

### DATABASE THEORY

**Lecture 12: Introduction to Datalog** 

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# Introduction to Datalog

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### 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

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

#### 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  $R(t_1, ..., t_n)$  with R a predicate symbol (or relation) of arity n, and  $t_1, ..., t_n$  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

```
\label{eq:alice} \begin{array}{l} \text{father(alice, bob)} \\ \text{mother(alice, carla)} \\ \text{mother(evan, carla)} \\ \text{father(carla, 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,y) \wedge \text{Parent}(y,w) \wedge \text{SameGeneration}(v,w) \end{array}
```

### **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)
  - $\sim$  universe  $\mathcal{U}$
- Variables can represent arbitrary constants from this set
  - → 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.

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## 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  $\theta$  such that

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

#### Notes:

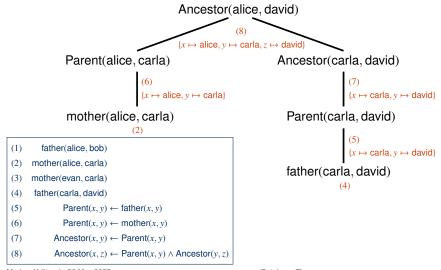
- n = 0 for ground facts, so they can always be derived (induction base)
- if variables in the head do not occur in the body, they can be any constant from the universe

slide 7 of 33

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## **Datalog Deductions as Proof Trees**

We can think of deductions as tree structures:



## 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  $T_P(I)$ :

- $T_P(I) = \{H \mid H \leftarrow B_1 \land \ldots \land B_n \in ground(P) \text{ and } B_1, \ldots, B_n \in I\}$
- 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

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

corresponds to the implication

$$\forall x, y, z. \mathsf{Parent}(x, y) \land \mathsf{Ancestor}(y, z) \rightarrow \mathsf{Ancestor}(x, z).$$

A set of FO implications may have many models

→ 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.

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### 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.

→ similar to active domain semantics in databases

## Datalog as a Query Language

How can we use Datalog to query databases?

- → View database as set of ground facts
- → 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*.

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

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# Datalog as a Generalisation of CQs

A conjunctive query  $\exists y_1, \dots, y_m.A_1 \land \dots \land A_\ell$  with answer variables  $x_1, \dots, x_n$  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.

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### Proof

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

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

"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  $\rho_1$ )
- such that  $R(t_1, \ldots, t_n)$  and  $R(s_1, \ldots, s_n)$  unify with most general unifier  $\sigma$ ,
- the resolvent of  $\rho_1$  and  $\rho_2$  with respect to  $\sigma$  is  $H\sigma \leftarrow B_1\sigma \wedge \ldots \wedge C_1\sigma \wedge \ldots \wedge C_\ell\sigma \wedge \ldots \wedge B_m\sigma$ .

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).

Now given a non-recursive Datalog program, unfold each non-answer predicate (in any order). → 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 → 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 <u>safe</u> 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

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## 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 Programs

#### Let's start with Datalog without variables

→ sets of ground rules a.k.a. propositional Horn logic program

### Naive computation of $T_P^{\infty}$ :

```
T_{P}^{0} := \emptyset
01
      i := 0
02
03
        repeat:
04
               T_{p}^{i+1} := \emptyset
               for H \leftarrow B_1 \wedge \ldots \wedge B_\ell \in P:
05
                       if \{B_1,\ldots,B_\ell\}\subseteq T_p^i:
06
                               T_{p}^{i+1} := T_{p}^{i+1} \cup \{H\}
07
08
               i := i + 1
09
        until T_p^{i-1} = T_p^i
10
        return T_p^i
```

#### How long does this take?

- At most |P| facts can be derived
- Algorithm terminates with  $i \le |P| + 1$
- In each iteration, we check each rule once (linear), and compare its body to  $T_P^i$  (quadratic)
- → 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  $T_p^{\infty}$  can be computed in linear time.

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 I
- (2) Compute  $T_{\text{ground}(P)}^{\infty}$

#### 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 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

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## **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 
→ propositional Horn logic programming

#### We restrict to a simple form of propositional Horn logic:

- facts have the usual form  $H \leftarrow$
- all other rules have the form  $H \leftarrow B_1 \wedge B_2$

Deciding fact entailment is still P-hard (exercise)

### We can store such programs in a database:

- For each fact  $H \leftarrow$ , the database has a tuple fact(H)
- For each rule H ← B<sub>1</sub> ∧ B<sub>2</sub>, the database has a tuple rule(H, B<sub>1</sub>, B<sub>2</sub>)

## 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:**

- 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

→ Datalog query answering is P-hard for data complexity

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## **ExpTime-Hardness of Query Complexity**

#### A direct proof:

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

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

- in our case, n = N is the number of database constants
- k is some constant
- $\rightarrow$  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  $\sigma$  after X steps
- $\rightarrow$  How to encode  $2^{N^k}$  time points X and tape positions Y?

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# Preparing for a Long Computation

We need to encode  $2^{N^k}$  time points and tape positions  $\rightarrow$  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

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

- $succ^{i}(X, Y)$ : X + 1 = Y, where X and Y are i-digit numbers
- first<sup>i</sup>(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  $\operatorname{succ}^{i}(X, Y)$ ,  $\operatorname{first}^{i}(X)$ , and  $\operatorname{last}^{i}(X)$  as follows:

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

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

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

### Initialising the Computation

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

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

$$\begin{array}{ll} \operatorname{state}_{q_0}(B_0) & \text{where } q_0 \text{ is the TM's initial state} \\ \operatorname{head}(B_0,B_0) & \\ \operatorname{symbol}_{\sigma_i}(B_0,B_i) & \text{for all } i \in \{1,\dots,n\} \\ \operatorname{symbol}_{\square}(B_0,Y) \leftarrow \leq^M(B_{n+1},Y) & \text{where } Y=y_1,\dots,y_M \end{array}$$

## TM Transition and Acceptance Rules

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

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

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

Further rules ensure the preservation of unaltered tape cells:

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

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

$$accept() \leftarrow state_{q_{acc}}(X)$$

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### 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
- 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 the size of  $\mathcal{M}$  and w (in fact: in logarithmic space), whereas k can be considered constant in this context

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## ExpTime-Hardness: Notes

#### Some further remarks on our construction:

- The constructed program does not use EDB predicates
  - → 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
  - ightharpoonup 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