

## DATABASE THEORY

**Lecture 13: Datalog Expressivity and Containment** 

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# Expressivity

## Review: Datalog

A rule-based recursive query language

```
\begin{aligned} & \text{father}(\text{alice}, \text{bob}) \\ & \text{mother}(\text{alice}, \text{carla}) \\ & & \text{Parent}(x, y) \leftarrow \text{father}(x, y) \\ & & \text{Parent}(x, y) \leftarrow \text{mother}(x, y) \\ & \text{SameGeneration}(x, x) \\ & \text{SameGeneration}(x, y) \leftarrow \text{Parent}(x, v) \land \text{Parent}(y, w) \land \text{SameGeneration}(v, w) \end{aligned}
```

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?

Datalog is more complex than FO query answering:

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

Next question: Is Datalog also more expressive than FO query answering?

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## The Big Picture

Where does Datalog fit in this picture?

```
Arbitrary Query Mappings everything undecidable

Polynomial Time Query Mappings

First-Order Queries
Data compl.: AC°, Comb./Query compl.: PSpace equivalence/containment/emptiness: undec.

Conjunctive Queries
Data compl.: AC°; everything else: NP

k-Bounded Hypertree Width everything (sub)polynomial

Tree CQs
```

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### **Expressivity of Datalog**

#### Datalog is P-complete for data complexity:

- $\bullet$  Entailments can be computed in polynomial time with respect to the size of the input database  ${\cal I}$
- There is a Datalog program P, such that all problems that can be solved in
  polynomial time can be reduced to the question whether P entails some fact over a
  database I that can be computed in logarithmic space.

 $\sim$  So Datalog can solve all polynomial problems?

No, it can't. Many problems in P that cannot be solved in Datalog:

- Parity: Is the number of elements in the database even?
- Connected graph?
- Is the input database a chain (or linear order)?

• ...

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## Limits of Datalog Expressiveness

Closure under homomorphism shows many limits of Datalog

**Special case:** there is a homomorphism from I to  $\mathcal{J}$  if  $I \subset \mathcal{J}$ 

- → Datalog entailments always remain true when adding more facts
  - Parity cannot be expressed
  - Connectivity cannot be expressed
  - It cannot be checked if the input database is a chain
  - Many FO queries with negation cannot be expressed (e.g.,  $\neg p(a)$ )
  - ...

#### However this criterion is not sufficient!

Datalog cannot even express all polynomial time query mappings that are closed under homomorphism

### Datalog Expressivity and Homomorphisms

How can we know that something is not expressible in Datalog?

A useful property: Datalog is "closed under homomorphisms"

**Theorem 13.1:** Consider a Datalog program P, an atom A, and databases I and  $\mathcal{J}$ . If P entails A over I, and there is a homomorphism  $\mu$  from I to  $\mathcal{J}$ , then  $\mu(P)$  entails  $\mu(A)$  over  $\mathcal{J}$ .

(By  $\mu(P)$  and  $\mu(A)$  we mean the program/atom obtained by replacing constants in P and A, respectively, by their  $\mu$ -images.)

#### Proof (sketch):

- · Closure under homomorphism holds for conjunctive queries
- Single rule applications are like conjunctive queries
- We can show the claim for all  $T_{P,T}^i$  by induction on i

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## Capturing PTime in Datalog

How could we extend Datalog to capture all query mappings in P? → semipositive Datalog on an ordered domain

**Definition 13.2:** Semipositive Datalog, denoted Datalog<sup>⊥</sup>, extends Datalog by allowing negated EDB atoms in rule bodies.

Datalog (semipositive or not) with a successor ordering assumes that there are special EDB predicates succ (binary), first and last (unary) that characterise a total order on the active domain.

Semipositive Datalog with a total order corresponds to standard Datalog on an extended version of the given database:

- For each ground fact  $r(c_1, \ldots, c_n)$  with  $I \not\models r(c_1, \ldots, c_n)$ , add a new fact  $\bar{r}(c_1, \ldots, c_n)$  to I, using a new EDB predicate  $\bar{r}$
- Replace all uses of  $\neg r(t_1, \ldots, t_n)$  in P by  $\bar{r}(t_1, \ldots, t_n)$
- Define extensions for the EDB predicates succ, first and last to characterise some (arbitrary) total order on the active domain.

