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12. Evaluation of Datalog (2)
13. Graph Databases and Path Queries
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See course homepage [⇒ link] for more information and materials
Review: Datalog

Datalog is a powerful recursive query language

Advantages:

- Natural extension of (U)CQs with recursion
- Can be extended with (EDB) negation
- Polynomial data complexity of query answering

Disadvantages:

- High query and combined complexity ($\text{ExpTime}$)
- Perfect optimisation is undecidable
- Somewhat complicated to write queries
Graph Databases

Our original motivation for going from FO queries to Datalog: Reachability of nodes in a (directed) graph $\leadsto$ let's focus on graphs

**Graph database**: a DBMS that supports “graphs” as its datamodel

There are many kinds of graphs:

- Directed or undirected?
- Labelled or unlabelled edges/nodes?
- What kinds of labels? Datatypes?
- Parallel edges (multi-graphs)? With same label?
- One graph or several graphs per database?

Two types of graph database models dominate the market today: Resource Description Framework (RDF) and Property Graph
RDF is a W3C standard for representing linked data on the Web

- Directed labelled graph; nodes are identified by their labels
- Labels are URIs or datatype literals
- Multiple parallel edges only when using different edge labels
- Supports multiple graphs in one database
- W3C standard; implementations for many programming languages
- Datatype support based on W3C XML Schema datatypes
- Graphs can be exchanged in many standard syntax formats
Property Graph

Property Graph is a popular data model of many graph databases

- Directed labelled multi-graph; labels do not identify nodes
- “Labels” can be lists of attribute-value pairs
- Multiple parallel edges with the exact same labels are possible
- No native multi-graph support (could be simulated with additional attributes)
- No standard definition of technical details; most common implementation: Tinkerpop/Blueprints API (Java)
- Datatype support varies by implementation
- No standard syntax for exchanging data
Representing Graphs

Graphs (of any type) are usually viewed as sets of edges

- RDF: triples of form subject-predicate-object
  - When managing multiple graphs, each triple is extended with a fourth component (graph ID) \( \sim \) quads
  - RDF databases are sometimes still called “triple stores”, although most modern systems effectively store quads

- Property Graph: edge objects with attribute lists
  - represented by Java objects in Blueprints

Graphs can be stored in relational databases

- RDF: table Triple[Subject,Predicate, Object]
- Property Graph: tables Edge[SourceId, EdgeId, TargetId] and Attributes[Id, Attribute, Value]
Property Graphs can represent RDF:

- use attributes to store RDF node and edge labels (URIs)
- use key constraints to ensure that no two distinct nodes can have same label
Representing Data in Graphs

Property Graphs can represent RDF:

- use attributes to store RDF node and edge labels (URIs)
- use key constraints to ensure that no two distinct nodes can have same label

RDF can represent Property Graphs:

- use additional nodes to represent Property Graph edges
- use RDF triples with special predicates to represent attributes

Either model can also represent hypergraphs/RDBs (exercise)

→ all models can represent all data in principle
→ supported query features and performance will vary
Querying Graphs

Preferred query language depends on graph model

- RDF: W3C SPARQL query language
- Property Graph: no uniform approach to data access
  - many tools prefer API access over a query language
  - proprietary query languages, e.g., “Cypher” for Neo4j

However, there are some common basics in almost all cases:\n
- Conjunctive queries
- Regular path queries

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1 Might not be true for Cypher, which – in contrast to most other database query languages – seems to be based on graph isomorphism rather than homomorphism. But since there is no clear documentation, it’s hard to be sure.

