Knowledge Bases and Databases
Part 1: First-Order Queries

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A.Y. 2007/2008

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Overview of Part 1: First-order queries

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Chapter I

First-Order Logic

Outline

1. Syntax of first-order logic

2. Semantics of first-order logic

3. First-order logic queries

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First-order logic

- First-order logic (FOL) is the logic to speak about objects, which are the domain of discourse or universe.

- FOL is concerned about properties of these objects and relations over objects (resp., unary and n-ary predicates).

- FOL also has functions including constants that denote objects.

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FOL syntax – Terms

We first introduce:

- A set $Vars = \{x_1, \ldots, x_n\}$ of individual variables (i.e., variables that denote single objects).
- A set of functions symbols, each of given arity ≥ 0. Functions of arity 0 are called constants.

Def.: The set of *Terms* is defined inductively as follows:

- $Vars \subseteq Terms$;
- If $t_1, \ldots, t_k \in Terms$ and f^k is a k-ary function symbol, then $f^k(t_1, \ldots, t_k) \in Terms$;
- Nothing else is in *Terms*.

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FOL syntax – Formulas

Def.: The set of *Formulas* is defined inductively as follows:

- If $t_1, \ldots, t_k \in Terms$ and P^k is a k-ary predicate, then $P^k(t_1, \ldots, t_k) \in Formulas$ (atomic formulas).
- If $t_1, t_2 \in Terms$, then $t_1 = t_2 \in Formulas$.
- If $\varphi \in Formulas$ and $\psi \in Formulas$ then
    - $\neg\varphi \in Formulas$
    - $\varphi \wedge \psi \in Formulas$
    - $\varphi \vee \psi \in Formulas$
    - $\varphi \rightarrow \psi \in Formulas$
- If $\varphi \in Formulas$ and $x \in Vars$ then
    - $\exists x.\varphi \in Formulas$
    - $\forall x.\varphi \in Formulas$
- Nothing else is in *Formulas*.

Note: a predicate of arity 0 is a proposition of propositional logic.

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Interpretations

Given an alphabet of predicates $P_1, P_2, \ldots$ and functions $f_1, f_2, \ldots$, each with an associated arity, a FOL interpretation is:

$$\mathcal{I} = (\Delta^{\mathcal{I}}, P_1^{\mathcal{I}}, P_2^{\mathcal{I}}, \ldots, f_1^{\mathcal{I}}, f_2^{\mathcal{I}}, \ldots)$$

where:

- $\Delta^{\mathcal{I}}$ is the domain (a set of objects)
- if P_i is a k-ary predicate, then $P_i^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}} \times \cdots \times \Delta^{\mathcal{I}}$ (k times)
- if f_i is a k-ary function, then $f_i^{\mathcal{I}} : \Delta^{\mathcal{I}} \times \cdots \times \Delta^{\mathcal{I}} \longrightarrow \Delta^{\mathcal{I}}$ (k times)
- if f_i is a constant (i.e., a 0-ary function), then $f_i^{\mathcal{I}} : () \longrightarrow \Delta^{\mathcal{I}}$ (i.e., f_i denotes exactly one object of the domain)

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Assignment

Let *Vars* be a set of (individual) variables.

> **Def.:** Given an interpretation $\mathcal{I}$, an assignment is a function
>
> $$\alpha : Vars \longrightarrow \Delta^{\mathcal{I}}$$
>
> that assigns to each variable $x \in Vars$ an object $\alpha(x) \in \Delta^{\mathcal{I}}$.

It is convenient to extend the notion of assignment to terms. We can do so by defining a function $\hat{\alpha} : Terms \longrightarrow \Delta^{\mathcal{I}}$ inductively as follows:

- $\hat{\alpha}(x) = \alpha(x)$, if $x \in Vars$
- $\hat{\alpha}(f(t_1, \ldots, t_k)) = f^{\mathcal{I}}(\hat{\alpha}(t_1), \ldots, \hat{\alpha}(t_k))$

Note: for constants $\hat{\alpha}(c) = c^{\mathcal{I}}$.

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Truth in an interpretation wrt an assignment

We define when a FOL formula φ is true in an interpretation $\mathcal{I}$ wrt an assignment α, written $\mathcal{I}, \alpha \models \varphi$:

- $\mathcal{I}, \alpha \models P(t_1, \ldots, t_k)$ if $(\hat{\alpha}(t_1), \ldots, \hat{\alpha}(t_k)) \in P^{\mathcal{I}}$
- $\mathcal{I}, \alpha \models t_1 = t_2$ if $\hat{\alpha}(t_1) = \hat{\alpha}(t_2)$
- $\mathcal{I}, \alpha \models \neg\varphi$ if $\mathcal{I}, \alpha \not\models \varphi$
- $\mathcal{I}, \alpha \models \varphi \wedge \psi$ if $\mathcal{I}, \alpha \models \varphi$ and $\mathcal{I}, \alpha \models \psi$
- $\mathcal{I}, \alpha \models \varphi \vee \psi$ if $\mathcal{I}, \alpha \models \varphi$ or $\mathcal{I}, \alpha \models \psi$
- $\mathcal{I}, \alpha \models \varphi \rightarrow \psi$ if $\mathcal{I}, \alpha \models \varphi$ implies $\mathcal{I}, \alpha \models \psi$
- $\mathcal{I}, \alpha \models \exists x.\varphi$ if for some $a \in \Delta^{\mathcal{I}}$ we have $\mathcal{I}, \alpha[x \mapsto a] \models \varphi$
- $\mathcal{I}, \alpha \models \forall x.\varphi$ if for every $a \in \Delta^{\mathcal{I}}$ we have $\mathcal{I}, \alpha[x \mapsto a] \models \varphi$

