Complexity Theory
VU 181.142, SS 2016

8. PSPACE

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21 June, 2016
Outline

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PSPACE

Motivation

PSPACE captures unrestricted alternation. Therefore, 

- it generalizes the polynomial hierarchy,
- it is the class of many strategy games, decision making, etc.,
- it has QSAT (QBF) as natural complete problem.
QSAT (QBF)

INSTANCE: Boolean expression \( \varphi \) in CNF with variables \( x_1, \ldots, x_n \).
QUESTION: Is there a truth value for the variable \( x_1 \) such that for both truth values of \( x_2 \) there is a truth value for \( x_3 \) and so on up to \( x_n \), such that \( \varphi \) is satisfied by the overall truth assignment?

Notation
An instance of QSAT is written as \( \exists x_1 \forall x_2 \exists x_3 \cdots Q x_n \varphi \), where \( Q \) is \( \forall \) if \( n \) is even and \( \exists \) if \( n \) is odd.

Theorem
QSAT is PSPACE-complete.
Proof of the PSPACE-Membership of QSAT

Remark. We only prove the PSPACE-membership here. The hardness will be proved below via the complexity of First-Order Logic.

Let an arbitrary QBF be given as $\psi \equiv \exists x_1 \forall x_2 \exists x_3 \cdots Q x_n \varphi$. All possible truth assignments of the variables can be represented by the leaves in a full binary tree of depth $n$ ("semantic tree"): The left subtree of the root contains all truth assignments $T$ with $T(x_1) = \text{false}$, while the right subtree of the root contains all truth assignments $T$ with $T(x_1) = \text{true}$.

Analogously, for every $i \geq 1$, the subtrees at depth $i + 1$, whose root is the first child of its parent, contains all truth assignments $T$ with $T(x_{i+1}) = \text{false}$, while the subtrees at depth $i + 1$, whose root is the second child of its parent, contains all truth assignments $T$ with $T(x_{i+1}) = \text{true}$. 
Proof of the PSPACE-Membership of QSAT (continued)

We can now turn this tree into a monotone Boolean circuit $C$ where all gates at the $i$-th level are
– OR-gates if $i$ is even (in particular, the root node at level 0) and
– AND-gates if $i$ is odd.

An input gate (i.e., a leaf node) is true if $\varphi$ evaluates to true in the truth assignment corresponding to this leaf node; and an input gate is false if $\varphi$ evaluates to false in this truth assignment.

Clearly, the QBF $\psi$ is true $\iff$ the Boolean circuit $C$ has the value true.

Notation. It will turn out to be convenient in the sequel to use strings over $\{0, 1\}$ (rather than natural numbers) as labels of the gates, i.e.: The output gate (= the root node) has as label the empty string $\epsilon$. Now suppose that some internal node $N$ has label $w \in \{0, 1\}^*$. Then the first child of $N$ has label $w0$ and the second child has label $w1.$
Proof of the PSPACE-Membership of QSAT (continued)

The Boolean circuit can be evaluated in space $O(n)$ by an algorithm which traverses the (tree-structured) circuit as follows:

- In order to evaluate an **AND-gate** $g$, we recursively evaluate its first child $g0$. If $g0$ is **false**, we know that $g$ is **false**. Otherwise, the evaluation continues with the second child $g1$ of $g$.

- **OR-gates** are treated analogously – with **true** and **false** reversed.

- The evaluation of a **NOT-gate** is clear (namely by recursively evaluating its unique child and returning the opposite truth value) but not needed for the monotone Boolean circuit $C$.

- Once the evaluation of a gate $g$ is finished, the algorithm continues with the parent node of $g$ (whose label is obtained by simply omitting the last bit of $g$’s label).
Proof of the PSPACE-Membership of QSAT (continued)

The linear space bound on the evaluation of the Boolean circuit follows immediately from the following observation: At any time, the algorithm only needs to store (the label of) exactly 1 gate of the tree, namely the current gate $g$ of the evaluation.

Implicitly, we thus have the entire path from $g$ to the root. If the path contains a gate which is the first child of its parent $h$, then it is clear that the second child of $h$ has not been visited yet. If the path contains a gate which is the second child of $h$, then it is clear that the value of the first child of $h$ is $\text{true}$ for an AND-gate $h$ and $\text{false}$ for an OR-gate $h$.

