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#### **Abstract**

We describe a technique and a tool called Qex for generating input tables and parameter values for a given parameterized SQL query. The evaluation semantics of an SQL query is translated into a specific background theory for a satisfiability modulo theories (SMT) solver as a set of equational axioms. Symbolic evaluation of a goal formula together with the background theory yields a model from which concrete tables and values are extracted. We use the SMT solver Z3 in the concrete implementation of Qex and provide an evaluation of its performance.

# 1 Introduction

The original motivation behind Qex comes from unit testing of relational databases, where a key challenge is the automatic generation of input tables and parameters for a given query and a given test condition, where a typical test condition is that the result of the query is a nonempty table. An early prototype of Qex as a proof-of-concept and an integration of Qex into the Visual Studio Database edition is discussed in [19, 24]. Here we present a new approach for encoding queries that uses algebraic datatypes and equational axioms, taking advatage of recent advances in SMT technology. The encoding is much simpler than the one described in [24], and boosted the performance of Qex by several orders of magnitude. In [24] algebraic datatypes were not available and queries were encoded into an intermediate background theory  $\mathscr{T}^{\Sigma}$  using bags and a summation operator. The resulting formula was eagerly expanded, for a given size of the database, into a quantifier free formula that was then asserted to the SMT solver. The expansion often caused an exponential blowup in the size of the expanded formula, even when some parts of the expansion were irrelevant with respect to the test condition. The new approach not only avoids the eager expansion but avoids also the need for nonlinear constraints that arise when dealing with multiplicities of rows in bags and aggregates over bags. Moreover, the axiomatic approach makes it possible to encode frequently occurring like-patterns through an automata based technique, and other string constraints. To this end, Qex now encodes strings faithfully as character sequences, whereas in [24] strings were abstracted to integers with no support for general string operations. Furthermore, algebraic datatypes provide a straightforward encoding for value types that allow null values. In addition, Qex now also handles table constraints and uses symmetry breaking formulas for search space reduction.

The core idea is as follows. A given SQL query q is translated into a term [q] over a rich background theory that comes with a collection of built-in (predefined) functions. Tables are represented by lists of tuples, where lists are built-in algebraic datatypes. In addition to built-in functions (such as arithmetical operations) the term [q] may also use functions whose meaning is governed by a set of additional axioms referred to as Th(q). These custom axioms describe the evaluation rules of SQL queries and are in most cases defined as recursive list axioms that resemble functional programs. Table 1 provides a rough overview of the SQL constructs supported in Qex and the corresponding theories used for mapping a given construct into a formula for Z3 [26, 10] that is used as the underlying SMT solver in the implementation of Qex. As indicated in the table, in all of the cases there is also an additional set of custom axioms that are used in addition to the built-in ones.

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Qex:	Symbolic	SQL query	explorer
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	Built-in theories						Custom
Features	Arithmetic	Bitvectors	Sets	Arrays	Algebraic d.t.	Tuples	theories
Table constraints	✓		✓		✓	✓	✓
SELECT clauses	✓				✓		✓
Aggregates	✓		✓	✓	✓	✓	✓
LIKE patterns		<b>√</b>			✓		✓
Null values					✓		✓

Table 1: Overview of features in Qex and related use of SMT theories.

For input tables and other parameters, the term  $[\![q]\!]$  uses uninterpreted constants. Given a condition  $\varphi$  over the result of  $[\![q]\!]$ , e.g.,  $[\![q]\!]\neq nil$  ( $[\![q]\!]$  is nonempty),  $\varphi$  is asserted to the SMT solver as a goal formula and Th(q) is asserted to the SMT solver as an additional set of axioms, sometimes called a *soft theory*. Next, a satisfiability check is performed together with *model generation*. If  $\varphi$  is satisfiable then the generated model is used to extract concrete values (interpretations) for the input table constants and other additional parameter constants.

The rest of the paper is structured as follows. Section 2 introduces some basic notions that are used throughout the paper. Section 3 defines a custom theory of axioms over lists that are used in Section 4 to translate queries into formulas. Section 5 discusses the implementation of Qex with a focus on its interaction with Z3. Section 6 provides some experimental evaluation of Qex. Section 7 is about related work, and Section 8 provides some final remarks.

## 2 Preliminaries

We assume that the reader is familiar with elementary concepts in logic and model theory, our terminology is consistent with [13] in this regard.

We are working in a fixed multi-sorted universe  $\mathscr{U}$  of values. For each sort  $\sigma$ ,  $\mathscr{U}^{\sigma}$  is a separate subuniverse of  $\mathscr{U}$ . The basic sorts needed in this paper are the Boolean sort  $\mathbb{B}$ ,  $(\mathscr{U}^{\mathbb{B}} = \{true, false\})$ , the integer sort  $\mathbb{Z}$ , and the n-tuple sort  $\mathbb{T}\langle \sigma_0, \dots, \sigma_{n-1} \rangle$  for  $n \geq 1$  of some given basic sorts  $\sigma_i$  for i < n. We also use other sorts but they are introduced at the point when they are first needed.

