SemMedDB-neo4j: A Graph Database of Biomedical Semantic Relations

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ABSTRACT

Semantic relations from the biomedical literature are increasingly used in knowledge management applications such as *literature-based discovery (LBD)* as well as in clinical decision-making support. *SemMedDB* is a repository of semantic predications extracted from all PubMed by *SemRep*. SemMedDB has been so far distributed only in MySQL format. However, for many biomedical applications, the domain knowledge is more naturally represented as a graph of concepts and semantic relationships between them. In this work, we describe our recent conversion of SemMedDB to a neo4j graph database (***SemMedDB-neo4j***). It contains additional aggregated and publication history data, which is especially suitable for discovery and evaluation in LBD.

AVAILABILITY

SemMedDB-neo4j is available at:

http://lbd.mf.uni-lj.si/semmeddb-neo4j

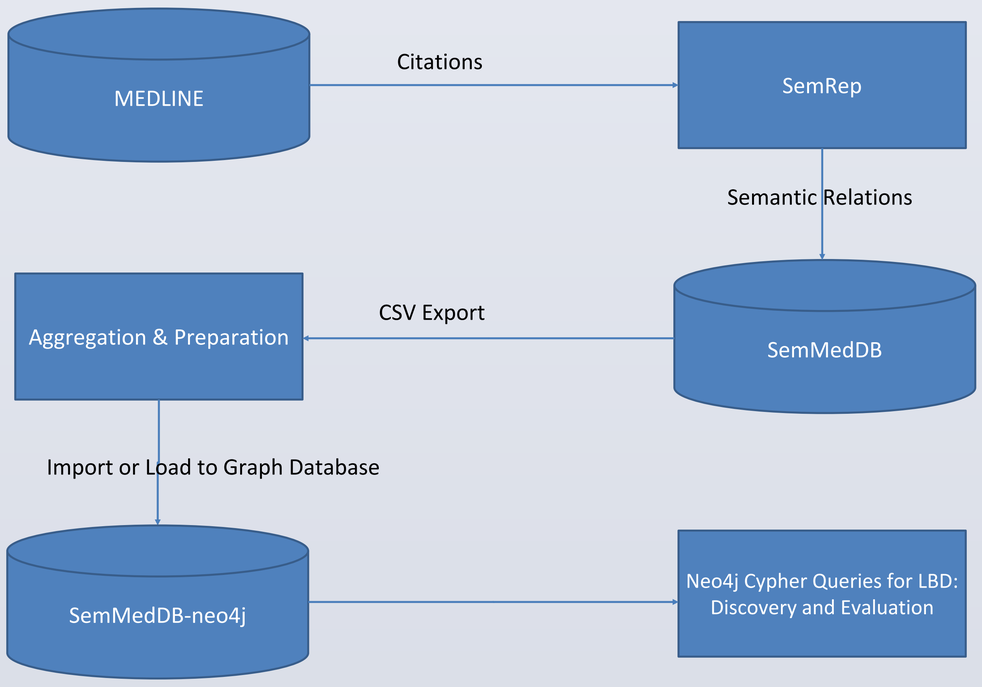
INTRODUCTION AND BACKGROUND

SemMedDB, a distribution of semantic relations extracted from full MEDLINE with SemRep (a natural language processing tool)

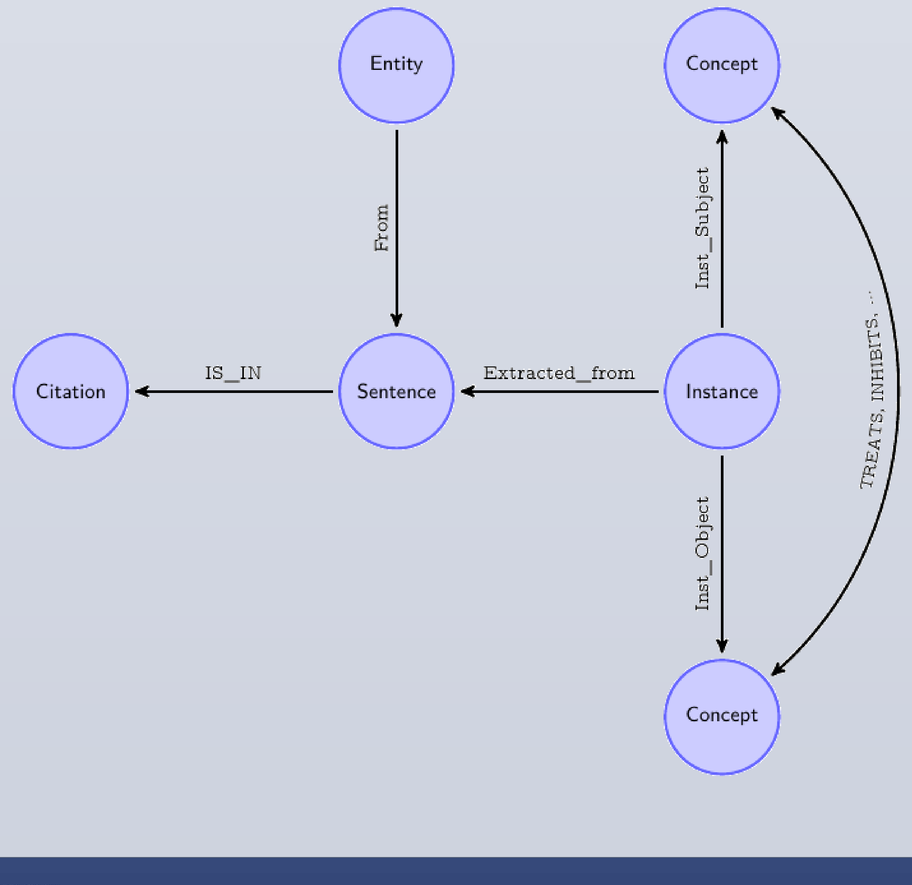
- Example: From "dexamethasone is a potent inducer of multidrug resistance-associated protein expression in rat hepatocytes" SemRep extracts:
  - Dexamethasone STIMULATES Multidrug Resistence-Associated Proteins
  - Multidrug Resistance-Associated Proteins PART_OF Rats
  - Hepatocytes PART_OF Rats