Here, $\alpha[x \mapsto a]$ stands for the new assignment obtained from α as follows:

$$\alpha[x \mapsto a](x) = a$$
$$\alpha[x \mapsto a](y) = \alpha(y) \quad \text{for } y \neq x$$

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Open vs. closed formulas

Definitions

- A variable x in a formula φ is free if x does not occur in the scope of any quantifier, otherwise it is bounded.
- An open formula is a formula that has some free variable.
- A closed formula, also called sentence, is a formula that has no free variables.

For closed formulas (but not for open formulas) we can define what it means to be true in an interpretation, written $\mathcal{I} \models \varphi$, without mentioning the assignment, since the assignment α does not play any role in verifying $\mathcal{I}, \alpha \models \varphi$.

Instead, open formulas are strongly related to queries — cf. relational databases.

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FOL queries

Def.: A FOL query is an (open) FOL formula.

When φ is a FOL query with free variables $(x_1, \ldots, x_k)$, then we sometimes write it as $\varphi(x_1, \ldots, x_k)$, and say that φ has arity k.

Given an interpretation $\mathcal{I}$, we are interested in those assignments that map the variables $x_1, \ldots, x_k$ (and only those). We write an assignment α s.t. $\alpha(x_i) = a_i$, for $i = 1, \ldots, k$, as $\langle a_1, \ldots, a_k \rangle$.

Def.: Given an interpretation $\mathcal{I}$, the answer to a query $\varphi(x_1, \ldots, x_k)$ is

$$\varphi(x_1, \ldots, x_k)^{\mathcal{I}} = \{(a_1, \ldots, a_k) \mid \mathcal{I}, \langle a_1, \ldots, a_k \rangle \models \varphi(x_1, \ldots, x_k)\}$$

Note: We will also use the notation $\varphi^{\mathcal{I}}$, which keeps the free variables implicit, and $\varphi(\mathcal{I})$ making apparent that φ becomes a functions from interpretations to set of tuples.

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FOL boolean queries

Def.: A FOL boolean query is a FOL query without free variables.

Hence, the answer to a boolean query $\varphi()$ is defined as follows:

$$\varphi()^{\mathcal{I}} = \{() \mid \mathcal{I}, \langle \rangle \models \varphi()\}$$

Such an answer is

- $()$, if $\mathcal{I} \models \varphi$
- $\emptyset$, if $\mathcal{I} \not\models \varphi$.

As an obvious convention we read $()$ as "true" and $\emptyset$ as "false".

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FOL formulas: logical tasks

Definitions

- **Validity**: φ is **valid** iff for all $\mathcal{I}$ and α we have that $\mathcal{I}, \alpha \models \varphi$.

- **Satisfiability**: φ is **satisfiable** iff there exists an $\mathcal{I}$ and α such that $\mathcal{I}, \alpha \models \varphi$, and **unsatisfiable** otherwise.

- **Logical implication**: φ **logically implies** ψ, written $\varphi \models \psi$ iff for all $\mathcal{I}$ and α, if $\mathcal{I}, \alpha \models \varphi$ then $\mathcal{I}, \alpha \models \psi$.

- **Logical equivalence**: φ is **logically equivalent** to ψ, iff for all $\mathcal{I}$ and α, we have that $\mathcal{I}, \alpha \models \varphi$ iff $\mathcal{I}, \alpha \models \psi$ (i.e., $\varphi \models \psi$ and $\psi \models \varphi$).

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FOL queries – Logical tasks

- **Validity**: if φ is valid, then $\varphi^{\mathcal{I}} = \Delta^{\mathcal{I}} \times \cdots \times \Delta^{\mathcal{I}}$ for all $\mathcal{I}$, i.e., the query always returns all the tuples of $\mathcal{I}$.

- **Satisfiability**: if φ is satisfiable, then $\varphi^{\mathcal{I}} \neq \emptyset$ for some $\mathcal{I}$, i.e., the query returns at least one tuple.

- **Logical implication**: if φ logically implies ψ, then $\varphi^{\mathcal{I}} \subseteq \psi^{\mathcal{I}}$ for all $\mathcal{I}$, written $\varphi \subseteq \psi$, i.e., the answer to φ is contained in that of ψ in every interpretation. This is called **query containment**.