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## A PTime Capturing Result

**Theorem 13.3:** A Boolean query mapping defines a language in P if and only if it can be described by a query in semipositive Datalog with a successor ordering.

```
Example 13.4: We can express Connectivity for binary graphs as follows: 

Reachable(x, x) \leftarrow 

Reachable(x, y) \leftarrow Reachable(y, x) 

Reachable(x, z) \leftarrow Reachable(x, y) \wedge edge(y, z) 

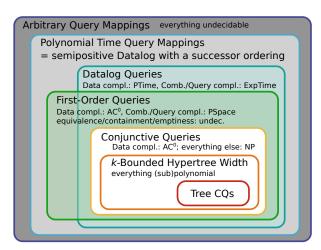
Connected(x) \leftarrow first(x) 

Connected(x) \leftarrow Connected(x) \wedge succ(x, y) \wedge Reachable(x, y) 

Accept() \leftarrow last(x) \wedge Connected(x)
```

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## The Big Picture



Note: languages that capture the same query mappings must have the same data complexity, but may differ in combined or in query complexity

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### Datalog Expressivity: Summary

The PTime capturing result is a powerful and exhaustive characterisation for semipositive Datalog with a successor ordering

Situation much less clear for other variants of Datalog (as of 2018):

- What exactly can we express in Datalog without EDB negation and/or successor ordering?
  - Does a weaker language suffice to capture PTime? → No!
  - When omitting negation, do we get query mappings closed under homomorphism?
     No!<sup>1</sup>
- How about query mappings in PTime that are closed under homomorphism?
  - Does plain Datalog capture these? → No!<sup>2</sup>
  - Does Datalog with successor ordering capture these? → No!<sup>3</sup>

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## **Datalog Containment**

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<sup>&</sup>lt;sup>1</sup>Counterexample on previous slide

<sup>&</sup>lt;sup>2</sup>[A. Dawar, S. Kreutzer, ICALP 2008]

<sup>&</sup>lt;sup>3</sup>[S. Rudolph, M. Thomazo, IJCAI 2016]: "We are somewhat baffled by this result: in order to express queries which satisfy the strongest notion of monotonicity, one cannot dispense with negation, the epitome of non-monotonicity."

## Datalog Implementation and Optimisation

How can Datalog query answering be implemented? How can Datalog queries be optimised?

Recall: static query optimisation

- Query equivalence
- Query emptiness
- Query containment

ightharpoonup all undecidable for FO queries, but decidable for (U)CQs

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### Checking Rule Entailment

The containment decision procedure for CQs suggests a procedure for single Datalog rules:

- Consider a Datalog program P and a rule  $H \leftarrow B_1 \wedge \ldots \wedge B_n$ .
- Define a database  $I_{B_1 \wedge ... \wedge B_n}$  as for CQs:
  - For every variable x in  $H \leftarrow B_1 \wedge ... \wedge B_n$ , we introduce a fresh constant  $c_x$ , not used anywhere yet
  - We define  $H^c$  to be the same as H but with each variable x replaced by  $c_x$ ; similarly we define  $B_i^c$  for each  $1 \le i \le n$
  - The database  $I_{B_1 \wedge ... \wedge B_n}$  contains exactly the facts  $B_i^c$   $(1 \leq i \leq n)$
- Now check if  $H^c \in T_P^{\infty}(\mathcal{I}_{B_1 \wedge ... \wedge B_n})$ :
  - If no, then there is a database on which  $H \leftarrow B_1 \wedge ... \wedge B_n$  produces an entailment that P does not produce.
  - If yes, then  $P \models H \leftarrow B_1 \land \ldots \land B_n$

## Learning from CQ Containment?

How did we manage to decide the question  $Q_1 \stackrel{?}{\sqsubseteq} Q_2$  for conjunctive queries  $Q_1$  and  $Q_2$ ?

#### Key ideas were:

- We want to know if all situations where  $Q_1$  matches are also matched by  $Q_2$ .
- We can simply view  $Q_1$  as a database  $I_{Q_1}$ : the most general database that  $Q_1$  can match to
- Containment  $Q_1 \stackrel{?}{\sqsubseteq} Q_2$  holds if  $Q_2$  matches the database  $I_{Q_1}$ .

→ decidable in NP

A CQ  $Q[x_1,\ldots,x_n]$  can be expressed as a Datalog query with a single rule  ${\sf Ans}(x_1,\ldots,x_n) \leftarrow Q$ 

→ Could we apply a similar technique to Datalog?

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### Example: Rule Entailment

Let P be the program

Ancestor
$$(x, y) \leftarrow \text{parent}(x, y)$$
  
Ancestor $(x, z) \leftarrow \text{parent}(x, y) \land \text{Ancestor}(y, z)$ 

and consider the rule  $Ancestor(x, z) \leftarrow parent(x, y) \land parent(y, z)$ .