Neo4j graph database used for Implementation

PROCESSING WORKFLOW



The Graph Data Model of SemMedDB-neo4j



The Graph Data Model of SemMedDB-neo4j (cont.)

Nodes types (neo4j labels)

- `Citation` (corresponds to a PubMed bibliographic record)
- `Sentence` (corresponds to a sentence in an abstract or a title of a bibliographic record)
- `Instance` (corresponds to a semantic predication extracted from a particular sentence)
- `Concept` (corresponds to UMLS biomedical concepts that refer to arguments (i.e., subject and object) of the semantic predication). Might have additional label(s) for UMLS semantic type(s) (e.g., `dsyn` for "Disease or Syndrome" or `phsu` for "Pharmacologic Substance")
- `Entity` (corresponds to an entity mention in a sentence)

Relations between the nodes

- `IS_IN` (a relation between a `Sentence` and a `Citation` nodes),
- `Extracted_From` (a relation between a predication `Instance` and a `Sentence` nodes),
- `Inst_Subject` (a relation between an `Instance` and the `Concept` which is the subject of that instance), and
- `Inst_Object` (a relation between an `Instance` and the `Concept` which is the object of that instance).
- All semantic predicates (e.g., `TREATS`, `INHIBITS`) are represented as aggregated relations between `Concept` nodes; for example, there is only one `INHIBITS` relation between a particular concept pair, but there could be many instances of that relation (`Instance` nodes).

Properties (in addition to SemMedDB)

Related to aggregated and publication history data

EXAMPLE CYPHER QUERIES

A generic implementation of the "inhibit the cause of the disease" LBD discovery pattern for finding novel treatments:

```
MATCH (drug:Concept:phsu)-[r1:INHIBITS]->(y:Concept)-[r2:CAUSES]->(disease:Concept:dsyn)
  WHERE NOT (drug)-(:TREATS)->(disease)
  RETURN drug, r1, y, r2, disease;
```

How many actual treatments could be predicted with the above LBD pattern before the treatments were asserted in the literature?

```
MATCH (drug:Concept:phsu)-[r3:TREATS]->(disease:Concept:dsyn),
      (drug)-[r1:INHIBITS]->(y:Concept)-[r2:CAUSES]->(disease)
  WHERE r1.min_pyear<r3.min_pyear AND r2.min_pyear<r3.min_pyear
  RETURN count(r3);
```

A generic query returning linked `Citation` to `Sentence` to `Instance` to (`Subject` and `Object`), and corresponding aggregated semantic relations:

```
MATCH (c:Citation)<-[r_in:IS_IN]-(s:Sentence)<-[r_extr:Extracted_From]-(i:Instance)
       -[r_sub:Inst_Subject]->(sub:Concept), (i)-[r_obj:Inst_Object]->(obj:Concept),
      (sub)-[rel]->(obj)
  RETURN c, r_in, s, r_extr, i, r_sub,sub, r_obj, obj,rel;
```

RESULTS

Graph Database Construction

- **284,472,714** nodes (excluding "entity" nodes)
- **408,532,660** relations (excluding "entity" relations)
- **29,137,782** MEDLINE citation records processed
- **67,599,778** semantic relation instances extracted with SemRep and aggregated into
- **18,283,847** semantic relations between
- **285,675** biomedical concept nodes

CONCLUSIONS

SemMedDB-neo4j is a graph database distribution of SemMedDB, with additional aggregated and temporal data, which makes it especially suitable for knowledge management applications such as literature-based discovery (LBD).

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