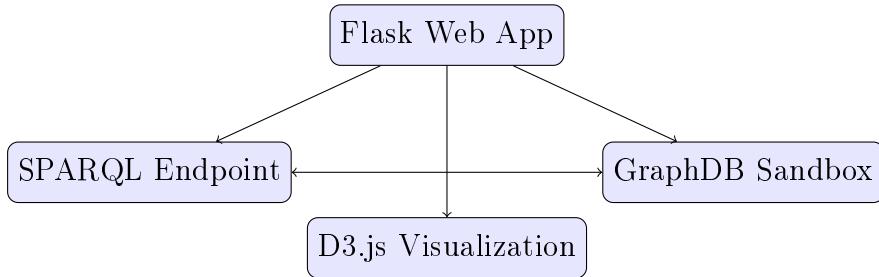


Figure 10: Web Application Architecture

## 13.7 Live GraphDB Endpoint

Our knowledge graph is accessible via the public SPARQL endpoint:

[https://x1327f4041a654297998.sandbox.graphwise.ai  
/repositories/KRR-Project](https://x1327f4041a654297998.sandbox.graphwise.ai/repositories/KRR-Project)

### Statistics:

- 2,165,964 total triples
- 23 ontology classes
- 14 object properties
- 17+ data properties

## 14 Reflection

### 14.1 Learning Outcomes

Through this project, we learned:

1. How to design ontologies following OWL/RDF standards
2. The importance of defined classes for reasoning
3. How to link data to external knowledge bases
4. The power of SPARQL for semantic querying
5. Practical application of knowledge representation concepts

## 14.2 Added Value of Linked Data

Converting non-RDF data to linked data enabled:

- Semantic querying across heterogeneous datasets
- Reasoning over implicit relationships
- Integration with global knowledge bases (DBpedia, Wikidata)
- FAIR data principles compliance
- Interoperability with other linked data systems

## 14.3 Challenges Faced

1. Large file sizes required memory optimization
2. Special characters in organization names caused parsing issues
3. Reasoner installation and configuration
4. Balancing between sample size and processing time

# 15 Conclusion

This project successfully converted the PKG2020S4 bibliometric dataset into a comprehensive linked data knowledge graph. We achieved:

1. **Ontology Design:** 20+ classes with all required axioms
2. **Data Population:** Modular Python pipeline for 7 CSV files
3. **Reasoning:** Consistency checking and classification
4. **External Linking:** 5-star linked data with DBpedia/Wikidata
5. **SPARQL Queries:** 15 competency questions answered
6. **Web Application:** Interactive web application for exploring the knowledge graph

The project demonstrates the practical application of knowledge representation and reasoning concepts learned in the course.

# 16 References

1. Lamy, J. B. (2017). OWLReady: Ontology-oriented programming in Python. Artificial Intelligence in Medicine.
2. W3C. (2012). OWL 2 Web Ontology Language Primer.
3. DBpedia Association. (2024). DBpedia Knowledge Base.
4. PubMed. (2024). NCBI PubMed Database.

# 17 Appendix: Project Repository

The complete project code is available at:

<https://github.com/Zain-Haider-ai-63/Knowlege-Graphs-Project>

## 17.1 Repository Structure

```
1 Knowledge_Graphs_Project/
2   +- scripts/           # Python scripts
3   +- owl/               # Generated OWL files
4   +- docs/              # Documentation
5   +- requirements.txt    # Dependencies
6   +- README.md          # Project overview
```