The only difficulty remaining is that the circuit $C$ has exponential size. Observe that both, the construction of $C$ and the evaluation of $C$ work in polynomial space. Hence, the combination of these two algorithms is feasible in PSPACE – by the same idea as in the proof that the composition of two log-space computations is feasible in log-space.
**Proposition**

QSAT is a generalization of the $\Sigma_i^P$-complete problem QSAT$_i$ for any value of $i$.

**Corollary**

$\text{PH} \subseteq \text{PSPACE}$

**Remark**

It is not known if PH is properly included in PSPACE. Most probably, $\text{PH} \subset \text{PSPACE}$ holds, because $\text{PH} = \text{PSPACE}$ would imply that the polynomial hierarchy collapses (since there exist PSPACE-complete problems).
Games

Observation

PSPACE is the class of many strategy games, decision making, etc.

QSAT can be considered as a two-person game:

- two players: $\exists$ and $\forall$
- players move alternatingly ($\exists$ first)
- a move: determining the truth value of a variable
- $\exists$ tries to make the formula $\varphi$ true while $\forall$ tries to make it false.
- after $n$ moves either $\exists$ or $\forall$ wins.

Decision making can sometimes be considered as a game against nature.
Complexity of Query Evaluation

### Decision Problems

For (Boolean) queries of a certain query language (e.g., SQL, datalog, XPath, XQuery, etc.), there are three main kinds of decision problems:

- **Data complexity** refers to the following decision problem:
  
  Let $Q$ be some *fixed* query.
  
  INSTANCE: An input database $D$.
  
  QUESTION: Does query $Q$ yield a non-empty result over the DB $D$?

- **Query complexity** refers to the following decision problem:
  
  Let $D$ be some *fixed* input database.
  
  INSTANCE: A query $Q$.
  
  QUESTION: Does query $Q$ yield a non-empty result over the DB $D$?

- **Combined complexity** refers to the following decision problem:
  
  INSTANCE: An input database $D$ and a query $Q$.
  
  QUESTION: Does query $Q$ yield a non-empty result over the DB $D$?
First-Order Queries

Definition

A term is a constant or a variable.

For a given input schema $\mathcal{R} = \{R_1, \ldots, R_n\}$, the base formulae are either equality atoms $s = t$ or atoms of the form $R(t_1, \ldots, t_\alpha)$, where the $t_i$ are terms and $\alpha$ is the arity of $R$. A first-order query over $\mathcal{R}$ is either a base formula or a formula of the following form:

1. $(\varphi \land \psi)$, where $\varphi$ and $\psi$ are formulae over $\mathcal{R}$;
2. $(\varphi \lor \psi)$, where $\varphi$ and $\psi$ are formulae over $\mathcal{R}$;
3. $\neg \varphi$, where $\varphi$ is a formula over $\mathcal{R}$;
4. $\exists x \varphi$, where $x$ is a variable and $\varphi$ is a formula over $\mathcal{R}$;
5. $\forall x \varphi$, where $x$ is a variable and $\varphi$ is a formula over $\mathcal{R}$.

Remark. First-order queries essentially correspond to SQL without GROUP BY, (aggregate) functions and arithmetic.
First-Order Queries

**Theorem**

The query complexity and the combined complexity of first-order queries are PSPACE-complete (even if we disallow negation and equality atoms). The data complexity is in \( L \) (actually, even in a lower class).

**Remark**

The decision problem for the query complexity is a special case of the decision problem for the combined complexity. Hence, it suffices to prove the following results:

- The combined complexity of first-order queries is in PSPACE.
- The query complexity of first-order queries is PSPACE-hard.
PSPACE-Hardness of First-Order Queries

Proof of the PSPACE-Hardness

We prove the hardness by reduction from an arbitrary language \( L \) in PSPACE. To this end, we define a fixed database \( D \). Moreover, we describe a reduction \( R \) which, for every string \( w \), constructs a First-Order sentence \( R(w) \) such that \( w \in L \iff R(w) \) evaluates to true over \( D \).

Let \( T = (K, \Sigma, \delta, s) \) be a single-string Turing machine that decides \( L \) in polynomial space. W.l.o.g., we assume that on any positive instance \( w \), the TM \( T \) has exactly one accepting configuration, say \( ("yes", \triangleright, \sqsubset \sqsubset \ldots) \). Assume that the computation on input \( w \) requires at most \( d \cdot n^k \) space with \( n = |w| \) and constants \( d, k \). Then the computation takes at most \( N = c^{d \cdot n^k} \) steps for some constant \( c \).