Then  $I_{\mathsf{parent}(x,y) \land \mathsf{parent}(y,z)} = \{\mathsf{parent}(c_x,c_y), \mathsf{parent}(c_y,c_z)\}$  (abbreviate as I) We can compute  $T_P^\infty(I)$ :

$$\begin{split} T_P^0(I) &= I \\ T_P^1(I) &= \{\mathsf{Ancestor}(c_x, c_y), \mathsf{Ancestor}(c_y, c_z)\} \cup I \\ T_P^2(I) &= \{\mathsf{Ancestor}(c_x, c_z) \cup T_P^1(I) \\ T_P^3(I) &= T_P^2(I) = T_P^\infty(I) \end{split}$$

Therefore, Ancestor $(x, z)^c$  = Ancestor $(c_x, c_z) \in T_P^{\infty}(I)$ , so P entails Ancestor $(x, z) \leftarrow \text{parent}(x, y) \land \text{parent}(y, z)$ .

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## **Deciding Datalog Containment?**

Idea for two Datalog programs  $P_1$  and  $P_2$ :

- If  $P_2 \models P_1$ , then every entailment of  $P_1$  is also entailed by  $P_2$
- In particular, this means that  $P_1$  is contained in  $P_2$
- We have  $P_2 \models P_1$  if  $P_2 \models H \leftarrow B_1 \land \ldots \land B_n$  for every rule  $H \leftarrow B_1 \land \ldots \land B_n \in P_1$
- We can decide  $P_2 \models H \leftarrow B_1 \land \ldots \land B_n$ .

Can we decide Datalog containment this way?

→ No! In fact, Datalog containment is undecidable. What's wrong?

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## Datalog as Second-Order Logic

Datalog is a fragment of second-order logic:

IDB predicates are like variables that can take any set of tuples as value!

**Example 13.5:** The previous query  $\langle A, P_1 \rangle$  can be expressed by the formula

$$\forall \mathsf{A}. \left( \begin{array}{ccc} \forall x, y. \mathsf{A}(x,y) & \leftarrow \mathsf{parent}(x,y) & \land \\ \forall x, y, z. \mathsf{A}(x,z) & \leftarrow \mathsf{parent}(x,y) \land \mathsf{A}(y,z) \end{array} \right) \rightarrow \mathsf{A}(v,w)$$

- This is a formula with two free variables *v* and *w*.
  - → query with two result variables
- Intuitive semantics: "⟨c,d⟩ is a query result if A(c,d) holds for all possible values of A that satisfy the rules"
  - → Datalog semantics in other words

We can express any Datalog query like this, with one second-order variable per IDB predicate.

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### Implication Entailment vs. Datalog Entailment

$$P_1: \qquad \qquad P_2: \\ \mathsf{A}(x,y) \leftarrow \mathsf{parent}(x,y) \qquad \qquad \mathsf{B}(x,y) \leftarrow \mathsf{parent}(x,y) \\ \mathsf{A}(x,z) \leftarrow \mathsf{parent}(x,y) \land \mathsf{A}(y,z) \qquad \qquad \mathsf{B}(x,z) \leftarrow \mathsf{parent}(x,y) \land \mathsf{B}(y,z)$$

Consider the Datalog queries  $\langle A, P_1 \rangle$  and  $\langle B, P_2 \rangle$ :

- Clearly,  $\langle A, P_1 \rangle$  and  $\langle B, P_2 \rangle$  are equivalent (and mutually contained in each other).
- However,  $P_2$  entails no rule of  $P_1$  and  $P_1$  entails no rule of  $P_2$ .

 $\sim$  IDB predicates do not matter in Datalog, but predicate names matter in first-order implications

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### First-Order vs. Second-Order Logic

A Datalog program looks like a set of first-order implications, but it has a second-order semantics

We have already seen that Datalog can express things that are impossible to express in FO queries – that's why we introduced it!<sup>1</sup>

Consequences for query optimisation:

- Entailment between sets of first-order implications is decidable (shown above)
- Containment between Datalog gueries is not decidable (shown next)

<sup>&</sup>lt;sup>1</sup>Possible confusion when comparing of FO and Datalog: entailments of first-order implications agree with answers of Datalog queries, so it seems we can break the FO locality restrictions; but query answering is model checking not entailment; FO model checking is much weaker than second-order model checking

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### Undecidability of Datalog Query Containment

A classical undecidable problem:

#### **Post Correspondence Problem:**

- Input: two lists of words  $\alpha_1, \ldots, \alpha_n$  and  $\beta_1, \ldots, \beta_n$
- Output: "yes" if there is a sequence of indices  $i_1, i_2, i_3, \ldots, i_m$  such that  $\alpha_{i_1}\alpha_{i_2}\alpha_{i_3}\cdots\alpha_{i_m}=\beta_{i_1}\beta_{i_2}\beta_{i_3}\cdots\beta_{i_m}$ .

