BIOQUERY-ASP: Querying Biomedical Databases and Ontologies using Answer Set Programming

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Motivation

- Biomedical data is stored in various structured forms and at different locations.
- With the current Web technologies, reasoning over these data is limited to answering simple queries by keyword search and by some direction of humans.
- Vital research, like drug discovery, requires deep reasoning (e.g., answering complex queries, generating explanations).

Complex Queries

- Q1 What are the genes that are targeted by the drug Epinephrine and that interact with the gene DLG4?
- Q2 What are the genes that are targeted by all the drugs that belong to the category Hmg-coa reductase inhibitors?
- Q3 What are the cliques of 5 genes, that contain the gene DLG4?
- Q4 What are the genes that are related to the gene ADRB1 via a gene-gene relation chain of length at most 3?
- Q5 What are the most similar 3 genes that are targeted by the drug Epinephrine?

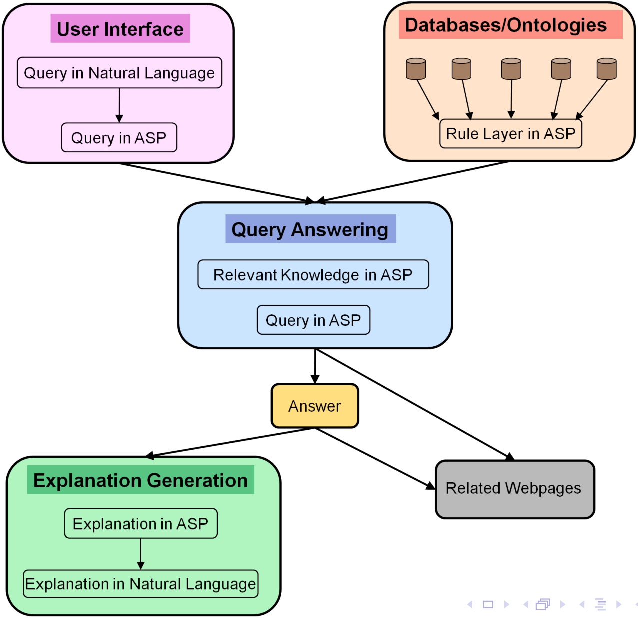
Challenges

- It is hard to represent a query in a formal language.
- Complex queries require recursive definitions, aggregates, etc..
- Databases/ontologies are in different formats/locations.
- Databases/ontologies are large.
- Experts may ask for further explanations.

Challenges

- It is hard to represent a query in a formal language.
  - Represent queries in a controlled natural language (CNL) – BIOQUERY-CNL* [EY09, EEO11].
- Complex queries require recursive definitions, aggregates, etc..
  - Represent queries in Answer Set Programming (ASP) [BCD+08, EEEO11].
- Databases/ontologies are in different formats/locations.
  - Integration of knowledge via a rule layer in ASP [BCD+08, EEO11].
- Databases/ontologies are large.
  - Extract the relevant part for faster reasoning [EEEO11].
- Experts may ask for further explanations.
  - Algorithm for generating shortest/different explanations [EEEO11].

BioQuery-ASP: System Overview



Answer Set Programming (ASP)

- Knowledge representation and automated reasoning paradigm.
- Theoretical basis: answer set semantics (Gelfond & Lifschitz, 1988).
- Expressive representation language: Defaults, recursive definitions, aggregates, preferences, etc.
- ASP solvers:
  - SMODELS (Helsinki University of Technology, 1996)
  - DLV (Vienna University of Technology, 1997)
  - CMODELS (University of Texas at Austin, 2002)
  - PBMODELS (University of Kentucky, 2005)
  - CLASP (University of Potsdam, 2006) – winning first places at ASP'07/09/11/12, PB'09/11/12, and SAT'09/11/12

Applications of ASP in Artificial Intelligence

- planning ([Lif02], [DEF+03], [SPS09], [TSGM11], [GKS12])
- theory update/revision ([IS95], [FGP07], [OC07], [EW08], [ZCRO10], [Del10])
- preferences ([SW01], [Bre07], [BNT08])
- diagnosis ([EFLP99], [BG03], [EBDT+09])
- learning ([Sak01], [Sak05], [SI09], [CSIR11])
- description logics and semantic web ([EGRH06], [CEO09], [Sim09], [PHE10], [SW11], [EKSX12])
- probabilistic reasoning ([BH07], [BGR09])
- data integration and question answering ([AFL10], [LGI+05])
- multi-agent systems ([VCP+05], [SPS09], [SS09], [BGSP10], [Sak11], [PSBG12])
- multi-context systems ([EBDT+09], [BEF11], [EFS11], [BEFW11], [DFS12])
- natural language processing/understanding ([BDS08], [BGG12], [LS12])
- argumentation ([EGW08], [WCG09], [EGW10], [Gag10])