Markus Krötzsch, 07 July 2016
Conjunctive Queries over Graphs

Basic descriptions of local patterns in a graph

Formally, it suffices to say:

CQs over RDF correspond to CQs over relational databases with a single table Triple[Subject, Predicate, Object]

(analogously for Property Graphs)

- All complexity results for query answering and optimisation carry over from RDBs (in particular, restricting to graphs does not make anything simpler)
- Details of representation of data in tables do not matter
- CQs are restricted to local patterns (no reachability . . . )
Regular Path Queries

Idea: use regular expressions to navigate over paths

Let’s consider a simplified graph model, where a graph is given by:

- Set of nodes $N$ (without additional labels)
- Set of edges $E$, labelled by a function $\lambda : E \rightarrow L$, where $L$ is a finite set of labels

**Definition**

A **regular expression** over a set of labels $L$ is an expression of the following form:

$$E ::= L \mid (E \circ E) \mid (E + E) \mid E^*$$

A **regular path query** (RPQ) is an expression of the form $E(s, t)$, where $E$ is a regular expression and $s$ and $t$ are terms (constants or variables).
Semantics of Regular Path Queries

As usual, a regular expression \( E \) matches a word \( w = \ell_1 \cdots \ell_n \) if any of the following conditions is satisfied:

- \( E \in L \) is a label and \( w = E \).
- \( E = (E_1 \circ E_2) \) and there is \( i \in \{0, \ldots, n\} \) such that \( E_1 \) matches \( \ell_1 \cdots \ell_i \) and \( E_2 \) matches \( \ell_{i+1} \cdots \ell_n \) (the words matched by \( E_1 \) and \( E_2 \) can be empty if \( i = 0 \) or \( i = n \), respectively).
- \( E = (E_1 + E_2) \) and \( w \) is matched by \( E_1 \) or by \( E_2 \)
- \( E = E_1^* \) and \( w \) has the form \( w_1 w_2 \cdots w_m \) for \( n \geq 0 \), where each word \( w_i \) is matched by \( E_1 \)

Definition

Let \( a \) and \( b \) be constants and \( x \) and \( y \) be variables. An RPQ \( E(a, b) \) is entailed by a graph \( G \) if there is a directed path from node \( a \) to node \( b \) that is labelled by a word matched by \( E \). The answers to RPQs \( E(x, y) \), \( E(x, b) \), and \( E(a, y) \) are defined in the obvious way.
Extending the Expressive Power of RPQs

Regular path queries can be used to express typical reachability queries, but are still quite limited \(\rightarrow\) extensions

**2-Way Regular Path Queries (2RPQs)**
- For every label \(\ell \in L\), also introduce a converse label \(\ell^-\)
- Allow converse labels in regular expressions
- Matched paths can follow edges forwards or backwards

**Conjunctive Regular Path Queries (CRPQs)**
- Extend conjunctive queries with RPQs
- RPQs can be used like binary query atoms
- Obvious semantics

**Conjunctive 2-Way Regular Path Queries (C2RPQs)** combine both extensions
C2RPQs: Examples

All ancestors of Alice:

$$((\text{father} + \text{mother}) \circ (\text{father} + \text{mother})^*)(\text{alice}, y)$$
C2RPQs: Examples

All ancestors of Alice:

$$[((\text{father} + \text{mother}) \circ (\text{father} + \text{mother})^*) (\text{alice}, y)$$

People with finite Erdös number:

$$(\text{authorOf} \circ \text{authorOf}^*)^* (x, \text{paulErdös})$$
C2RPQs: Examples

All ancestors of Alice:

$$(((\text{father} + \text{mother}) \circ (\text{father} + \text{mother})^*)(\text{alice}, y))$$

People with finite Erdös number:

$$(\text{authorOf} \circ \text{authorOf}^-)^* (x, \text{paulErdös})$$

Pairs of stops connected by tram lines 3 and 8:

$$(\text{nextStop3} \circ \text{nextStop3}^*)(x, y) \land (\text{nextStop8} \circ \text{nextStop8}^*)(x, y)$$
A nondeterministic algorithm for Boolean RPQs:

- Transform regular expression into a finite automaton
- Starting from the first node, guess a matching path
- When moving along path, advance state of automaton
- Accept if the second node is reached in an accepting state
- Reject if path is longer than size of graph \( \times \) size of automaton

Space requirements when assuming query (and automaton) fixed:

- Pointer to current node in graph
- Pointer to current state of automaton
- Counter for length of path

Conversely, reachability in an unlabelled graph is hard for \( \text{NL} \)