- **Logical equivalence**: if φ is logically equivalent to ψ, then $\varphi^{\mathcal{I}} = \psi^{\mathcal{I}}$ for all $\mathcal{I}$, written $\varphi \equiv \psi$, i.e., the answer to the two queries is the same in every interpretation. This is called **query equivalence** and corresponds to query containment in both directions.

Note: These definitions can be extended to the case where we have **axioms**, i.e., **constraints** on the admissible interpretations.

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Chapter II

First-Order Query Evaluation

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Query evaluation

Let us consider:

- a finite alphabet, i.e., we have a finite number of predicates and functions, and
- a finite interpretation $\mathcal{I}$, i.e., an interpretation (over the finite alphabet) for which $\Delta^{\mathcal{I}}$ is finite.

Then we can consider query evaluation as an algorithmic problem, and study its computational properties.

Note: To study the computational complexity of the problem, we need to define a corresponding decision problem.

Query evaluation problem

Definitions

- Query answering problem: given a finite interpretation $\mathcal{I}$ and a FOL query $\varphi(x_1, \ldots, x_k)$, compute

$$\varphi^{\mathcal{I}} = \{(a_1, \ldots, a_k) \mid \mathcal{I}, \langle a_1, \ldots, a_k \rangle \models \varphi(x_1, \ldots, x_k)\}$$

- Recognition problem (for query answering): given a finite interpretation $\mathcal{I}$, a FOL query $\varphi(x_1, \ldots, x_k)$, and a tuple $(a_1, \ldots, a_k)$, with $a_i \in \Delta^{\mathcal{I}}$, check whether $(a_1, \ldots, a_k) \in \varphi^{\mathcal{I}}$, i.e., whether

$$\mathcal{I}, \langle a_1, \ldots, a_k \rangle \models \varphi(x_1, \ldots, x_k)$$

Note: The recognition problem for query answering is the decision problem corresponding to the query answering problem.

Query evaluation algorithm

We define now an algorithm that computes the function $\texttt{Truth}(\mathcal{I}, \alpha, \varphi)$ in such a way that $\texttt{Truth}(\mathcal{I}, \alpha, \varphi) = \texttt{true}$ iff $\mathcal{I}, \alpha \models \varphi$.

We make use of an auxiliary function $\texttt{TermEval}(\mathcal{I}, \alpha, t)$ that, given an interpretation $\mathcal{I}$ and an assignment α, evaluates a term t returning an object $o \in \Delta^{\mathcal{I}}$:

```
Δᴵ TermEval(I,α,t) {
    if (t is x ∈ Vars)
        return α(x);
    if (t is f(t_1,...,t_k))
        return fᴵ(TermEval(I,α,t_1),...,TermEval(I,α,t_k));
}
```

Then, $\texttt{Truth}(\mathcal{I}, \alpha, \varphi)$ can be defined by structural recursion on φ.

Query evaluation algorithm (cont'd)

```
boolean Truth(I,α,φ) {
  if (φ is t_1 = t_2)
    return TermEval(I,α,t_1) = TermEval(I,α,t_2);
  if (φ is P(t_1,...,t_k))
    return P^I(TermEval(I,α,t_1),...,TermEval(I,α,t_k));
  if (φ is ¬ψ)
    return ¬Truth(I,α,ψ);
  if (φ is ψ ∘ ψ')
    return Truth(I,α,ψ) ∘ Truth(I,α,ψ');
  if (φ is ∃x.ψ) {
    boolean b = false;
    for all (a ∈ Δ^I)
      b = b ∨ Truth(I,α[x ↦ a],ψ);
    return b;
  }
  if (φ is ∀x.ψ) {
    boolean b = true;
    for all (a ∈ Δ^I)
      b = b ∧ Truth(I,α[x ↦ a],ψ);
    return b;
  }
}
```

Query evaluation – Results

Theorem (Termination of $\mathtt{Truth}(I, \alpha, \varphi)$)

The algorithm `Truth` terminates.

Proof. Immediate. □

Theorem (Correctness)

The algorithm `Truth` is sound and complete, i.e., $I, \alpha \models \varphi$ if and only if $\mathtt{Truth}(I, \alpha, \varphi) = \mathtt{true}$.

Proof. Easy, since the algorithm is very close to the semantic definition of $I, \alpha \models \varphi$. □

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Query evaluation – Time complexity I

Theorem (Time complexity of $\mathtt{Truth}(I, \alpha, \varphi)$)

The time complexity of $\mathtt{Truth}(I, \alpha, \varphi)$ is $(|I| + |\alpha| + |\varphi|)^{|\varphi|}$, i.e., polynomial in the size of I and exponential in the size of φ.

Proof.

- f^I (of arity k) can be represented as k-dimensional array, hence accessing the required element can be done in time linear in $|I|$.

- $\mathtt{TermEval}(\ldots)$ visits the term, so it generates a polynomial number of recursive calls, hence is time polynomial in $(|I| + |\alpha| + |\varphi|)$.

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Query evaluation – Time complexity II

- $P^{\mathcal{I}}$ (of arity k) can be represented as k-dimensional boolean array, hence accessing the required element can be done in time linear in $|\mathcal{I}|$.

