TECHNISCHE UNIVERSITÄT DRESDEN

DATABASE THEORY

Lecture 12: Introduction to Datalog

Markus Krötzsch

Knowledge-Based Systems

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Introduction to Datalog

Introduction to Datalog

Datalog introduces recursion into database queries

- Use deterministic rules to derive new information from given facts
- Inspired by logic programming (Prolog)
- However, no function symbols and no negation
- Studied in AI (knowledge representation) and in databases (query language)

Example 12.1: Transitive closure C of a binary relation r

$$C(x, y) \leftarrow r(x, y)$$
$$C(x, z) \leftarrow C(x, y) \wedge r(y, z)$$

Intuition:

- some facts of the form $r(x, y)$ are given as input, and the rules derive new conclusions $C(x, y)$
- variables range over all possible values (implicit universal quantifier)

Syntax of Datalog

Recall: A term is a constant or a variable. An atom is a formula of the form $R(t_1, \ldots, t_n)$ with R a predicate symbol (or relation) of arity n, and $t_1, \ldots, t_n$ terms.

Definition 12.2: A Datalog rule is an expression of the form:

$$H \leftarrow B_1 \wedge \ldots \wedge B_m$$

where H and $B_1, \ldots, B_m$ are atoms. H is called the head or conclusion; $B_1 \wedge \ldots \wedge B_m$ is called the body or premise. A rule with empty body ($m = 0$) is called a fact. A ground rule is one without variables (i.e., all terms are constants).

A set of Datalog rules is a Datalog program.

Datalog: Example

$$
\begin{aligned}
\text{father}(\text{alice}, \text{bob}) & \\
\text{mother}(\text{alice}, \text{carla}) & \\
\text{mother}(\text{evan}, \text{carla}) & \\
\text{father}(\text{carla}, \text{david}) & \\
\text{Parent}(x, y) & \leftarrow \text{father}(x, y) \\
\text{Parent}(x, y) & \leftarrow \text{mother}(x, y) \\
\text{Ancestor}(x, y) & \leftarrow \text{Parent}(x, y) \\
\text{Ancestor}(x, z) & \leftarrow \text{Parent}(x, y) \wedge \text{Ancestor}(y, z) \\
\text{SameGeneration}(x, x) & \\
\text{SameGeneration}(x, y) & \leftarrow \text{Parent}(x, v) \wedge \text{Parent}(y, w) \wedge \text{SameGeneration}(v, w)
\end{aligned}
$$

Datalog Semantics by Deduction

What does a Datalog program express?

Usually we are interested in entailed ground atoms

What can be entailed? Informally:

- Restrict to set of constants that occur in program (finite)
  $\leadsto$ universe $\mathcal{U}$
- Variables can represent arbitrary constants from this set
  $\leadsto$ ground substitutions map variables to constants
- A rule can be applied if its body is satisfied for some ground substitution

  Example 12.3: The rule Parent$(x, y) \leftarrow$ mother(x, y) can be applied to mother(alice, carla) under substitution $\{x \mapsto$ alice$, y \mapsto$ carla$\}$.

- If a rule is applicable under some ground substitution, then the according instance of the rule head is entailed.

Datalog Semantics by Deduction (2)

An inductive definition of what can be derived:

Definition 12.4: Consider a Datalog program P. The set of ground atoms that can be derived from P is the smallest set of atoms A for which there is a rule $H \leftarrow B_1 \wedge \ldots \wedge B_n$ and a ground substitution θ such that

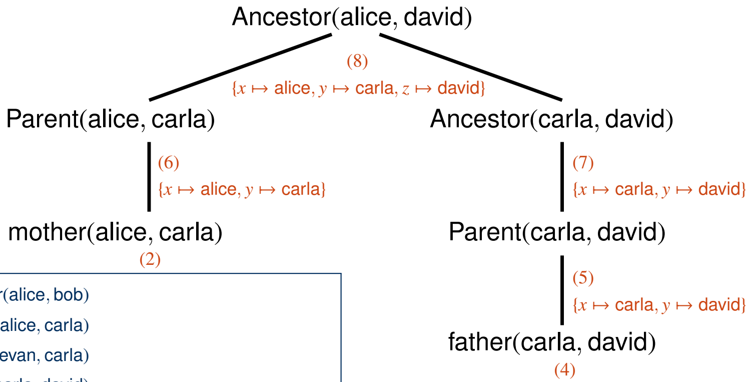
- $A = H\theta$, and
- for each $i \in \{1, \ldots, n\}$, $B_i\theta$ can be derived from P.

