

DATABASE THEORY

Lecture 13: Datalog Expressivity and Containment

Markus Krötzsch Knowledge-Based Systems

TU Dresden, 2 June 2025

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/e

Review: Datalog

A rule-based recursive query language

```
\begin{aligned} & \text{father(alice, bob)} \\ & \text{mother(alice, 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?

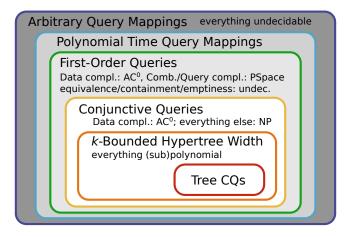
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Expressivity

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The Big Picture

Where does Datalog fit in this picture?



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Expressivity of Datalog

Datalog is P-complete for data complexity:

- ullet 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.

→ So Datalog can solve all polynomial problems?

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 database I that can be computed in logarithmic space.
- → 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?
- CONNECTIVITY: Is the input database a connected graph?
- Is the input database a chain (or linear order)?
- ...

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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 μ 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 μ -images.)

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Proof (sketch):

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

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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

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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., $\neg p(a)$)

• ...

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Limits of Datalog Expressiveness

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 - Parity cannot be expressed
 - Connectivity cannot be expressed
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 - ...

However this criterion is not sufficient!

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

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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[⊥], 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 an (arbitrary) total order on the active domain.

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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 a query in semipositive Datalog with a successor ordering.

^aWhere "described by" means that there is a program that decides the BCQ for every database and every choice of successor ordering.

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A PTime Capturing Result

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^aWhere "described by" means that there is a program that decides the BCQ for every database and every choice of successor ordering.

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

```
\begin{aligned} & \mathsf{Reachable}(x,x) \leftarrow \\ & \mathsf{Reachable}(x,y) \leftarrow \mathsf{Reachable}(y,x) \\ & \mathsf{Reachable}(x,z) \leftarrow \mathsf{Reachable}(x,y) \land \mathsf{edge}(y,z) \\ & \mathsf{Connected}(x) \leftarrow \mathsf{first}(x) \\ & \mathsf{Connected}(y) \leftarrow \mathsf{Connected}(x) \land \mathsf{succ}(x,y) \land \mathsf{Reachable}(x,y) \\ & \mathsf{Accept}() \leftarrow \mathsf{last}(x) \land \mathsf{Connected}(x) \end{aligned}
```

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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 2025):

- 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!¹ (but they are closed under bijective homomorphisms)
- How about query mappings in PTime that are closed under homomorphism?
 - Does plain Datalog capture these? → No!²
 - Does Datalog with successor ordering capture these? → No!³

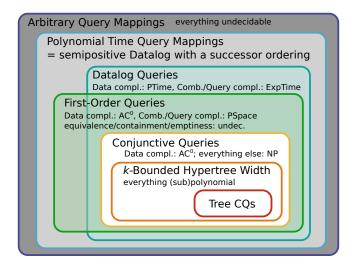
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¹Counterexample on previous slide

²[A. Dawar, S. Kreutzer, ICALP 2008]

³[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."

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 Containment

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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

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

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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 \mathcal{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

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Learning from CQ Containment?

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→ decidable in NP

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

→ Could we apply a similar technique to Datalog?

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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 $H \leftarrow B_1 \wedge ... \wedge B_n$.
- Define a database $I_{B_1 \wedge ... \wedge B_n}$ as for CQs:
 - − For every variable x in $H \leftarrow B_1 \land ... \land B_n$, 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 $H \leftarrow B_1 \land ... \land B_n$ produces an entailment that P does not produce.
 - If yes, then $P \models H \leftarrow B_1 \land \ldots \land B_n$

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

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Let *P* be the program

```
Ancestor(x, y) \leftarrow \text{parent}(x, y)
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Then $I_{parent(x,y) \land parent(y,z)} = \{parent(c_x, c_y), parent(c_y, c_z)\}$ (abbreviate as I)

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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 $I_P^\infty(I)$:

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

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Let P be the program

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

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Therefore, Ancestor $(x,z)^c = \text{Ancestor}(c_x,c_z) \in T_P^{\infty}(I)$, 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?