RPQ matching is \( \text{NL} \)-complete (data complexity)

(Combined/query complexity is in \( \text{P} \), as we will see below)
Complexity of RPQs

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- Reject if path is longer than size of graph $\times$ size of automaton

Space requirements when assuming query (and automaton) fixed: pointer to current node in graph, pointer to current state of automaton, counter for length of path $\sim$ NL algorithm

Conversely, reachability in an unlabelled graph is hard for NL $\sim$ RPQ matching is NL-complete (data complexity)

(Combined/query complexity is in P, as we will see below)
Complexity of C2RPQs

We already know:

- CQ matching is in $\text{AC}^0$ (data complexity) and $\text{NP}$-complete (query and combined complexity)
- RPQ matching is $\text{NL}$-complete (data) and in $\text{P}$ (query/combined)
- $\text{AC}^0 \subset \text{NL}$ and $\text{NL} \subseteq \text{NP}$

$\Rightarrow$ C2RPQs are $\text{NP}$-hard (combined/query) and $\text{NL}$-hard (data)
Complexity of C2RPQs

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$\Rightarrow$ C2RPQs are $\text{NP}$-hard (combined/query) and $\text{NL}$-hard (data)

It’s not hard to show that these bounds are tight:

**Theorem**

C2RPQ matching is $\text{NP}$-complete for combined and query complexity, and $\text{NL}$-complete for data complexity.
How do path queries relate to Datalog?

We already know:

- Datalog is \textit{ExpTime}-complete (combined/query) and \textit{P}-complete (data)
- C2RPQs are \textit{NP}-complete (combined/query) and \textit{NL}-complete (data)

\rightarrow maybe Datalog is more expressive than C2RPQs . . .
(C2)RPQs and Datalog

How do path queries relate to Datalog?

We already know:

- Datalog is \textit{ExpTime}-complete (combined/query) and \textit{P}-complete (data)
- C2RPQs are \textit{NP}-complete (combined/query) and \textit{NL}-complete (data)

\(\Rightarrow\) maybe Datalog is more expressive than C2RPQs …

Indeed, we can express regular expressions in Datalog

For simplicity, assume that we have a binary EDB predicate \(p_\ell\) for each label \(\ell \in L\) (other encodings would work just as well)
We transform a regular expression $E$ to a Datalog query $\langle Q_E, P_E \rangle$:

- If $E = \ell \in L$ is a label, then $P_E = \{ Q_E(x, y) ← p_\ell(x, y) \}$
- If $E = \ell^\dagger$ is the converse of a label $\ell \in L$, then $P_E = \{ Q_E(x, y) ← p_\ell(y, x) \}$
- If $E = (E_1 \circ E_2)$ then $P_E = P_{E_1} \cup P_{E_2} \cup \{ Q_E(x, z) ← Q_{E_1}(x, y) \land Q_{E_2}(y, z) \}$
- If $E = (E_1 + E_2)$ then $P_E = P_{E_1} \cup P_{E_2} \cup \{ Q_E(x, y) ← Q_{E_1}(x, y), Q_{E_2}(x, y) \}$
- If $E = E^*$ then $P_E = P_{E_1} \cup \{ Q_E(x, x) ←, Q_E(x, z) ← Q_{E_1}(x, y) \land Q_{E_1}(y, z) \}$
2-Way Regular Expressions in Datalog

We transform a regular expression $E$ to a Datalog query $\langle Q_E, P_E \rangle$:

If $E = \ell \in L$ is a label, then $P_E = \{ Q_E(x, y) \leftarrow p_\ell(x, y) \}$
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$$P_E = \{Q_E(x, y) \leftarrow p_\ell(y, x)\}$$
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If $E = (E_1 \circ E_2)$ then

$$P_E = P_{E_1} \cup P_{E_2} \cup \{ Q_E(x, z) \leftarrow Q_{E_1}(x, y) \land Q_{E_2}(y, z) \}$$
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If $E = (E_1 + E_2)$ then

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2-Way Regular Expressions in Datalog

