Overview

1. Introduction | Relational data model
2. First-order queries
3. Complexity of query answering
4. Complexity of FO query answering
5. Conjunctive queries
6. Tree-like conjunctive queries
7. Query optimisation
8. Conjunctive Query Optimisation / First-Order Expressiveness
9. First-Order Expressiveness / Introduction to Datalog
10. Expressive Power and Complexity of Datalog
11. Implementation techniques for Datalog
12. Path queries
13. Constraints
14. Outlook: database theory in practice

See course homepage [⇒ link] for more information and materials
Review: EF Games

Ehrenfeucht-Fraïssé games characterise expressivity of FO formulas:

- the quantifier rank needed to distinguish structure corresponds to
- the number of rounds needed by Spoiler to win the game
How to show that a query mapping $M$ can not be FO-defined:

- Let $C_M$ be the class of all databases recognised by $M$
- Find sequences of databases $I_1, I_2, I_3, \ldots \in C_M$ and databases $J_1, J_2, J_3, \ldots \notin C_M$, such that $I_i \sim J_i$

$\sim$ for any formula $\varphi$ (however large its quantifier rank $r$), there is a counterexample $I_r \in C_M$ and $J_r \notin C_M$ that $\varphi$ cannot distinguish

Problems:

- How to find such sequences of $I_i$ and $J_i$?
  $\sim$ No general strategy exists
- Given suitable sequences, how to show that $I_i \sim J_i$?
  $\sim$ Can be difficult, but doable for some special cases
Expressiveness on Linear Orders

Let’s look at some very simple structures:

**Definition**
A structure $\mathcal{I}$ is a **linear order** if it has a single binary predicate $\leq$ interpreted as a total, transitive, reflexive and asymmetric relation.

**Example:**

$L_6 : 1 \leq 2 \leq 3 \leq 4 \leq 5 \leq 6$

$L_7 : 1 \leq 2 \leq 3 \leq 4 \leq 5 \leq 6 \leq 7$

Spoiler can win the 3-round EF game:

**Spoiler** plays 4 in $L_7$

- **Duplicator** plays 4 in $L_6$: **Spoiler** plays 6 in $L_7$
  - **Duplicator** plays 5 in $L_6$: **Spoiler** plays 5 in $L_7$ and wins
  - **Duplicator** plays 6 in $L_6$: **Spoiler** plays 7 in $L_7$ and wins
- **Duplicator** plays 3 in $L_6$: symmetric game (flipped horizontally)
Expressiveness on Linear Orders

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**Definition**

A structure $\mathcal{I}$ is a **linear order** if it has a single binary predicate $\leq$ interpreted as a total, transitive, reflexive and asymmetric relation.

**Example:**

$L_7 : 1 \leq 2 \leq 3 \leq 4 \leq 5 \leq 6 \leq 7$

$L_8 : 1 \leq 2 \leq 3 \leq 4 \leq 5 \leq 6 \leq 7 \leq 8$

**Spoiler cannot win the 3-round EF game:**

*Spoiler* plays 4 in $L_8$: *Duplicator* plays 4 in $L_7$
*Spoiler* plays 6 in $L_8$: *Duplicator* plays 6 in $L_7$; spoiler cannot win
*Spoiler* plays 7 in $L_8$: *Duplicator* plays 6 in $L_7$; spoiler cannot win

Other cases similar: Spoiler never wins
Theorem

The following are equivalent:

• \( L_m \sim_r L_n \)
• either (1) \( m = n \), or (2) \( m \geq 2^r - 1 \) and \( n \geq 2^r - 1 \)

Proof: see board
FO-Definability of Parity

**Theorem**

Parity is not FO-definable for linear orders, hence it is not FO-definable for arbitrary databases.

**Proof:**

- Suppose for a contradiction that Parity is FO-definable by some query $\varphi$.
- Let $r$ be the quantifier rank of $\varphi$.
- Consider databases $L_m$ and $L_n$ with $m = 2^r$ and $n = 2^r + 1$.
- We know that $L_m \sim_r L_n$, and therefore $L_m \equiv_r L_n$.
- Hence, $L_m \models \varphi$ if and only if $L_n \models \varphi$.
- But $L_m \in \text{Parity}$ while $L_n \notin \text{Parity}$.
- Therefore, $\varphi$ does not FO-define Parity. Contradiction.
FO-Definability of Connectivity

The Connectivity problem over finite graphs is as follows:

- **Input:** A finite graph (relational structure with one binary relation “edge”)
- **Output:** “true” if there is an (undirected) path between any pair of vertices

**Theorem**

Connectivity is not FO-definable.