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Can we decide Datalog containment this way?

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

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Implication Entailment vs. Datalog Entailment

$$\begin{aligned} P_1: & P_2: \\ \mathsf{A}(x,y) \leftarrow \mathsf{parent}(x,y) & \mathsf{B}(x,y) \leftarrow \mathsf{parent}(x,y) \\ \mathsf{A}(x,z) \leftarrow \mathsf{parent}(x,y) \land \mathsf{A}(y,z) & \mathsf{B}(x,z) \leftarrow \mathsf{parent}(x,y) \land \mathsf{B}(y,z) \end{aligned}$$

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

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Implication Entailment vs. Datalog Entailment

```
P_1: P_2:  \mathsf{A}(x,y) \leftarrow \mathsf{parent}(x,y) \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 \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 .

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Implication Entailment vs. Datalog Entailment

$$\begin{aligned} P_1: & P_2: \\ A(x,y) \leftarrow \mathsf{parent}(x,y) & \mathsf{B}(x,y) \leftarrow \mathsf{parent}(x,y) \\ A(x,z) \leftarrow \mathsf{parent}(x,y) \land \mathsf{A}(y,z) & \mathsf{B}(x,z) \leftarrow \mathsf{parent}(x,y) \land \mathsf{B}(y,z) \end{aligned}$$

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

- Clearly, \(\lambda , P_1 \rangle \) and \(\lambda B, P_2 \rangle \) 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 .

→ IDB predicates do not matter in Datalog, but predicate names matter in first-order implications

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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!

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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

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

- This is a formula with two free variables v and w.
 - → query with two result variables
- Intuitive semantics: " $\langle c,d \rangle$ 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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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!¹

Consequences for query optimisation:

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

¹Possible 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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slide 20 of 27

Undecidability of Datalog Query Containment

A classical undecidable problem:

Post Correspondence Problem:

- Input: two lists of words $\alpha_1, \ldots, \alpha_n$ and β_1, \ldots, β_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 σ , we use a binary EDB predicate letter[σ]
- We assume that the words α_i have the form $a_1^i\cdots a_{|\alpha_i|}^i$, and that the words β_i have the form $b_1^i\cdots b_{|\beta_i|}^i$

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Solving PCP with Datalog Containment

A program P_1 to recognise potential PCP solutions.

Rules to recognise words α_i and β_i for every $i \in \{1, ..., n\}$:

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

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

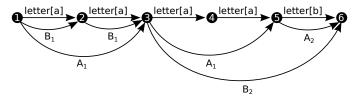
$$\begin{aligned} \mathsf{PCP}(x,y_1,y_2) &\leftarrow A_i(x,y_1) \land B_i(x,y_2) \\ \mathsf{PCP}(x,z_1,z_2) &\leftarrow \mathsf{PCP}(x,y_1,y_2) \land A_i(y_1,z_1) \land B_i(y_2,z_2) \\ \mathsf{Accept}() &\leftarrow \mathsf{PCP}(x,z,z) \end{aligned}$$

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Solving PCP with Datalog Containment (2)

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

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



Additional IDB facts that are derived (among others):

$$PCP(1,3,2)$$
 $PCP(1,5,3)$ $PCP(1,6,6)$ Accept()

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Solving PCP with Datalog Containment (3)

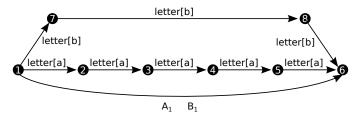
Example: $\alpha_1 = aaaaa, \beta_1 = bbb$

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Solving PCP with Datalog Containment (3)

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

Problem: P_1 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 σ, σ'):

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

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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Solving PCP with Datalog Containment (5)

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

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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".

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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".

→ 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 easy to decide in polynomial time)

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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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