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If $E = (E_1 + E_2)$ then

$$P_E = P_{E_1} \cup P_{E_2} \cup \{ Q_E(x, y) \leftarrow Q_{E_1}(x, y), Q_E(x, y) \leftarrow Q_{E_2}(x, y) \}$$

If $E = E_1^*$ then

$$P_E = P_{E_1} \cup \{ Q_E(x, x) \leftarrow, Q_E(x, z) \leftarrow Q_E(x, y) \land Q_{E_1}(y, z) \}$$
As a side effect, the previous translation shows that 2RPQs can be evaluated in $P$ combined complexity:

- Each (2-way) regular expression $E$ leads to a Datalog query $\langle Q_E, P_E \rangle$ of polynomial size
- Each rule in $P_E$ has at most three variables
  - the grounding of $P_E$ for a graph with nodes $N$ is of size $|P_E| \times |N|^3$
- propositional logic rules can be evaluated in polynomial time

$\sim$ polynomial time decision procedure
Expressing C2RPQs in Datalog

It is now easy to express C2RPQs in Datalog:

- Use the encoding of CQs in Datalog as shown in the exercise
- Express 2RPQ atoms in Datalog as just shown

Can every Datalog query over binary “labelled-edge” EDB predicates be expressed with (C2)RPQs?
Expressing C2RPQs in Datalog

It is now easy to express C2RPQs in Datalog:

- Use the encoding of CQs in Datalog as shown in the exercise
- Express 2RPQ atoms in Datalog as just shown

Can every Datalog query over binary “labelled-edge” EDB predicates be expressed with (C2)RPQs?

- This would imply $P = NL$ (but not that $NP = ExpTime$!): unlikely but not known to be false
- However, there are stronger direct arguments that show the limits of C2RPQs (exercise)
Expressing 2RPQs in Datalog requires only restricted forms of Datalog:

**Definition**

A Datalog program is **linear** if each of its rules has at most one IDB atom in its body. A Datalog program is **binary** if all of its IDB predicates have arity at most two.

The following complexity results are known:

**Theorem**

Query answering in linear Datalog is $\text{NL}$-complete for data complexity, and $\text{PSPACE}$-complete for combined and query complexity.

Combined complexity further drops to $\text{NP}$ for binary Datalog.

$\Rightarrow$ complexity results that are more similar to (C2)RPQs ...
2RPQs and Linear Datalog

The Datalog translation of 2RPQs does not lead to linear Datalog, but we can fix this.

We transform a regular expression $E$ to a linear Datalog query $\langle Q_E, P_E^{\text{lin}} \rangle$:

- Construct a non-deterministic automaton $\mathcal{A}_E$ for $E$
- For every state $q$ of $\mathcal{A}_E$, we use a binary IDB predicate $S_q$
- For the starting state $q_0$ of $\mathcal{A}_E$, we add a rule $S_{q_0}(x, x) \leftarrow$
- For every transition $q \xrightarrow{\ell} q'$ of $\mathcal{A}_E$, we add a rule
  \[ S_{q'}(x, z) \leftarrow S_q(x, y) \land p_\ell(y, z) \]
- For every final state $q_f$ of $\mathcal{A}_E$, we add a rule
  \[ Q_E(x, y) \leftarrow S_{q_f}(x, y) \]

Two-way queries can be captured by allowing two-way transitions.
Linear Datalog vs. 2RPQs

So all 2RPQs can be expressed in linear Datalog
Is the converse also true?

Query \( (x, z) \leftarrow p_a(x, y) \land p_b(y, z) \)

Query \( (x, z) \leftarrow p_a(x, x') \land \text{Query} \( (x', z') \land p_b(z', z) \)

The linear Datalog program matches paths with labels from a \( a \) \( n \) \{ context-free, non-regular language \}

\{ not expressible in (C2)RPQs \}

Intuition: linear Datalog generalises context-free languages
Linear Datalog vs. 2RPQs

So all 2RPQs can be expressed in linear Datalog
Is the converse also true?