We first define the (fixed) input database \( D \): it just contains two unary relations \( K \) and \( \Sigma \) with the states and symbols, respectively, of \( T \).
PSPACE-Hardness of First-Order Queries

Proof of the PSPACE-Hardness (continued)

Now let $w$ be an arbitrary instance of $L$. We have to construct an FO formula $R(w)$. This construction is based on well-known ideas.

**Idea 1.** Recall the NL-completeness proof of REACHABILITY. Our PSPACE-hardness proof also makes use of the configuration graph $G(T, w)$ of TM $T$ on input $w$: The nodes are all possible configurations of $T$ (with space bound $d \cdot n^k$). There is an edge between two nodes (i.e., two configurations) $C_1$ and $C_2$ iff the TM $T$ has a transition in one step from $C_1$ to $C_2$. We have $w \in L$ iff there exists a path from the unique initial configuration $(s, \triangleright, w)$ to (“yes”, $\triangleright, \sqcap \sqcup \ldots$).

**Idea 2.** Recall the proof of Savitch’s Theorem, where we search for a path between two nodes via middle-first search. The crucial idea of this proof was to define a predicate $PATH(a, b, i)$ with the intended meaning that $PATH(a, b, i)$ is true iff there is a path from $a$ to $b$ of length at most $2^i$. The main task of our PSPACE-hardness proof will be to encode predicates $PATH(a, b, i)$ for $i \in \{0, \ldots, \log N\}$ as FO formulas.
PSPACE-Hardness of First-Order Queries

Proof of the PSPACE-Hardness (continued)

Configurations. Every configuration can be represented by a vector of length $M = d \cdot n^k + 1$: we represent $(q, u, v)$ with $u = u_1, \ldots, u_\alpha$ and $v = v_1, \ldots, v_\beta$ as $(u_1, \ldots, u_\alpha, q, v_1, \ldots, v_\beta, \sqcup, \sqcup, \ldots)$.

Encoding of $PATH(a, b, i)$. For every $i \in \{0, \ldots, \log N\}$ we define a formula $\psi_i(x_1, \ldots, x_M, y_1, \ldots, y_M)$ with free variables $x_1, \ldots, x_M$, $y_1, \ldots, y_M$, s.t. $\psi_i$ is true in $D$ iff $(x_1, \ldots, x_M)$ is instantiated to (the representation of) some configuration $C_1$, $(y_1, \ldots, y_M)$ is instantiated to (the representation of) some configuration $C_2$, and there is a path of length at most $2^i$ from $C_1$ to $C_2$ in the configuration graph $G(T, w)$.

Reduction from $L$ to FO evaluation. Suppose that we have defined the predicates $\psi_i(x_1, \ldots, x_M, y_1, \ldots, y_M)$. Let $j = \log N$. Moreover, let $(a_1, \ldots, a_M)$ be the (representation of the) initial configuration $C_0$ on input $w$ and let $(b_1, \ldots, b_M)$ be the accepting configuration $C_{\text{"yes"}}$.

We define $\psi^* = \psi_j(a_1, \ldots, a_M, b_1, \ldots, b_M)$.

Then we have $x \in L \iff \psi^*$ is true over $D$. 
# PSPACE-Hardness of First-Order Queries

## Proof of the PSPACE-Hardness (continued)

### Base Case.

ψ₀(x₁, ..., xₘ, y₁, ..., yₘ) is defined as a big quantifier-free formula in DNF where each disjunct represents a valid combination of values for (x₁, ..., xₘ) and (y₁, ..., yₘ), i.e., either they represent the same configuration or they correspond to the transition of T in one step. For every ℓ ∈ {1, ..., M − 1}, ψ₀ thus contains disjuncts

\[
D = \Sigma(x₁) \land \cdots \land \Sigma(xₖ) \land K(xₖ₊₁) \land \Sigma(xₖ₊₂) \land \cdots \land \Sigma(xₘ) \land x₁ = y₁ \land \cdots \land xₘ = yₘ.
\]

For each transition (q, a, q’, b, →) in δ, ψ₀ contains the following disjuncts (cursor movements ← and → are treated analogously).

\[
D = \Sigma(x₁) \land x₁ = y₁ \land \cdots \land \Sigma(xₖ₋₁) \land xₖ₋₁ = yₖ₋₁ \land xₖ = a \land xₖ₊₁ = q \land \Sigma(xₖ₊₂) \land yₖ = b \land yₖ₊₁ = xₖ₊₂ \land yₖ₊₂ = q' \land \Sigma(xₖ₊₃) \land xₖ₊₃ = yₖ₊₃ \land \cdots \land \Sigma(xₘ) \land xₘ = yₘ.
\]
PSPACE-Hardness of First-Order Queries

Proof of the PSPACE-Hardness (continued)

Notation. We use vector notation \( \vec{z} \) as a short-hand for \( (z_1, \ldots, z_M) \). We also write \( \vec{x} = \vec{y} \) for the conjunction \( x_1 = y_1 \land \cdots \land x_M = y_M \).