- $\texttt{Truth}(\ldots)$ for the boolean cases simply visits the formula, so generates either one or two recursive calls.

- $\texttt{Truth}(\ldots)$ for the quantified cases $\exists x.\varphi$ and $\forall x.\psi$ involves looping for all elements in $\Delta^{\mathcal{I}}$ and testing the resulting assignments.

- The total number of such testings is $O(|\mathcal{I}|^{\sharp Vars})$.

Hence the claim holds. $\qquad\Box$

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Query evaluation – Space complexity I

Theorem (Space complexity of $\texttt{Truth}(\mathcal{I}, \alpha, \varphi)$)

The space complexity of $\texttt{Truth}(\mathcal{I}, \alpha, \varphi)$ is $|\varphi| \cdot (|\varphi| \cdot \log|\mathcal{I}|)$, i.e., logarithmic in the size of $\mathcal{I}$ and polynomial in the size of φ.

Proof.
- $f^{\mathcal{I}}(\ldots)$ can be represented as k-dimensional array, hence accessing the required element requires $O(\log|\mathcal{I}|)$;
- $\texttt{TermEval}(\ldots)$ simply visits the term, so it generates a polynomial number of recursive calls. Each activation record has a constant size, and we need $O(|\varphi|)$ activation records;
- $P^{\mathcal{I}}(\ldots)$ can be represented as k-dimensional boolean array, hence accessing the required element requires $O(\log|\mathcal{I}|)$;

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Query evaluation – Space complexity II

- $\texttt{Truth}(\ldots)$ for the boolean cases simply visits the formula, so generates either one or two recursive calls, each requiring constant size;
- $\texttt{Truth}(\ldots)$ for the quantified cases $\exists x.\varphi$ and $\forall x.\psi$ involves looping for all elements in $\Delta^{\mathcal{I}}$ and testing the resulting assignments;
- The total number of activation records that need to be at the same time on the stack is $O(\sharp Vars) \leq O(|\varphi|)$.

Hence the claim holds. $\qquad\Box$

Note: the worst case form for the formula is

$$\forall x_1.\exists x_2.\cdots\forall x_{n-1}.\exists x_n.P(x_1, x_2, \ldots, x_{n-1}, x_n).$$

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Query evaluation – Complexity measures [Var82]

Definition (Combined complexity)

The combined complexity is the complexity of $\{\langle \mathcal{I}, \alpha, \varphi \rangle \mid \mathcal{I}, \alpha \models \varphi\}$, i.e., interpretation, tuple, and query are all considered part of the input.

Definition (Data complexity)

The data complexity is the complexity of $\{\langle \mathcal{I}, \alpha \rangle \mid \mathcal{I}, \alpha \models \varphi\}$, i.e., the query φ is fixed (and hence not considered part of the input).

Definition (Query complexity)

The query complexity is the complexity of $\{\langle \alpha, \varphi \rangle \mid \mathcal{I}, \alpha \models \varphi\}$, i.e., the interpretation $\mathcal{I}$ is fixed (and hence not considered part of the input).

Query evaluation – Combined, data, query complexity

Theorem (Combined complexity of query evaluation)

The complexity of $\{\langle \mathcal{I}, \alpha, \varphi \rangle \mid \mathcal{I}, \alpha \models \varphi\}$ is:

- time: exponential
- space: PSpace-complete — see [Var82] for hardness

Theorem (Data complexity of query evaluation)

The complexity of $\{\langle \mathcal{I}, \alpha \rangle \mid \mathcal{I}, \alpha \models \varphi\}$ is:

- time: polynomial
- space: in LogSpace

Theorem (Query complexity of query evaluation)

The complexity of $\{\langle \alpha, \varphi \rangle \mid \mathcal{I}, \alpha \models \varphi\}$ is:

- time: exponential
- space: PSpace-complete — see [Var82] for hardness

Evaluation of conjunctive queries
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Chap. 3: Conjunctive Queries

Chapter III

Conjunctive Queries

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Conjunctive queries (CQs)

Def.: A conjunctive query (CQ) is a FOL query of the form

$$\exists \vec{y}.conj(\vec{x}, \vec{y})$$

where $conj(\vec{x}, \vec{y})$ is a conjunction (i.e., an "and") of atoms and equalities, over the free variables $\vec{x}$, the existentially quantified variables $\vec{y}$, and possibly constants.

Note:

- CQs contain no disjunction, no negation, no universal quantification, and no function symbols besides constants.
- Hence, they correspond to relational algebra select-project-join (SPJ) queries.
- CQs are the most frequently asked queries.

Conjunctive queries and SQL – Example

Relational alphabet:
$\mathsf{Person(name, age)}, \quad \mathsf{Lives(person, city)}, \quad \mathsf{Manages(boss, employee)}$

Query: return name and age of all persons that live in the same city as their boss.