No. Counterexample:

\[
\text{Query}(x, z) \leftarrow p_a(x, y) \land p_b(y, z) \\
\text{Query}(x, z) \leftarrow p_a(x, x') \land \text{Query}(x', z') \land p_b(z', z)
\]

The linear Datalog program matches paths with labels from \(a^n b^n\)
\(\Rightarrow\) context-free, non-regular language
\(\Rightarrow\) not expressible in (C2)RPQs

Intuition: linear Datalog generalises context-free languages
Recall the basic static optimisation problems of database theory:

- Query containment
- Query equivalence
- Query emptiness

Which of these are decidable for (C2)RPQs?
Recall the basic static optimisation problems of database theory:

- Query containment
- Query equivalence
- Query emptiness

Which of these are decidable for (C2)RPQs?

Observation: query emptiness is trivial
Containment for RPQs

Containment of Regular Path Queries corresponds to containment of regular expressions \( \sim \) known to be decidable in \( \text{PSPACE} \)

Proof sketch for checking \( E_1 \subseteq E_2 \):

(1) Construct non-deterministic automata (NFAs), \( A_1 \) and \( A_2 \) for the regular expressions \( E_1 \) and \( E_2 \), respectively

(2) Construct an automaton \( \bar{A}_2 \) that accepts the complement of \( A_2 \).

(3) Construct the intersection \( A_1 \cap \bar{A}_2 \) of \( A_1 \) and \( \bar{A}_2 \)

(4) Check if \( A_1 \cap \bar{A}_2 \) accepts a word (if yes, then there is a counterexample that disproves \( E_1 \subseteq E_2 \); if no, then the containment holds)

Complexity estimate:

\( A_1 \cap \bar{A}_2 \) is exponential (blow-up by powerset construction in step (2)) but step (4) is possible by checking reachability on the state graph

\( \sim \) \( \text{NL} \) algorithm on an exponential state graph

\( \sim \) \( \text{NPSPACE} \) algorithm (construct the state graph on the fly)

\( \sim \) \( \text{PSPACE} \) algorithm (Savitch’s Theorem)
Containment for (C)2RPQs

Things are more tricky when adding converses and conjunctions

Theorem

- Containment of 2RPQs is $\text{PSPACE}$-complete
- Containment of C2RPQs is $\text{EXPSPACE}$-complete

The proofs are more involved.

Automata-theoretic constructions are used, but with more complicated automata models and for somewhat different languages (there is no good “language of possible C2RPQ matches on a graph” $\rightarrow$ consider language of possible proofs instead)
Query Optimisation for Path Queries

Decidable in $\text{PSPACE}$ (2RPQs) and $\text{EXPSPACE}$ (C2RPQs)

Should be compared to linear Datalog:

**Theorem**
Query containment for linear Datalog queries is undecidable.

Proof: see Lecture 11 (Post Correspondence Problem in Datalog – in fact, in linear Datalog)

Essentially no adoption in practice

∼ maybe the complexities are too high . . .

∼ or maybe path query optimisers are just too primitive
Path Queries: Final Remarks on Expressivity

We have seen that C2RPQs are $\text{NL}$-complete for data

$\leadsto$ can all $\text{NL}$-complete queries be captured by a C2RPQ?
We have seen that C2RPQs are NL-complete for data.  

\( \sim \) can all NL-complete queries be captured by a C2RPQ?  

**No.** For many reasons.  

- C2RPQs have no disjunction (\( \sim \) Unions of C2RPQs)  
- C2RPQs have no negation  

FO-queries with a binary transitive closure operator capture NL  

Several (regular) extensions of path queries:  

- Nested unary 2RPQs in regular expressions (“test operators”)  
- Nested binary C2RPQs in regular expressions  
- Other more expressive fragments of “regular Datalog”, e.g., Monadically Defined Queries
Summary and Outlook

Graph databases as an important class of “noSQL” databases

Two main data models

- Resource Description Framework (RDF)
- Property Graph

Path queries as common foundation of all graph query languages

- higher data complexities than CQs/FO queries
- lower complexities than Datalog queries
- decidable query optimisation

Next topics:

- Applications
- Summary