Applications of ASP in Other Areas

- product configuration ([SN98], [TSNS03])
- Linux package configuration ([Syr00], [GKS11])
- wire routing ([ELW00], [ET01])
- combinatorial auctions ([BU01])
- game theory ([VV02], [VV04])
- decision support systems ([NBG$^+$01])
- logic puzzles ([FMT02], [BD12])
- bioinformatics ([BCD$^+$08], [EY09], [EEB10], [EEEO11])
- phylogenetics ([ELR06], [BEE$^+$07], [Erd09], [EEEF09], [CEE11], [Erd11])
- haplotype inference ([EET09], [TE08])
- systems biology ([TB04], [GGI$^+$10], [ST09], [TAL$^+$10], [GSTV11])
- automatic music composition ([BBVF09],[BBVF11])
- assisted living ([MMB08], [MMB09], [MSMB11])
- team building ([RGA$^+$12])
- robotics ([CHO$^+$09], [EHP$^+$11], [AEEP11], [EHPU12], [APE12])
- software engineering ([EIO$^+$11])
- bounded model checking ([HN03], [TT07])
- verification of cryptographic protocols ([DGH09])
- e-tourism ([RDG$^+$10])

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- decision support systems ([NBG$^+$01]): used by United Space Alliance
- logic puzzles ([FMT02], [BD12])
- bioinformatics ([BCD$^+$08], [EY09], [EEB10], [EEEO11])
- phylogenetics ([ELR06], [BEE$^+$07], [Erd09], [EEEF09], [CEE11], [Erd11])
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- team building ([RGA$^+$12]): used by Gioia Tauro seaport
- robotics ([CHO$^+$09], [EHP$^+$11], [AEEP11], [EHPU12], [APE12])
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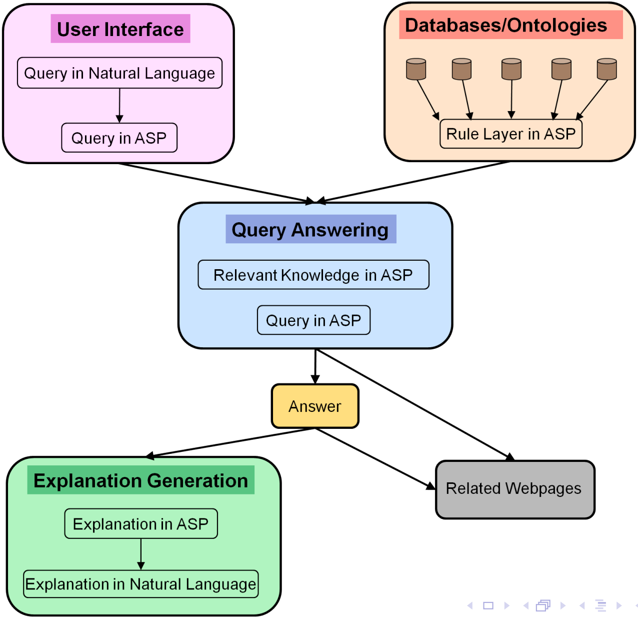


BioQuery-CNL*: A CNL for biomedical queries

BioQuery-CNL* Grammar:

Query → WhatQuery QuestionMark
WhatQuery → What are OfRelation NestedPredicateRelation
OfRelation → *Noun*() of *Type*()
NestedPredicateRelation → (...)* that PredicateRelation
PredicateRelation → InstanceRelation (...)*
InstanceRelation → (Neg)? *Verb*() the *Type*() *Instance*()
QuestionMark → ?

Ontology functions:

Type() returns the type information, e.g., gene, disease, drug
Instance(T) returns instances of the type T, e.g., Asthma for type disease
Verb(T, T') returns the verbs where type T is the subject and type T' is the object, e.g., drug treat disease
Noun(T) returns the nouns that are related to the type T, e.g., side-effects of type drug

Example: What are the side-effects of the drugs that treat the disease Asthma?