Expressed in SQL:

```
SELECT P.name, P.age
FROM Person P,  Manages M,  Lives L1,  Lives L2
WHERE P.name = L1.person  AND  P.name = M.employee  AND
      M.boss = L2.person  AND  L1.city = L2.city
```

Expressed as a CQ:

$\exists b, e, p_1, c_1, p_2, c_2.\mathsf{Person}(n, a) \wedge \mathsf{Manages}(b, e) \wedge \mathsf{Lives}(p1, c1) \wedge \mathsf{Lives}(p2, c2) \wedge$
$$n = p1 \ \wedge \ n = e \ \wedge \ b = p2 \ \wedge \ c1 = c2$$

Or simpler: $\exists b, c.\mathsf{Person}(n, a) \wedge \mathsf{Manages}(b, n) \wedge \mathsf{Lives}(n, c) \wedge \mathsf{Lives}(b, c)$

Datalog notation for CQs

A CQ $q = \exists \vec{y}.conj(\vec{x}, \vec{y})$ can also be written using datalog notation as

$$q(\vec{x}_1) \leftarrow conj'(\vec{x}_1, \vec{y}_1)$$

where $conj'(\vec{x}_1, \vec{y}_1)$ is the list of atoms in $conj(\vec{x}, \vec{y})$ obtained by equating the variables $\vec{x}$, $\vec{y}$ according to the equalities in $conj(\vec{x}, \vec{y})$.

As a result of such an equality elimination, we have that $\vec{x}_1$ and $\vec{y}_1$ can contain constants and multiple occurrences of the same variable.

Def.: In the above query q, we call:

- $q(\vec{x}_1)$ the head;
- $conj'(\vec{x}_1, \vec{y}_1)$ the body;
- the variables in $\vec{x}_1$ the distinguished variables;
- the variables in $\vec{y}_1$ the non-distinguished variables.

Conjunctive queries – Example

- Consider an interpretation $\mathcal{I} = (\Delta^{\mathcal{I}}, E^{\mathcal{I}})$, where $E^{\mathcal{I}}$ is a binary relation – *note that such interpretation is a (directed) graph*.
- The following CQ q returns all nodes that participate to a triangle in the graph:

$$\exists y, z.E(x, y) \wedge E(y, z) \wedge E(z, x)$$

- The query q in datalog notation becomes:

$$q(x) \leftarrow E(x, y), E(y, z), E(z, x)$$

- The query q in SQL is (we use Edge(f,s) for $E(x, y)$):

```
SELECT E1.f
FROM Edge E1, Edge E2, Edge E3
WHERE E1.s = E2.f AND E2.s = E3.f AND E3.s = E1.f
```

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Nondeterministic evaluation of CQs

Since a CQ contains only existential quantifications, we can evaluate it by:

1. guessing a truth assignment for the non-distinguished variables;
2. evaluating the resulting formula (that has no quantifications).

```
boolean ConjTruth(I,α,∃y⃗.conj(x⃗,y⃗)) {
  GUESS assignment α[y⃗ ↦ a⃗] {
    return Truth(I,α[y⃗ ↦ a⃗],conj(x⃗,y⃗));
  }
}
```

where $\text{Truth}(\mathcal{I},\alpha,\varphi)$ is defined as for FOL queries, considering only the required cases.

Evaluation of conjunctive queries
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Nondeterministic CQ evaluation algorithm

```
boolean Truth(I,α,φ) {
  if (φ is t_1 = t_2)
    return TermEval(I,α,t_1) = TermEval(I,α,t_2);
  if (φ is P(t_1,...,t_k))
    return P^I(TermEval(I,α,t_1),...,TermEval(I,α,t_k));
  if (φ is ψ ∧ ψ')
    return Truth(I,α,ψ) ∧ Truth(I,α,ψ');
}

Δ^I TermEval(I,α,t) {
  if (t is a variable x) return α(x);
  if (t is a constant c) return c^I;
}
```

Evaluation of conjunctive queries
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CQ evaluation – Combined, data, and query complexity

Theorem (Combined complexity of CQ evaluation)

$\{\langle \mathcal{I}, \alpha, q \rangle \mid \mathcal{I}, \alpha \models q\}$ is NP-complete — see below for hardness.

- time: exponential
- space: polynomial

Theorem (Data complexity of CQ evaluation)

$\{\langle \mathcal{I}, \alpha \rangle \mid \mathcal{I}, \alpha \models q\}$ is in LogSpace

- time: polynomial
- space: logarithmic

Theorem (Query complexity of CQ evaluation)

$\{\langle \alpha, q \rangle \mid \mathcal{I}, \alpha \models q\}$ is NP-complete — see below for hardness.

- time: exponential
- space: polynomial

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3-colorability

A graph is k-colorable if it is possible to assign to each node one of k colors in such a way that every two nodes connected by an edge have different colors.

Def.: 3-colorability is the following decision problem

Given a graph $G = (V, E)$, is it 3-colorable?

Theorem

3-colorability is NP-complete.

We exploit 3-colorability to show NP-hardness of conjunctive query evaluation.