**Proof:**

- Suppose for a contradiction that Connectivity is FO-definable using a query $\varphi$.
- We show that this would make Parity FO-definable on linear orders.
- For a linear order $L$ with order predicate $\leq$, we define a finite graph $G(L)$ over a binary predicate “edge” such that $G(L)$ is connected if and only if $L$ has an even number of elements.
Defining a Graph From a Linear Order

We use abbreviations for the following FO formulas:

\[\text{succ}[x, y] = (x \leq y) \land \neg(y \leq x) \land \forall z.(z \leq x \lor y \leq z)\]

\[\text{min}[x] = \forall z.x \leq z\]

\[\text{max}[x] = \forall z.z \leq x\]

\[\text{succ}^\circ[x, y] = \text{succ}[x, y] \lor (\text{max}[x] \land \text{min}[y])\]

We now define the formula \(\psi\) that derives edges from a linear order:

\[\forall x, y. \text{edge}(x, y) \iff \exists z. \text{succ}^\circ[x, z] \land \text{succ}^\circ[z, y]\]
Illustration: Graphs From Linear Orders

Markus Krötzsch, 15 June 2015
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Observation:
The graph $\mathcal{G}(\mathcal{L})$ is connected if and only if $\mathcal{L}$ has odd parity.

Therefore, if $\varphi$ FO-defines $\text{Connectivity}$ on graphs with predicate edge, then $\neg(\varphi \land \psi)$ FO-defines $\text{Parity}$ on linear orders.

Since $\text{Parity}$ is not FO-definable, no such $\varphi$ can exist.
Beyond Linear Orders: Locality

Intuition: Duplicator can win an EF game if selected nodes have the same “neighbourhood”

\[ \sim \text{let’s define this for graphs (structures with binary predicates)} \]

**Definition**

Consider a graph \( G \). For a natural number \( d \geq 0 \) and a vertex \( v \), the \( d \)-neighbourhood of \( v \), \( N(v, d) \), is defined inductively:

- \( N(v, 0) = \{v\} \)
- \( N(v, d + 1) = N(v, d) \cup \{w \mid w \text{ is a direct neighbour of some } w' \in N(v, d)\} \)

Two vertices \( v \) and \( w \) have the same \( d \)-type if the subgraphs \( G|_{N(v,d)} \) and \( G|_{N(w,d)} \) are isomorphic.

Two graphs are \( d \)-equivalent if, for every \( d \)-type, they have the same number of \( d \)-neighbourhoods of this type.
Locality and FO-definability

A special case of Gaifman’s Locality Theorem of first-order logic:

**Theorem**

For every integer $r \geq 1$:

- if $G_1$ is $3^{r-1}$-equivalent to $G_2$
- then $G_1 \sim_r G_2$, and thus $G_1 \equiv_r G_2$

$\sim$ Intuition: FO can only express local properties

How to show that a query mapping $M$ can not be FO-defined:

- Let $C_M$ be the class of all databases recognised by $M$
- Find sequences of graphs $I_1, I_2, I_3, \ldots \in C_M$ and graphs $J_1, J_2, J_3, \ldots \notin C_M$, such that $I_i$ is $i$-equivalent to $J_i$

$\sim$ for any formula $\varphi$ (however large its quantifier rank $r$), there is a counterexample $I_{3^{r-1}} \in C_M$ and $J_{3^{r-1}} \notin C_M$ that $\varphi$ cannot distinguish
Connectivity is not FO-definable (Proof 2)

**Theorem**

Connectivity is not FO-definable.

Proof: counterexample for quantifier rank $r$: set $d = 3^r$

- the only $d$-type is a path of $2d + 1$ nodes
- $\mathcal{I}_d$ and $\mathcal{J}_d$ are $d$-equivalent
2-COLOURABILITY

Theorem

2-COLOURABILITY is not FO-definable.

Proof: counterexample for quantifier rank $r$: set $d = 3^r$ (odd number)

- the only $d$-type is a path of $2d + 1$ nodes
- $I_d$ and $J_d$ are $d$-equivalent
Acyclicity

Theorem

Acyclicity is not FO-definable.

Proof: counterexample for quantifier rank $r$: set $d = 3^r$

- $d$-types are paths of $\leq 2d + 1$ nodes
- $I_d$ and $J_d$ are $d$-equivalent
Summary: Limits of FO-Queries

FO queries (and hence Relational Calculus) cannot express properties that require a “global” view:
  • properties where one needs to follow paths
  • properties where one needs to count elements

Remember Lecture 1?

“Stops at distance 2 from Helmholtzstr.”

\[ R_2 = \delta_{\text{To}\rightarrow \text{From}}(\pi_{\text{To}}(\text{Connect} \bowtie R_1)) \]

What about all stops reachable from Helmholtzstr.?
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Remember Lecture 1?

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What about all stops reachable from Helmholtzstr.?

\[ \not\exists \]

Not expressible in Relational Calculus

Yet, all examples we saw are in \( P \)

\[ \not\exists \]

Is there another query language that could help us?
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: 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 $R(t_1, \ldots, t_n)$ with $R$ a predicate symbol (or relation) of arity $n$, and $t_1, \ldots, t_n$ terms.