Definition of \( \psi_{i+1} \). We define \( \psi_{i+1} \) inductively from \( \psi_i \). It is tempting to define \( \psi_{i+1}(\vec{x}, \vec{y}) \) as
\[
\psi_{i+1}(\vec{x}, \vec{y}) := (\exists \vec{z})\psi_i(\vec{x}, \vec{z}) \land \psi_i(\vec{z}, \vec{y}).
\]
However, this is not allowed since it would produce an exponentially big formula \( \psi^* \). Instead, we have to “reuse” the definition of \( \psi_i \) as follows.
\[
\psi_{i+1}(\vec{x}, \vec{y}) := (\exists \vec{z})(\forall \vec{u})(\forall \vec{v}) \left( [(\vec{u} = \vec{x} \land \vec{v} = \vec{z}) \lor (\vec{u} = \vec{z} \land \vec{v} = \vec{y})] \rightarrow \psi_i(\vec{u}, \vec{v}) \right)
\]
It can be easily verified that this reduction works in polynomial time; actually even logarithmic space suffices. For the correctness of this reduction, we have to prove by induction on \( i \) that \( \psi_i \) has the intended meaning, i.e., \( \psi_i(\vec{a}, \vec{b}) \) is true over \( D \iff \) there is a path of length at most \( 2^i \) from configuration \( \vec{a} \) to configuration \( \vec{b} \) in \( G(T, w) \).
Proof of the PSPACE-Membership

Let $D$ be an arbitrary input database and let $\varphi$ be an arbitrary first-order sentence. Moreover, let all constants in $\varphi$ and all elements in $D$ be from the domain $\text{dom}$. We prove the PSPACE-membership by reducing the problem of evaluating $\varphi$ over $D$ to the QSAT problem.

1. Restricting the domain to $\{0, 1\}$. Let $\text{dom} = \{a_1, \ldots, a_n\}$. Then these elements can be encoded by bit-vectors of size $m = \lceil \log(n) \rceil$. Let $\vec{b}_i$ denote the encoding of $a_i$. Then we transform $D$ into $D'$ by replacing any $\alpha$-ary relation $r$ by an $(\alpha \cdot m)$-ary relation $r'$. 
PSPACE-Membership of First-Order Queries

Proof of the PSPACE-Membership (continued)

Every tuple \((a_{i1}, \ldots, a_{i\alpha})\) in \(r\) is transformed into the tuple \((\bar{b}_{i1}, \ldots, \bar{b}_{i\alpha})\) in \(r\). Likewise, we transform \(\varphi\) to \(\varphi'\) by replacing every constant \(a_i\) by its encoding \(\bar{b}_i\) and by replacing any variable \(x_j\) by a vector \((x_{j1}, \ldots, x_{jm})\) of fresh variables.

2. Eliminating all atoms \(R(t_1, \ldots, t_k)\) from \(\varphi'\). Let \(R\) be a \(k\)-ary relation symbol occurring in \(\varphi'\) and suppose that the corresponding relation in \(D'\) contains the tuples \((c_{11}, \ldots, c_{1k}), (c_{21}, \ldots, c_{2k}), \ldots, (c_{N1}, \ldots, c_{Nk})\). Then we transform \(\varphi'\) into the formula \(\varphi''\) by replacing all atoms of the form \(R(t_1, \ldots, t_k)\) by the following disjunction:

\[
\bigvee_{j=1}^{N} (t_1 = c_{j1} \land \cdots \land t_k = c_{jk})
\]
PSPACE-Membership of First-Order Queries

Proof of the PSPACE-Membership (continued)