→ we will reduce PCP to Datalog containment

We need to define Datalog programs that work on databases that encode words:

- We represent words by chains of binary predicates
- Binary EDB predicates represent letters
- For each letter  $\sigma$ , we use a binary EDB predicate letter[ $\sigma$ ]
- We assume that the words  $\alpha_i$  have the form  $a_1^i\cdots a_{|\alpha_i|}^i$ , and that the words  $\beta_i$  have the form  $b_1^i\cdots b_{|\beta_i|}^i$

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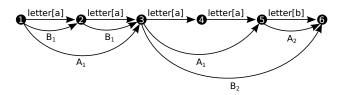
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## Solving PCP with Datalog Containment (2)

**Example:**  $\alpha_1 = aa, \, \beta_1 = a, \, \alpha_2 = b, \, \beta_2 = aab$ 

Example for an indented database and least model (selected parts):



Additional IDB facts that are derived (among others):

### Solving PCP with Datalog Containment

A program  $P_1$  to recognise potential PCP solutions.

Rules to recognise words  $\alpha_i$  and  $\beta_i$  for every  $i \in \{1, ..., m\}$ :

$$\begin{aligned} &\mathsf{A}_i(x_0,x_{|\alpha_i|}) \leftarrow \mathsf{letter}[a_1^i](x_0,x_1) \wedge \ldots \wedge \mathsf{letter}[a_{|\alpha_i|}^i](x_{|\alpha_i|-1},x_{|\alpha_i|}) \\ &\mathsf{B}_i(x_0,x_{|\beta_i|}) \leftarrow \mathsf{letter}[b_1^i](x_0,x_1) \wedge \ldots \wedge \mathsf{letter}[b_{|\beta_i|}^i](x_{|\beta_i|-1},x_{|\beta_i|}) \end{aligned}$$

Rules to check for synchronised chains (for all  $i \in \{1, ..., m\}$ ):

$$\begin{aligned} \mathsf{PCP}(x,y_1,y_2) &\leftarrow A_i(x,y_1) \land B_i(x,y_2) \\ \mathsf{PCP}(x,z_1,z_2) &\leftarrow \mathsf{PCP}(x,y_1,y_2) \land A_i(y_1,z_1) \land B_i(y_2,z_2) \\ \mathsf{Accept}() &\leftarrow \mathsf{PCP}(x,z,z) \end{aligned}$$

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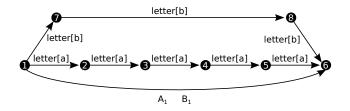
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## Solving PCP with Datalog Containment (3)

**Example:**  $\alpha_1 = aaaaa, \beta_1 = bbb$ 

**Problem:** P<sub>1</sub> also accepts some unintended cases



Additional IDB facts that are derived:

PCP(1, 6, 6) Accept()

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### Solving PCP with Datalog Containment (4)

**Solution:** specify a program  $P_2$  that recognises all unwanted cases

 $P_2$  consists of the following rules (for all letters  $\sigma, \sigma'$ ):

$$\begin{split} & \mathsf{EP}(x,x) \leftarrow \\ & \mathsf{EP}(y_1,y_2) \leftarrow \mathsf{EP}(x_1,x_2) \land \mathsf{letter}[\sigma](x_1,y_1) \land \mathsf{letter}[\sigma](x_2,y_2) \\ & \mathsf{Accept}() \leftarrow \mathsf{EP}(x_1,x_2) \land \mathsf{letter}[\sigma](x_1,y_1) \land \mathsf{letter}[\sigma'](x_2,y_2) \\ & \mathsf{NEP}(x_1,y_2) \leftarrow \mathsf{EP}(x_1,x_2) \land \mathsf{letter}[\sigma](x_2,y_2) \\ & \mathsf{NEP}(x_1,y_2) \leftarrow \mathsf{NEP}(x_1,x_2) \land \mathsf{letter}[\sigma](x_2,y_2) \\ & \mathsf{Accept}() \leftarrow \mathsf{NEP}(x,x) \end{split}$$

#### Intuition:

- EP defines equal paths (forwards, from one starting point)
- NEP defines paths of different length (from one starting point to the same end point)

 $\rightarrow$   $P_2$  accepts all databases with distinct parallel paths

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### Summary and Outlook

Datalog cannot express all query mappings in P ...

... but semipositive Datalog with a successor ordering can

First-order rule entailment is decidable . . .

... but Datalog containment is not.

#### **Next question:**

· How can we implement Datalog in practice?

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### Solving PCP with Datalog Containment (5)

What does it mean if  $\langle Accept, P_1 \rangle$  is contained in  $\langle Accept, P_2 \rangle$ ?

The following are equivalent:

- All databases with potential PCP solutions also have distinct parallel paths.
- Databases without distinct parallel paths have no PCP solutions.
- Linear databases (words) have no PCP solutions.
- The answer to the PCP is "no".

ightarrow If we could decide Datalog containment, we could decide PCP

Theorem 13.6: Containment and equivalence of Datalog queries are undecidable.

(Note that emptiness of Datalog queries is trivial)

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