Notes:

- $n = 0$ for ground facts, so they can always be derived (induction base)
- if variables in the head do not occur in the body, they can be any constant from the universe

Datalog Deductions as Proof Trees

We can think of deductions as tree structures:



(1) father(alice, bob)
(2) mother(alice, carla)
(3) mother(evan, carla)
(4) father(carla, david)
(5) $\text{Parent}(x, y) \leftarrow \text{father}(x, y)$
(6) $\text{Parent}(x, y) \leftarrow \text{mother}(x, y)$
(7) $\text{Ancestor}(x, y) \leftarrow \text{Parent}(x, y)$
(8) $\text{Ancestor}(x, z) \leftarrow \text{Parent}(x, y) \wedge \text{Ancestor}(y, z)$

Datalog Semantics by Least Fixed Point

Instead of using substitutions, we can also ground programs:

Definition 12.5: The grounding ground(P) of a Datalog program P is the set of all ground rules that can be obtained from rules in P by uniformly replacing variables with constants from the universe.

Derivations are described by the immediate consequence operator T_P that maps sets of ground facts I to sets of ground facts $T_P(I)$:

- $T_P(I) = \{H \mid H \leftarrow B_1 \wedge \ldots \wedge B_n \in \text{ground}(P) \text{ and } B_1, \ldots, B_n \in I\}$
- Least fixed point of T_P: smallest set L such that $T_P(L) = L$
- Bottom-up computation: $T_P^0 = \emptyset$ and $T_P^{i+1} = T_P(T_P^i)$
- The least fixed point of T_P is $T_P^\infty = \bigcup_{i \geq 0} T_P^i$ (exercise)

Observation: Ground atom A is derived from P if and only if $A \in T_P^\infty$

Datalog Semantics by Least Model

We can also read Datalog rules as universally quantified implications

Example 12.6: The rule

$$\text{Ancestor}(x, z) \leftarrow \text{Parent}(x, y) \wedge \text{Ancestor}(y, z)$$

corresponds to the implication

$$\forall x, y, z.\text{Parent}(x, y) \wedge \text{Ancestor}(y, z) \rightarrow \text{Ancestor}(x, z).$$

A set of FO implications may have many models
$\rightsquigarrow$ consider least model over the domain defined by the universe

Theorem 12.7: A fact is entailed by the least model of a Datalog program if and only if it can be derived from the Datalog program.

Datalog Semantics: Overview

There are three equivalent ways of defining Datalog semantics:

- Proof-theoretic: What can be proven deductively?
- Operational: What can be computed bottom up?
- Model-theoretic: What is true in the least model?

In each case, we restrict to the universe of given constants.
$\leadsto$ similar to active domain semantics in databases

Datalog as a Query Language

How can we use Datalog to query databases?
$\leadsto$ View database as set of ground facts
$\leadsto$ Specify which predicate yields the query result

Definition 12.8: A Datalog query is a pair $\langle R, P\rangle$, where P is a Datalog program and R is the answer predicate.
The result of the query is the set of R-facts entailed by P.

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Datalog queries distinguish "given" relations from "derived" ones:

- predicates that occur in a head of P are intensional database (IDB) predicates
- predicates that only occur in bodies are extensional database (EDB) predicates

Requirement: database relations used as EDB predicates only

Datalog as a Generalisation of CQs

A conjunctive query $\exists y_1, \ldots, y_m.A_1 \wedge \ldots \wedge A_\ell$ with answer variables $x_1, \ldots, x_n$ can be expressed as a Datalog query $\langle \mathsf{Ans}, P \rangle$ where P has the single rule:

$$\mathsf{Ans}(x_1, \ldots, x_n) \leftarrow A_1 \wedge \ldots \wedge A_\ell$$

Unions of CQs can also be expressed (how?)

Intuition: Datalog generalises UCQs by adding recursion.

Datalog and UCQs

We can make the relationship of Datalog and UCQs more precise:

Definition 12.9: For a Datalog program P:

- An IDB predicate R depends on an IDB predicate S if P contains a rule with R in the head and S in the body.
- P is non-recursive if there is no cyclic dependency.

Theorem 12.10: UCQs have the same expressivity as non-recursive Datalog.

That is: a query mapping can be expressed by some UCQ if and only if it can be expressed by a non-recursive Datalog program.

However, Datalog can be exponentially more succinct (shorter), as illustrated in an exercise.