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Chap. 3: Conjunctive Queries

Reduction from 3-colorability to CQ evaluation

Let $G = (V, E)$ be a graph. We define:

- An Interpretation: $\mathcal{I} = (\Delta^{\mathcal{I}}, E^{\mathcal{I}})$ where:
  - $\Delta^{\mathcal{I}} = \{r, g, b\}$
  - $E^{\mathcal{I}} = \{(r, g), (g, r), (r, b), (b, r), (g, b), (b, g)\}$
- A conjunctive query: Let $V = \{x_1, \ldots, x_n\}$, then consider the boolean conjunctive query defined as:

$$q_G \ = \ \exists x_1, \ldots, x_n. \bigwedge_{(x_i, x_j) \in E} E(x_i, x_j) \wedge E(x_j, x_i)$$

Theorem

G is 3-colorable iff $\mathcal{I} \models q_G$.

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NP-hardness of CQ evaluation

The previous reduction immediately gives us the hardness for combined complexity.

Theorem

CQ evaluation is NP-hard in combined complexity.

Note: in the previous reduction, the interpretation does not depend on the actual graph. Hence, the reduction provides also the lower-bound for query complexity.

Theorem

CQ evaluation is NP-hard in query (and combined) complexity.

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Homomorphism

Let $\mathcal{I} = (\Delta^{\mathcal{I}}, P^{\mathcal{I}}, \ldots, c^{\mathcal{I}}, \ldots)$ and $\mathcal{J} = (\Delta^{\mathcal{J}}, P^{\mathcal{J}}, \ldots, c^{\mathcal{J}}, \ldots)$ be two interpretations over the same alphabet (for simplicity, we consider only constants as functions).

Def.: A homomorphism from $\mathcal{I}$ to $\mathcal{J}$

is a mapping $h : \Delta^{\mathcal{I}} \to \Delta^{\mathcal{J}}$ such that:

- $h(c^{\mathcal{I}}) \ = \ c^{\mathcal{J}}$
- $h(P^{\mathcal{I}}(a_1, \ldots, a_k)) = P^{\mathcal{J}}(h(a_1), \ldots, h(a_k))$

Note: An isomorphism is a homomorphism that is one-to-one and onto.

Theorem

FOL is unable to distinguish between interpretations that are isomorphic.

Proof. See any standard book on logic. □

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Recognition problem and boolean query evaluation

Consider the recognition problem associated to the evaluation of a query q of arity k. Then

$$\mathcal{I}, \alpha \models q(x_1, \ldots, x_k) \qquad \text{iff} \qquad \mathcal{I}_{\alpha, \vec{c}} \models q(c_1, \ldots, c_k)$$

where $\mathcal{I}_{\alpha, \vec{c}}$ is identical to $\mathcal{I}$ but includes new constants $c_1, \ldots, c_k$ that are interpreted as $c_i^{\mathcal{I}_{\alpha, \vec{c}}} = \alpha(x_i)$.

That is, we can reduce the recognition problem to the evaluation of a boolean query.

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Canonical interpretation of a (boolean) CQ

Let q be a conjunctive query $\quad \exists x_1, \ldots, x_n . conj$

Def.: The canonical interpretation $\mathcal{I}_q$ associated with q

is the interpretation $\mathcal{I}_q = (\Delta^{\mathcal{I}_q}, P^{\mathcal{I}_q}, \ldots, c^{\mathcal{I}_q}, \ldots)$, where

- $\Delta^{\mathcal{I}_q} = \{x_1, \ldots, x_n\} \cup \{c \mid c \text{ constant occurring in } q\}$, i.e., all the variables and constants in q;
- $c^{\mathcal{I}_q} = c$, for each constant c in q;
- $(t_1, \ldots, t_k) \in P^{\mathcal{I}_q}$ iff the atom $P(t_1, \ldots, t_k)$ occurs in q.

Sometimes the procedure for obtaining the canonical interpretation is called freezing of q.

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Canonical interpretation of a (boolean) CQ – Example

Consider the boolean query q

$$q(c) \leftarrow E(c, y), E(y, z), E(z, c)$$

Then, the canonical interpretation $\mathcal{I}_q$ is defined as

$$\mathcal{I}_q = (\Delta^{\mathcal{I}_q}, E^{\mathcal{I}_q}, c^{\mathcal{I}_q})$$

where

- $\Delta^{\mathcal{I}_q} = \{y, z, c\}$
- $E^{\mathcal{I}_q} = \{(c, y), (y, z), (z, c)\}$
- $c^{\mathcal{I}_q} = c$

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Canonical interpretation and (boolean) CQ evaluation

Theorem ([CM77])

For boolean CQs, $\mathcal{I} \models q$ iff there exists a homomorphism from $\mathcal{I}_q$ to $\mathcal{I}$.

Proof.
"$\Rightarrow$" Let $\mathcal{I} \models q$, let α be an assignment to the existential variables that makes q true in $\mathcal{I}$, and let $\hat{\alpha}$ be its extension to constants. Then $\hat{\alpha}$ is a homomorphism from $\mathcal{I}_q$ to $\mathcal{I}$.