Representing Queries in ASP

Query Q2 in BIOQUERY-CNL*: What are the genes that are targeted by all the drugs that belong to the category Hmg-coa reductase inhibitors?

Query Q2 in ASP:

$$notcommon(gn_1) \leftarrow not\ drug\_gene(d_2, gn_1), condition_1(d_2)$$
$$condition_1(d) \leftarrow drug\_category(d, \text{``}Hmg - coa\ reductase\ inhibitors\text{''})$$

$$what\_be\_genes(gn_1) \leftarrow not\ notcommon(gn_1), notcommon\_exists$$
$$notcommon\_exists \leftarrow notcommon(x)$$

$$answer\_exists \leftarrow what\_be\_genes(gn)$$

Extraction and Integration of Knowledge using ASP

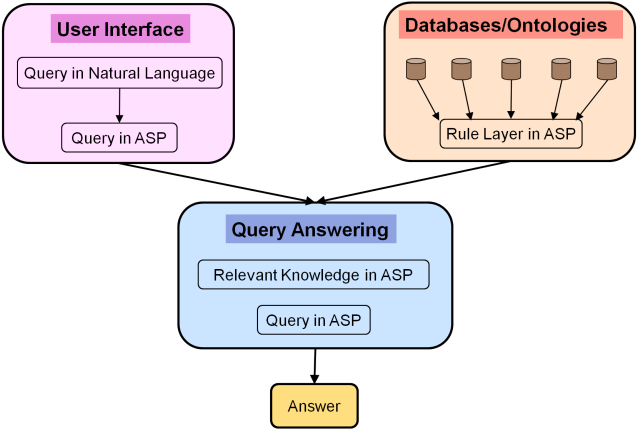
Knowledge from RDF(S)/OWL ontologies can be extracted using "external predicates" supported by the ASP solver DLVHEX [EGRH06]:

$$
\begin{array}{l}
triple\_gene(x, y, z) \leftarrow \&rdf[\text{``}URIforGeneOntology\text{''}](x, y, z) \\
gene\_gene(g_1, g_2) \leftarrow triple\_gene(x, \text{``}geneproperties : name\text{''}, g_1), \\
\qquad triple\_gene(x, \text{``}geneproperties : related\_genes\text{''}, b), \ldots
\end{array}
$$

ASP rules integrate the extracted knowledge, or define new concepts:

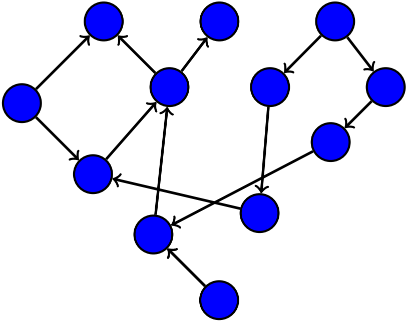
$$
\begin{array}{l}
gene\_reachable\_from(x, 1) \leftarrow gene\_gene(x, y), start\_gene(y) \\
gene\_reachable\_from(x, n+1) \leftarrow gene\_gene(x, z), \\
\qquad gene\_reachable\_from(z, n), max\_chain\_length(l) \quad (0 < n, n < l)
\end{array}
$$

Query Answering in ASP



- Generally, only a small part of the underlying databases/ontologies and the rule layer is related to the given query.
- We introduce a method to identify the relevant part of the ASP program for more efficient query answering.

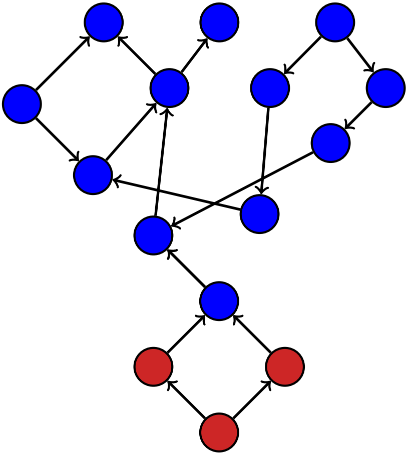
Identifying the Relevant Part of a Program