Proof

Theorem 12.10: UCQs have the same expressivity as non-recursive Datalog.

Proof: "Non-recursive Datalog can express UCQs": Just discussed.

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"UCQs can express non-recursive Datalog": Obtained by resolution:

- Given rules $\rho_1 : R(s_1, \ldots, s_n) \leftarrow C_1 \wedge \ldots \wedge C_\ell$ and
  $\rho_2 : H \leftarrow B_1 \wedge \ldots \wedge R(t_1, \ldots, t_n) \wedge \ldots \wedge B_m$
  (w.l.o.g. having no variables in common with ρ_1)
- such that $R(t_1, \ldots, t_n)$ and $R(s_1, \ldots, s_n)$ unify with most general unifier σ,
- the resolvent of ρ_1 and ρ_2 with respect to σ is
  $H\sigma \leftarrow B_1\sigma \wedge \ldots \wedge C_1\sigma \wedge \ldots \wedge C_\ell\sigma \wedge \ldots \wedge B_m\sigma$.

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Unfolding of R means to simultaneously resolve all occurrences of R in bodies of any rule, in all possible ways. After adding all these resolvents, we can delete all rules that contain R in body or head (assuming that R is not the answer predicate).

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Now given a non-recursive Datalog program, unfold each non-answer predicate (in any order). $\rightsquigarrow$ program with only the answer predicate in heads (requires non-recursiveness). This is easy to express as UCQ (using equality to handle constants in heads). □

Datalog and Domain Independence

Domain independence was considered useful for FO queries
$\leadsto$ results should not change if domain changes

Several solutions:

- Active domain semantics: restrict to elements mentioned in database or query
- Domain-independent queries: restrict to query where domain does not matter
- Safe-range queries: decidable special case of domain independence

Our definition of Datalog uses the active domain (=Herbrand universe) to ensure domain independence

Safe Datalog Queries

Similar to safe-range FO queries, there are also simple syntactic conditions that ensure domain independence for Datalog:

Definition 12.11: A Datalog rule is safe if all variables in its head also occur in its body. A Datalog program/query is safe if all of its rules are.

Simple observations:

- safe Datalog queries are domain independent
- every Datalog query can be expressed as a safe Datalog query ...
- ... and un-safe queries are not much more succinct either (exercise)

Some texts require Datalog queries to be safe in general
but in most contexts there is no real need for this

Complexity

Complexity of Datalog

How hard is answering Datalog queries?

Recall:

- Combined complexity: based on query and database
- Data complexity: based on database; query fixed
- Query complexity: based on query; database fixed

Plan:

- First show upper bounds (outline efficient algorithm)
- Then establish matching lower bounds (reduce hard problems)

A Simpler Problem: Ground Progams

Let's start with Datalog without variables
$\leadsto$ sets of ground rules a.k.a. propositional Horn logic program

Naive computation of T_P^∞:

```
T_P^0 := ∅
i := 0
repeat :
    T_P^{i+1} := ∅
    for H ← B_1 ∧ ... ∧ B_ℓ ∈ P :
        if {B_1, ..., B_ℓ} ⊆ T_P^i :
            T_P^{i+1} := T_P^{i+1} ∪ {H}
    i := i + 1
until T_P^{i-1} = T_P^i
return T_P^i
```