"$\Leftarrow$" Let h be a homomorphism from $\mathcal{I}_q$ to $\mathcal{I}$. Then restricting h to the variables only we obtain an assignment to the existential variables that makes q true in $\mathcal{I}$. □

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Canonical interpretation and (boolean) CQ evaluation

The previous result can be rephrased as follows:

(The recognition problem associated to) query evaluation can be reduced to finding a homomorphism.

Finding a homomorphism between two interpretations (aka relational structures) is also known as solving a Constraint Satisfaction Problem (CSP), a problem well-studied in AI – see also [KV98].

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Query containment

Def.: Query containment

Given two FOL queries φ and ψ of the same arity, φ is contained in ψ, denoted $\varphi \subseteq \psi$, if for all interpretations $\mathcal{I}$ and all assignments α we have that

$$\mathcal{I}, \alpha \models \varphi \quad \text{implies} \quad \mathcal{I}, \alpha \models \psi$$

(In logical terms: $\varphi \models \psi$.)

Note: Query containment is of special interest in query optimization.

Theorem

For FOL queries, query containment is undecidable.

Proof.: Reduction from FOL logical implication. □

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Query containment for CQs

For CQs, query containment $q_1(\vec{x}) \subseteq q_2(\vec{x})$ can be reduced to query evaluation.

1. **Freeze the free variables**, i.e., consider them as constants. This is possible, since $q_1(\vec{x}) \subseteq q_2(\vec{x})$ iff
   - $\mathcal{I}, \alpha \models q_1(\vec{x})$ implies $\mathcal{I}, \alpha \models q_2(\vec{x})$, for all $\mathcal{I}$ and α;   or equivalently
   - $\mathcal{I}_{\alpha,\vec{c}} \models q_1(\vec{c})$ implies $\mathcal{I}_{\alpha,\vec{c}} \models q_2(\vec{c})$, for all $\mathcal{I}_{\alpha,\vec{c}}$, where $\vec{c}$ are new constants, and $\mathcal{I}_{\alpha,\vec{c}}$ extends $\mathcal{I}$ to the new constants with $c^{\mathcal{I}_{\alpha,\vec{c}}} = \alpha(x)$.

2. **Construct the canonical interpretation** $\mathcal{I}_{q_1(\vec{c})}$ of the CQ $q_1(\vec{c})$ on the left hand side ...

3. ... and **evaluate on** $\mathcal{I}_{q_1(\vec{c})}$ the CQ $q_2(\vec{c})$ on the right hand side, i.e., check whether $\mathcal{I}_{q_1(\vec{c})} \models q_2(\vec{c})$.

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Chap. 3: Conjunctive Queries

Reducing containment of CQs to CQ evaluation

Theorem ([CM77])

For CQs, $q_1(\vec{x}) \subseteq q_2(\vec{x})$ iff $\mathcal{I}_{q_1(\vec{c})} \models q_2(\vec{c})$, where $\vec{c}$ are new constants.

Proof.
"⇒" Assume that $q_1(\vec{x}) \subseteq q_2(\vec{x})$.
 - Since $\mathcal{I}_{q_1(\vec{c})} \models q_1(\vec{c})$ it follows that $\mathcal{I}_{q_1(\vec{c})} \models q_2(\vec{c})$.

"⇐" Assume that $\mathcal{I}_{q_1(\vec{c})} \models q_2(\vec{c})$.
 - By [CM77] on hom., for every $\mathcal{I}$ such that $\mathcal{I} \models q_1(\vec{c})$ there exists a homomorphism h from $\mathcal{I}_{q_1(\vec{c})}$ to $\mathcal{I}$.
 - On the other hand, since $\mathcal{I}_{q_1(\vec{c})} \models q_2(\vec{c})$, again by [CM77] on hom., there exists a homomorphism h' from $\mathcal{I}_{q_2(\vec{c})}$ to $\mathcal{I}_{q_1(\vec{c})}$.
 - The mapping $h \circ h'$ (obtained by composing h and h') is a homomorphism from $\mathcal{I}_{q_2(\vec{c})}$ to $\mathcal{I}$. Hence, once again by [CM77] on hom., $\mathcal{I} \models q_2(\vec{c})$.

So we can conclude that $q_1(\vec{c}) \subseteq q_2(\vec{c})$, and hence $q_1(\vec{x}) \subseteq q_2(\vec{x})$. □

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Query containment for CQs

For CQs, we also have that (boolean) query evaluation $\mathcal{I} \models q$ can be reduced to query containment.

Let $\mathcal{I} = (\Delta^{\mathcal{I}}, P^{\mathcal{I}}, \ldots, c^{\mathcal{I}}, \ldots)$.

We construct the (boolean) CQ $q_{\mathcal{I}}$ as follows:

- $q_{\mathcal{I}}$ has no existential variables (hence no variables at all);
- the constants in $q_{\mathcal{I}}$ are the elements of $\Delta^{\mathcal{I}}$;
- for each relation P interpreted in $\mathcal{I}$ and for each fact $(a_1, \ldots, a_k) \in P^{\mathcal{I}}$, $q_{\mathcal{I}}$ contains one atom $P(a_1, \ldots, a_k)$ (note that each $a_i \in \Delta^{\mathcal{I}}$ is a constant in $q_{\mathcal{I}}$).