**Definition**

A Datalog rule is an expression of the form:

$$H ← B_1 ∧ \ldots ∧ B_m$$

where $H$ and $B_1, \ldots, B_m$ are atoms. $H$ is called the head or conclusion; $B_1 ∧ \ldots ∧ B_m$ 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.
father(alice, bob)
mother(alice, carla)
mother(evan, carla)
father(carla, david)

\[
\text{Parent}(x, y) \leftarrow \text{father}(x, y)
\]

\[
\text{Parent}(x, y) \leftarrow \text{mother}(x, y)
\]

\[
\text{Ancestor}(x, y) \leftarrow \text{Parent}(x, y)
\]

\[
\text{Ancestor}(x, z) \leftarrow \text{Parent}(x, y) \land \text{Ancestor}(y, z)
\]

SameGeneration(x, x)

SameGeneration(x, y) \leftarrow \text{Parent}(x, v) \land \text{Parent}(y, w) \land \text{SameGeneration}(v, w)
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 $U$

- Variables can represent arbitrary constants from this set
  $\sim$ ground substitutions map variables to constants

- A rule can be applied if its body is satisfied for some ground substitution
  Example: rule $\text{Parent}(x, y) \leftarrow \text{mother}(x, y)$ can be applied to
  $\text{mother}(\text{alice}, \text{carla})$ under substitution $\{x \mapsto \text{alice}, y \mapsto \text{carla}\}$

- If a rule is applicable under some ground substitution, then
  the according instance of the rule head is entailed.
An inductive definition of what can be derived:

**Definition**

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 $H \leftarrow B_1 \land \ldots \land B_n$ and a ground substitution $\theta$ 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
We can think of deductions as tree structures:

\[
\begin{align*}
&\text{Ancestor}(\text{alice}, \text{david}) \\
&\text{Parent}(\text{alice}, \text{carla}) \\
&\quad \text{mother}(\text{alice}, \text{carla}) \\
&\quad \quad \text{father}(\text{alice}, \text{bob}) \\
&\quad \quad \text{mother}(\text{alice}, \text{carla}) \\
&\quad \quad \quad \text{mother}(\text{evan}, \text{carla}) \\
&\quad \quad \quad \text{father}(\text{carla}, \text{david}) \\
&\quad \quad \quad \quad \text{Parent}(x, y) \leftarrow \text{father}(x, y) \\
&\quad \quad \quad \quad \text{Parent}(x, y) \leftarrow \text{mother}(x, y) \\
&\quad \quad \quad \quad \text{Ancestor}(x, y) \leftarrow \text{Parent}(x, y) \\
&\quad \quad \quad \quad \text{Ancestor}(x, z) \leftarrow \text{Parent}(x, y) \land \text{Ancestor}(y, z) \\
&\quad \quad \quad \text{Parent}(\text{carla}, \text{david}) \\
&\quad \quad \quad \quad \text{father}(\text{carla}, \text{david})
\end{align*}
\]
Instead of using substitutions, we can also ground programs:

**Definition**

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 \(T_P(I)\):

- \(T_P(I) = \{ H \mid H \leftarrow B_1 \land \ldots \land B_n \in \text{ground}(P) \text{ and } B_1, \ldots, B_n \in I \}\)
- 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 \(A \in T_P^\infty\)
We can also read Datalog rules as universally quantified implications.

Example: \( \text{Ancestor}(x, z) \leftarrow \text{Parent}(x, y) \land \text{Ancestor}(y, z) \) corresponds to implication

\[ \forall x, y, z. \text{Parent}(x, y) \land \text{Ancestor}(y, z) \rightarrow \text{Ancestor}(x, z). \]

A set of FO implications may have many models.
\( \sim \) consider least model over the domain defined by the universe.

**Theorem**

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.

\( \sim \) similar to active domain semantics in databases
Datalog as a Query Language

How can we use Datalog to query databases?

1. View database as set of ground facts
2. Specify which predicate yields the query result

**Definition**

A Datalog query is a pair \( \langle R, P \rangle \), where \( P \) is a Datalog program and \( R \) is the answer predicate.

Results of the query: \( R \)-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
Datalog as a Generalisation of CQs

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

\[
\text{Ans}(x_1, \ldots, x_n) \leftarrow A_1 \land \ldots \land A_\ell
\]

Unions of CQs can also be expressed (exercise)

Intuition: Datalog generalises UCQs with recursion

Open questions:

- How hard is it to answer Datalog queries?
- Can Datalog express all queries in \( \mathbb{P} \)?
- What about query containment and equivalence?
Summary and Outlook

FO-queries can only express “local” properties

Possible proof techniques:
  • Ehrenfeucht-Fraïssé Games
  • Locality Theorems
  • For more approaches see Chapter 17 of [Abiteboul, Hull, Vianu 1994]

Datalog can overcome some of these limitations

Next topics:
  • Complexity and expressive power of Datalog
  • Implementation techniques for Datalog