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return T_P^i
```

How long does this take?

- At most $|P|$ facts can be derived
- Algorithm terminates with $i \leq |P| + 1$
- In each iteration, we check each rule once (linear), and compare its body to T_P^i (quadratic)

$\leadsto$ polynomial runtime

Complexity of Propositional Horn Logic

Much better algorithms exist:

Theorem 12.12 (Dowling & Gallier, 1984): For a propositional Horn logic program P, the set T_P^∞ can be computed in linear time.

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Nevertheless, the problem is not trivial:

Theorem 12.13: For a propositional Horn logic program P and a proposition (or ground atom) A, deciding if $A \in T_P^\infty$ is a P-complete problem.

Remark:
all P problems can be reduced to propositional Horn logic entailment
yet not all problems in P (or even in NL) can be solved in linear time!

Datalog Complexity: Upper Bounds

A straightforward approach:

(1) Compute the grounding ground(P) of P w.r.t. the database $\mathcal{I}$

(2) Compute $T^{\infty}_{\text{ground}(P)}$

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Complexity estimation:

- The number of constants N for grounding is linear in P and $\mathcal{I}$
- A rule with m distinct variables has N^m ground instances
- Step (1) creates at most $|P| \cdot N^M$ ground rules, where M is the maximal number of variables in any rule in P
  - ground(P) is polynomial in the size of $\mathcal{I}$
  - ground(P) is exponential in P
- Step (2) can be executed in linear time in the size of ground(P)

Summing up: the algorithm runs in P data complexity and in ExpTime query and combined complexity

Datalog Complexity

These upper bounds are tight:

Theorem 12.14: Datalog query answering is:

- ExpTime-complete for combined complexity
- ExpTime-complete for query complexity
- P-complete for data complexity

It remains to show the lower bounds.

P-Hardness of Data Complexity

We need to reduce a P-hard problem to Datalog query answering
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- all other rules have the form $H \leftarrow B_1 \wedge B_2$

Deciding fact entailment is still P-hard (exercise)

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We can store such programs in a database:

- For each fact $H \leftarrow$, the database has a tuple Fact(H)
- For each rule $H \leftarrow B_1 \wedge B_2$,
  the database has a tuple Rule(H, B_1, B_2)

P-Hardness of Data Complexity (2)

The following Datalog program acts as an interpreter for propositional Horn logic programs:

$$\mathsf{True}(x) \leftarrow \mathsf{Fact}(x)$$

$$\mathsf{True}(x) \leftarrow \mathsf{Rule}(x, y, z) \land \mathsf{True}(y) \land \mathsf{True}(z)$$

Easy observations:

- $\mathsf{True}(A)$ is derived if and only if A is a consequence of the original propositional program
- The encoding of propositional programs as databases can be computed in logarithmic space
- The Datalog program is the same for all propositional programs

$\leadsto$ Datalog query answering is P-hard for data complexity

ExpTime-Hardness of Query Complexity

A direct proof:

Encode the computation of a deterministic Turing machine for up to exponentially many steps

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Encode the computation of a deterministic Turing machine for up to exponentially many steps

Recall that ExpTime = $\bigcup_{k\geq 1}$ Time(2^{n^k})

- in our case, n is the length of the input
- k is some constant

$\leadsto$ we need to simulate up to 2^{n^k} steps (and tape cells)

Main ingredients of the encoding:

- state$_q(X)$: the TM is in state q after X steps
- head(X, Y): the TM head is at tape position Y after X steps
- symbol$_\sigma(X, Y)$: the tape cell at position Y holds symbol σ after X steps

$\leadsto$ How to encode 2^{n^k} time points X and tape positions Y?

Preparing for a Long Computation

We need to encode 2^{n^k} time points and tape positions
$\leadsto$ use binary numbers with n^k digits

So X and Y in atoms like head(X, Y) are really lists of variables $X = x_1, \ldots, x_{n^k}$ and $Y = y_1, \ldots, y_{n^k}$, and the arity of head is $2 \cdot n^k$.

TODO: define predicates that capture the order of n^k-digit binary numbers

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TODO: define predicates that capture the order of n^k-digit binary numbers

For each number $i \in \{1, \ldots, n^k\}$, we use predicates:

- succ$^i(X, Y)$: $X + 1 = Y$, where X and Y are i-digit numbers
- first$^i(X)$: X is the i-digit encoding of 0