% Databases and Ontologies:
fact 1.
fact 2.
fact 3.
⋮

% Rule Layer:
rule 1.
rule 2.
rule 3.
⋮

Identifying the Relevant Part of a Program

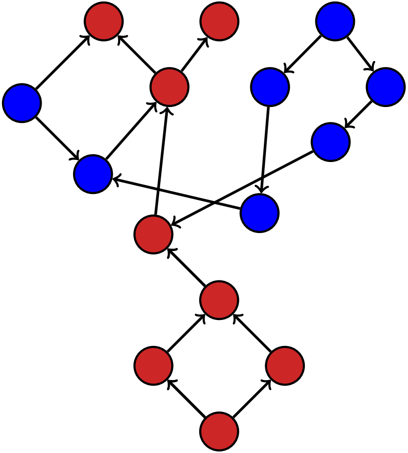


% Databases and Ontologies:
fact 1.
fact 2.
fact 3.
⋮

% Rule Layer:
rule 1.
rule 2.
rule 3.
⋮

% Query:
rule 1.
rule 2.
⋮

Identifying the Relevant Part of a Program



% Databases and Ontologies:
fact 1.
fact 2.
fact 3.
⋮

% Rule Layer:
rule 1.
rule 2.
rule 3.
⋮

% Query:
rule 1.
rule 2.
⋮

Experimental Results: Databases & Ontologies

Source	Relation (number of ASP facts)
BioGrid	gene-gene (372.293)
DrugBank	drug-drug (21.756) drug-category (4.743)
Sider	drug-sideeffect (61.102)
PharmGKB	drug-disease (3.740) drug-gene (15.805) disease-gene (9.417)
CTD	drug-disease (704.590) drug-gene (259.048) disease-gene (8.909.071)
	Total : 10.3 M

Experimental Results

Query	Complete	Relevant
Q1	271.39 Rules: 21059323	**13.08** Rules: 1961789
Q2	266.06 Rules: 21059909	**14.34** Rules: 2084579
Q3	266.62 Rules: 21059248	**9.85** Rules: 1567401
Q4	**273.93** Rules: 21059353	321.11 Rules: 19450525
Q5	265.91 Rules: 21061727	**9.93** Rules: 1460831
Q6	**269.69** Rules: 21111842	320.56 Rules: 19512500
Q7	270.05 Rules: 21062006	**6.07** Rules: 1023061
Q8	275.19 Rules: 21079275	**7.02** Rules: 1040406
Q9	272.48 Rules: 21059597	**3.48** Rules: 547545
Q10	266.37 Rules: 21077252	**11.25** Rules: 1594891

Example: Explanation Generation

Query in BioQuery-CNL*: What are the genes that are targeted by the drug Epinephrine and that interact with the gene DLG4?

An Answer: `ADRB1`

Shortest Explanation in ASP:

$$what\_be\_genes(ADRB1) \leftarrow drug\_gene(Epinephrine, ADRB1), gene\_gene(ADRB1, DLG4)$$

$$drug\_gene(Epinephrine, ADRB1) \leftarrow drug\_gene\_ctd(Epinephrine, ADRB1)$$

$$drug\_gene\_ctd(Epinephrine, ADRB1) \leftarrow$$

$$gene\_gene(ADRB1, DLG4) \leftarrow gene\_gene(DLG4, ADRB1)$$

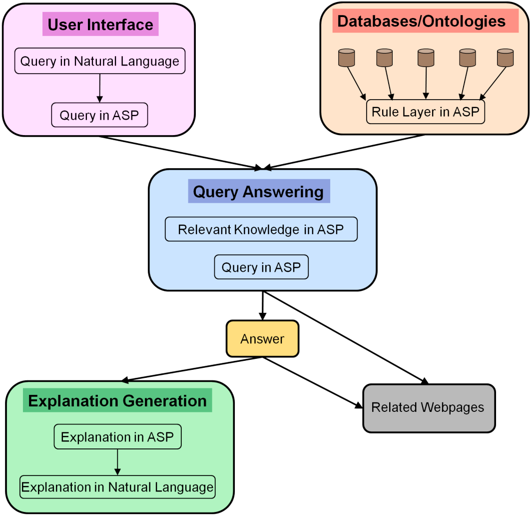
$$gene\_gene(DLG4, ADRB1) \leftarrow gene\_gene\_biogrid(DLG4, ADRB1)$$

$$gene\_gene\_biogrid(DLG4, ADRB1) \leftarrow$$

Explanation in Natural Language:

`The drug Epinephrine targets the gene ADRB1 according to CTD.`
`The gene DLG4 interacts with the gene ADRB1 according to BioGrid.`

BIOQUERY-ASP



http://krr.sabanciuniv.edu/projects/BioQuery-ASP/

Related Publications

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