TECHNISCHE UNIVERSITÄT DRESDEN

DATABASE THEORY

Lecture 16: Graph Databases and Path Queries

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Knowledge-Based Systems

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More recent versions of this slide deck might be available.
For the most current version of this course, see
`https://iccl.inf.tu-dresden.de/web/Database_Theory/en`

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 (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

Resource Description Framework (RDF)

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) $\leadsto$ 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]

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

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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)

$\leadsto$ all models can represent all data in principle
$\leadsto$ 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:[1]

- Conjunctive queries
- Regular path queries

[1] Might not be true for Cypher, which – in contrast to most other database query languages – is based on a variant of graph isomorphism rather than homomorphism; and which supports only specific path expressions

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]"

(and 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 $\lambda : E \to L$, where L is a finite set of labels

Definition 16.1: 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 16.2: 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 $\leadsto$ extensions

2-Way Regular Path Queries (2RPQs)

- For every label $\ell \in L$, also introduce a converse label ℓ^-
- 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:

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

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Pairs of stops connected by tram lines 3 and 8:

$$(\text{nextStop3} \circ \text{nextStop3}^*)(x, y) \wedge (\text{nextStop8} \circ \text{nextStop8}^*)(x, y)$$

Complexity of RPQs

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

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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
⇝ NL algorithm

Conversely, reachability in an unlabelled graph is hard for NL
⇝ 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 AC^0 (data complexity) and NP-complete (query and combined complexity)
- RPQ matching is NL-complete (data) and in P (query/combined)
- $\mathrm{AC}^0 \subset \mathrm{NL}$ and $\mathrm{NL} \subseteq \mathrm{NP}$

$\leadsto$ C2RPQs are NP-hard (combined/query) and NL-hard (data)

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- $AC^0 \subset NL$ and $NL \subseteq NP$

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

Theorem 16.3: C2RPQ matching is NP-complete for combined and query complexity, and NL-complete for data complexity.

(C2)RPQs and Datalog

How do path queries relate to Datalog?

We already know:

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

$\rightsquigarrow$ maybe Datalog is more expressive that C2RPQs . . .

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Indeed, we can express regular expressions in Datalog

For simplicity, assume that we have a binary EDB predicate p_ℓ for each label $\ell \in L$
(other encodings would work just as well)

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If $E = E_1^*$ then

$$P_E = P_{E_1} \cup \{\mathsf{Q}_E(x, x) \leftarrow, \mathsf{Q}_E(x, z) \leftarrow \mathsf{Q}_E(x, y) \wedge \mathsf{Q}_{E_1}(y, z)\}$$

Reprise: Combined Complexity of 2RPQs

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
  $\leadsto$ 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

$\leadsto$ 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?

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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)

Linear Datalog and Binary Datalog

Expressing 2RPQs in Datalog requires only restricted forms of Datalog:

Definition 16.4: 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 16.5: Query answering in linear Datalog is NL-complete for data complexity, and PSpace-complete for combined and query complexity.
Combined complexity further drops to NP for binary Datalog.

$\leadsto$ 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 $\langle \mathsf{Q}_E, P_E^{\mathsf{lin}} \rangle$:

- 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 $\mathsf{S}_{q_0}(x, x) \leftarrow$
- For every transition $q \xrightarrow{\ell} q'$ of $\mathcal{A}_E$, we add a rule

$$\mathsf{S}_{q'}(x, z) \leftarrow \mathsf{S}_q(x, y) \wedge \mathsf{p}_\ell(y, z)$$

- For every final state q_f of $\mathcal{A}_E$, we add a rule

$$\mathsf{Q}_E(x, y) \leftarrow \mathsf{S}_{q_f}(x, y)$$

Two-way queries can be captured by allowing two-way transitions.

Linear Datalog vs. 2RPQs

So all 2RPQs can be expessed in linear Datalog

Is the converse also true?

Linear Datalog vs. 2RPQs

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

No. Counterexample:

$$\mathsf{Query}(x,z) \leftarrow \mathsf{p}_a(x,y) \wedge \mathsf{p}_b(y,z)$$
$$\mathsf{Query}(x,z) \leftarrow \mathsf{p}_a(x,x') \wedge \mathsf{Query}(x',z') \wedge \mathsf{p}_b(z',z)$$

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

Intuition: linear Datalog generalises context-free languages

Query Optimisation for C2RPQs

Recall the basic static optimisation problems of database theory:

- Query containment
- Query equivalence
- Query emptiness

Which of these are decidable for (C2)RPQs?

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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 $\rightsquigarrow$ known to be decidable in PSpace

Proof sketch for checking $E_1 \sqsubseteq E_2$:

(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 $E_1 \sqsubseteq E_2$; 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
$\rightsquigarrow$ NL algorithm on an exponential state graph
$\rightsquigarrow$ NPSpace algorithm (construct the state graph on the fly)
$\rightsquigarrow$ PSpace algorithm (Savitch's Theorem)

Containment for (C)2RPQs

Things are more tricky when adding converses and conjunctions

Theorem 16.6:

- Containment of 2RPQs is PSpace-complete
- Containment of C2RPQs is 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” $\rightsquigarrow$ consider language of possible proofs instead)

Query Optimisation for Path Queries

Decidable in PSpace (2RPQs) and ExpSpace (C2RPQs)

Should be compared to linear Datalog:

Theorem 16.7: Query containment for linear Datalog queries is undecidable.

Proof: see Lecture 13 (Post Correspondence Problem in Datalog – in fact, in linear Datalog) □

Query containment of (C2)RPQs is seeing essentially no adoption in practice
$\leadsto$ maybe the complexities are too high . . .
$\leadsto$ or maybe path query optimisers are just too primitive . . .
$\leadsto$ or maybe (current) real-world queries do not look as if they would benefit from this effort

Path Queries: Final Remarks on Expressivity

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

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We have seen that C2RPQs are NL-complete for data
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No. For many reasons.

- C2RPQs have no disjunction ($\leadsto$ 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:

- Logical dependencies
- Query answering under constraints