- last$^i(X)$: X is the i-digit encoding of $2^i - 1$

Finally, we can define the actual order for $i = n^k$

- $\leq^i (X, Y)$: $X \leq Y$, where X and Y are i-digit numbers

Defining a Long Chain

We can define $\mathsf{succ}^i(X, Y)$, $\mathsf{first}^i(X)$, and $\mathsf{last}^i(X)$ as follows:

$$\mathsf{succ}^1(0, 1) \quad \mathsf{first}^1(0) \quad \mathsf{last}^1(1)$$

$$\left.\begin{aligned}
\mathsf{succ}^{i+1}(0, X, 0, Y) &\leftarrow \mathsf{succ}^i(X, Y) \\
\mathsf{succ}^{i+1}(1, X, 1, Y) &\leftarrow \mathsf{succ}^i(X, Y) \\
\mathsf{succ}^{i+1}(0, X, 1, Y) &\leftarrow \mathsf{last}^i(X) \wedge \mathsf{first}^i(Y) \\
\mathsf{first}^{i+1}(0, X) &\leftarrow \mathsf{first}^i(X) \\
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\end{aligned}\right\}
\begin{array}{l}\text{for } X = x_1, \ldots, x_i \\ \text{and } Y = y_1, \ldots, y_i \\ \text{lists of } i \text{ variables}\end{array}$$

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Now for $M = n^k$, we define $\leq^M(X, Y)$ as the reflexive, transitive closure of $\mathsf{succ}^M(X, Y)$:

$$\leq^M(X, X) \leftarrow$$
$$\leq^M(X, Z) \leftarrow \leq^M(X, Y) \wedge \mathsf{succ}^M(Y, Z)$$

Initialising the Computation

We can now encode the initial configuration of the Turing Machine for an input word $\sigma_1 \cdots \sigma_n \in (\Sigma \setminus \{\llcorner\!\lrcorner\})^*$.

We write B_i for the binary encoding of a number i with $M = n^k$ digits.

$\mathsf{state}_{q_0}(B_0)$	where q_0 is the TM's initial state
$\mathsf{head}(B_0, B_0)$	
$\mathsf{symbol}_{\sigma_i}(B_0, B_i)$	for all $i \in \{1, \ldots, n\}$
$\mathsf{symbol}_{\llcorner\!\lrcorner}(B_0, Y) \leftarrow \leq^M(B_{n+1}, Y)$	where $Y = y_1, \ldots, y_M$

TM Transition and Acceptance Rules

For each transition $\langle q, \sigma, q', \sigma', d\rangle \in \Delta$, we add rules:

$$\mathsf{symbol}_{\sigma'}(X', Y) \leftarrow \mathsf{succ}^M(X, X') \wedge \mathsf{head}(X, Y) \wedge \mathsf{symbol}_{\sigma}(X, Y) \wedge \mathsf{state}_q(X)$$
$$\mathsf{state}_{q'}(X') \leftarrow \mathsf{succ}^M(X, X') \wedge \mathsf{head}(X, Y) \wedge \mathsf{symbol}_{\sigma}(X, Y) \wedge \mathsf{state}_q(X)$$

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Similar rules are used for inferring the new head position (depending on d)

Further rules ensure the preservation of unaltered tape cells:

$$\begin{aligned}\mathsf{symbol}_{\sigma}(X', Y) \leftarrow\ & \mathsf{succ}^M(X, X') \wedge \mathsf{symbol}_{\sigma}(X, Y) \wedge \\ & \mathsf{head}(X, Z) \wedge \mathsf{succ}^M(Z, Z') \wedge \leq^M(Z', Y) \\ \mathsf{symbol}_{\sigma}(X', Y) \leftarrow\ & \mathsf{succ}^M(X, X') \wedge \mathsf{symbol}_{\sigma}(X, Y) \wedge \\ & \mathsf{head}(X, Z) \wedge \mathsf{succ}^M(Z', Z) \wedge \leq^M(Y, Z')\end{aligned}$$

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& \mathsf{head}(X, Z) \wedge \mathsf{succ}^M(Z', Z) \wedge \leq^M(Y, Z')
\end{aligned}$$

The TM accepts if it ever reaches the accepting state q_{acc}:

$$\mathsf{accept}() \leftarrow \mathsf{state}_{q_{\mathsf{acc}}}(X)$$

Hardness Results

Lemma 12.15: A deterministic TM accepts an input in Time(2^{n^k}) if and only if the Datalog program defined above entails the fact accept().

We obtain ExpTime-hardness of Datalog query answering:

- The decision problem of any language in ExpTime can be solved by a deterministic TM in Time(2^{n^k}) for some constant k
- In particular, there are ExpTime-hard languages $\mathcal{L}$ with suitable deterministic TM $\mathcal{M}$ and constant k
- For any input word w, we can reduce acceptance of w by $\mathcal{M}$ in Time(2^{n^k}) to entailment of accept() by a Datalog program $P(w, \mathcal{M}, k)$
- $P(w, \mathcal{M}, k)$ is polynomial in k and the size of $\mathcal{M}$ and w (in fact, it can be constructed in logarithmic space)

ExpTime-Hardness: Notes

Some further remarks on our construction:

- The constructed program does not use EDB predicates
  $\leadsto$ database can be empty
- Therefore, hardness extends to query complexity
- Using a fixed (very small) database, we could have avoided the use of constants
- We used IDB predicates of unbounded arity
  $\leadsto$ they are essential for the claimed hardness

Summary and Outlook

Datalog can overcome some of the limitations of first-order queries

Non-recursive Datalog can express UCQs

Datalog is more complex than FO query answering:

- ExpTime-complete for query and combined complexity
- P-complete for data complexity

Open questions:

- Expressivity of Datalog
- Query containment for Datalog
- Implementation techniques for Datalog