3. Replacing first-order variables by propositional variables. The only atoms occurring in $\varphi''$ are equality atoms $s = t$, where the terms $s, t$ are either variables (which can take the value 0 or 1) or the constants 0, 1. We identify 0 with the truth value false and 1 with the truth value true. Then we can transform $\varphi''$ into the QSAT formula $\psi$ by replacing the equality atoms by “equivalent” propositional formulae in the obvious way:

$$
\begin{align*}
&x = y \iff x \leftrightarrow y \\
&x = 0, \ 0 = x \iff \neg x \\
&0 = 1, \ 1 = 0 \iff \text{false} \ (\text{or } x \land \neg x) \\
&0 = 0, \ 1 = 1 \iff \text{true} \ (\text{or } x \lor \neg x)
\end{align*}
$$

Clearly, $\varphi$ evaluates to true over $D$ $\iff$ $\varphi'$ evaluates to true over $D'$ $\iff$ $\varphi''$ evaluates to true independently of any database $\iff \psi$ is true.
Discussion

Easy Consequences

PSPACE-hardness of QSAT. The above proof of the PSPACE-hardness of FO evaluation together with the above reduction from FO evaluation to QSAT immediately yields the PSPACE-hardness of QSAT.

Narrowing FO evaluation and PSPACE-hardness.

- The first 2 steps in the above reduction from FO evaluation to QSAT allowed us to transform an arbitrary FO formula $\varphi$ over a database with arbitrary finite domain into an FO formula $\psi$ over the domain $\{0, 1\}$, s.t. the atomic formulas of $\psi$ are equalities only. Moreover, negation can be shifted immediately in front of the equalities.

- Equalities and negated equalities over $\{0, 1\}$ can be represented by relations eq and noteq in the obvious way (this works for any finite domain), i.e., $\text{eq} = \{(0, 0), (1, 1)\}$ and $\text{noteq} = \{(0, 1), (1, 0)\}$.

- It follows that FO evaluation remains PSPACE-hard even if we disallow equalities and negation in the FO formulas.
Conjunctive Queries

**Definition**

Conjunctive queries (CQs) are a special case of first-order queries whose only connective is $\land$ and whose only quantifier is $\exists$ (i.e., $\lor$, $\neg$ and $\forall$ are excluded). Alternatively, CQs can be considered as a single datalog rule

$$Q : r(u) \leftarrow r_1(u_1) \land \ldots \land r_n(u_n)$$

where $n \geq 0$; $r_1, \ldots, r_n$ are (not necessarily distinct) extensional relation symbols and $u, u_1, \ldots, u_n$ are lists of terms of appropriate length. Moreover, all variables in $u$ occur in at least one $u_i$.

In a Boolean conjunctive query, the head of the rule $Q$ is the 0-ary intensional relation symbol $true()$ (rather than some arbitrary term $r(u)$).

**Remark.** Conjunctive queries correspond to select-project-join queries in the relational algebra, i.e., unnested select-from-where queries in SQL.
Conjunctive Queries

Theorem

The query complexity and the combined complexity of conjunctive queries are NP-complete.

Proof

NP-Membership (of the combined complexity). For each variable $u$ of the query, we guess a domain element to which $u$ is instantiated. Then we check whether all the resulting ground atoms in the query body exist in $D$. This check is obviously feasible in polynomial time.

Hardness (of the query complexity). We reduce the NP-complete 3-Colorability problem to our problem. For this purpose, we consider an input database over the binary relation symbol $Edge$. 
NP-Hardness of query complexity

Since we are considering the query complexity, the database $D$ is fixed (but arbitrarily chosen). We choose $D$ with a single relation $\text{Edge} = \{\langle 1, 2 \rangle, \langle 1, 3 \rangle, \langle 2, 1 \rangle, \langle 2, 3 \rangle, \langle 3, 1 \rangle, \langle 3, 2 \rangle\}$

Now let $G = (V, E)$ be an arbitrary instance of the 3-Colorability problem. From this, we define the Boolean conjunctive query $Q$ as follows. $Q$ contains the variables $X = \{x_i \mid v_i \in V\}$. Moreover, we set

$$\text{ans}() \leftarrow \bigwedge_{[v_i, v_j] \in E} \text{Edge}(x_i, x_j)$$

Clearly, this reduction is feasible in logarithmic space. The correctness is seen as follows: $Q$ is true over the DB $D$ $\iff$ The variables in $X$ can be instantiated to values $\{1, 2, 3\}$, s.t. $Q$ contains only ground atoms occurring in $D$ $\iff$ The graph $G$ has a valid 3-coloring.
Learning Objectives

- The power of unrestricted alternation (in QBF)
- PSPACE as the complexity class of many strategy games
- The relationship of PSPACE and PH
- Complexity of query evaluation, first-order queries