Theorem

For CQs, $\mathcal{I} \models q$ iff $q_{\mathcal{I}} \subseteq q$.

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Query containment for CQs – Complexity

From the previous results and NP-completenss of combined complexity of CQ evaluation, we immediately get:

Theorem

Containment of CQs is NP-complete.

Since CQ evaluation is NP-complete even in query complexity, the above result can be strengthened:

Theorem

Containment $q_1(\vec{x}) \subseteq q_2(\vec{x})$ of CQs is NP-complete, even when q_1 is considered fixed.

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Union of conjunctive queries (UCQs)

Def.: A union of conjunctive queries (UCQ) is a FOL query of the form

$$\bigvee_{i=1,\ldots,n} \exists \vec{y}_i . conj_i(\vec{x}, \vec{y}_i)$$

where each $conj_i(\vec{x}, \vec{y}_i)$ is a conjunction of atoms and equalities with free variables $\vec{x}$ and $\vec{y}_i$, and possibly constants.

Note: Obviously, each conjunctive query is also a of union of conjunctive queries.

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Datalog notation for UCQs

A union of conjunctive queries

$$q \;=\; \bigvee_{i=1,\ldots,n} \exists \vec{y_i}.conj_i(\vec{x}, \vec{y_i})$$

is written in datalog notation as

$$\{ \quad q(\vec{x}) \quad \leftarrow \quad conj_1'(\vec{x}, \vec{y_1}') $$
$$\vdots$$
$$q(\vec{x}) \quad \leftarrow \quad conj_n'(\vec{x}, \vec{y_n}') \quad \}$$

where each element of the set is the datalog expression corresponding to the conjunctive query $q_i = \exists \vec{y_i}.conj_i(\vec{x}, \vec{y_i})$.

Note: in general, we omit the set brackets.

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Evaluation of UCQs

From the definition of FOL query we have that:

$$\mathcal{I}, \alpha \;\models\; \bigvee_{i=1,\ldots,n} \exists \vec{y_i}.conj_i(\vec{x}, \vec{y_i})$$

if and only if

$$\mathcal{I}, \alpha \;\models\; \exists \vec{y_i}.conj_i(\vec{x}, \vec{y_i}) \qquad \text{for some } i \in \{1, \ldots, n\}.$$

Hence to evaluate a UCQ q, we simply evaluate a number (linear in the size of q) of conjunctive queries in isolation.

Hence, evaluating UCQs has the same complexity as evaluating CQs.

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UCQ evaluation – Combined, data, and query complexity

Theorem (Combined complexity of UCQ evaluation)

$\{\langle \mathcal{I}, \alpha, q \rangle \mid \mathcal{I}, \alpha \models q\}$ is NP-complete.

- time: exponential
- space: polynomial

Theorem (Data complexity of UCQ evaluation)

$\{\langle \mathcal{I}, q \rangle \mid \mathcal{I}, \alpha \models q\}$ is in LOGSPACE (query q fixed).

- time: polynomial
- space: logarithmic

Theorem (Query complexity of UCQ evaluation)

$\{\langle \alpha, q \rangle \mid \mathcal{I}, \alpha \models q\}$ is NP-complete (interpretation $\mathcal{I}$ fixed).

- time: exponential
- space: polynomial

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Query containment for UCQs

Theorem

For UCQs, $\{q_1, \ldots, q_k\} \subseteq \{q_1', \ldots, q_n'\}$ iff for each q_i there is a q_j' such that $q_i \subseteq q_j'$.

Proof.

"⇐" Obvious.

"⇒" If the containment holds, then we have $\{q_1(\vec{c}), \ldots, q_k(\vec{c})\} \subseteq \{q_1'(\vec{c}), \ldots, q_n'(\vec{c})\}$, where $\vec{c}$ are new constants:

- Now consider $\mathcal{I}_{q_i(\vec{c})}$. We have $\mathcal{I}_{q_i(\vec{c})} \models q_i(\vec{c})$, and hence $\mathcal{I}_{q_i(\vec{c})} \models \{q_1(\vec{c}), \ldots, q_k(\vec{c})\}$.
- By the containment, we have that $\mathcal{I}_{q_i(\vec{c})} \models \{q_1'(\vec{c}), \ldots, q_n'(\vec{c})\}$. I.e., there exists a $q_j'(\vec{c})$ such that $\mathcal{I}_{q_i(\vec{c})} \models q_j'(\vec{c})$.
- Hence, by [CM77] on containment of CQs, we have that $q_i \subseteq q_j'$.
  □

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Query containment for UCQs – Complexity

From the previous result, we have that we can check
$\{q_1, \ldots, q_k\} \subseteq \{q'_1, \ldots, q'_n\}$ by at most $k \cdot n$ CQ containment checks.

We immediately get:

Theorem

Containment of UCQs is NP-complete.

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