There is a collection of functions with a fixed meaning associated with the universe, e.g., arithmetical operations over  $\mathscr{U}^{\mathbb{Z}}$ . These functions and the corresponding function symbols are called *built-in*. Each function symbol f of arity  $n \geq 0$  has a fixed domain sort  $\sigma_0 \times \cdots \times \sigma_{n-1}$  and a fixed range sort  $\sigma_0 \times \cdots \times \sigma_{n-1} \to \sigma$ . For example, there is a built-in *relation* or *predicate* (Boolean function) symbol  $\langle : \mathbb{Z} \times \mathbb{Z} \to \mathbb{B}$  that denotes the standard order on integers. One can also declare *fresh* (new) *uninterpreted* function symbols f of arity f of a given domain sort and a given range sort. Using model theoretic terminology, these new symbols *expand* the signature.

Terms and formulas (or Boolean terms) are defined by induction as usual and are assumed to be well-sorted. We write FV(t) for the set of free variables in a term (or formula) t. A term or formula without free variables is closed.

A *model* is a mapping from function symbols to their interpretations (values). The built-in function symbols have the same interpretation in all models that we are considering, keeping that in mind, we may omit mentioning them in a model. A model *M* satisfies a closed formula  $\varphi$ ,  $M \models \varphi$ , if it provides an interpretation for all the uninterpreted function symbols in  $\varphi$  that makes  $\varphi$  true. For example, let  $f: \mathbb{Z} \to \mathbb{Z}$  be an uninterpreted function symbol and  $c: \mathbb{Z}$  be an uninterpreted constant. Let M be a

model where  $c^M$  (the interpretation of c in M) is 0 and  $f^M$  is a function that maps all values to 1. Then  $M \models 0 < f(c)$  but  $M \not\models 0 < c$ .

A closed formula  $\varphi$  is *satisfiable* if it has a model. A formula  $\varphi$  with  $FV(\varphi) = \bar{x}$  is *satisfiable* if its existential closure  $\exists \bar{x} \varphi$  is satisfiable. We write  $\models_{\mathscr{U}} \varphi$ , or  $\models \varphi$ , if  $\varphi$  is *valid* (true in all models). Some examples:  $0 < 1 \land 2 < 10$  is valid;  $4 < x \land x < 5$ , where  $x : \mathbb{Z}$  is a free variable, is unsatisfiable because there exists no integer between 4 and 5;  $0 < x \land x < 3$ , where  $x : \mathbb{Z}$  is a free variable, is satisfiable.

# 3 Equational axioms over lists

The representation of a table in Qex is a list of rows, where a row is a tuple. While bags of rows rather than lists would model the semantics of SQL more directly (order of rows is irrelevant, but multiple occurrences of the same row are relevant), the inductive structure of a list provides a way to define the evaluation semantics of queries by recursion. The mapping of queries to axioms, discussed in Section 4, uses a collection of axioms over lists that are defined next. Intuitively, the axioms correspond to definitions of standard (higher order) functionals that are typical in functional programming. The definitions of the axioms below, although more concise, correspond precisely to their actual implementation in Qex using the Z3 API. Before describing the actual axioms, we explain the intuition behind a particular kind of axioms, that we call *equational*, when used in an SMT solver.

### 3.1 Equational axioms and *E*-matching in SMT solvers

During proof search in an SMT solver, axioms are triggered by matching subexpressions in the goal. Qex uses particular kinds of axioms, all of which are equations of the form

$$\forall \bar{x}(t_{\text{lhs}} = t_{\text{rhs}}) \tag{1}$$

where  $FV(t_{lhs}) = \bar{x}$  and  $FV(t_{rhs}) \subseteq \bar{x}$ . The left-hand-side  $t_{lhs}$  of (1) is called the *pattern* of (1).

While SMT solvers support various kinds of patterns in general, in this paper we use the convention that the pattern of an equational axiom is always its left-hand-side.

The high-level idea behind E-matching is as follows. The axiom (1) is *triggered* by the current goal  $\psi$  of the solver, if  $\psi$  contains a subterm u and there exists a substitution  $\theta$  such that  $u =_E t_{\text{lhs}}\theta$ , i.e., u matches the pattern of the axiom (modulo the built-in theories E). If (1) is triggered, then the current goal is replaced by the *logically equivalent* formula where u has been replaced by  $t_{\text{rhs}}\theta$ .

Thus, the axioms that are used in Qex can be viewed as "rewrite rules", and each application of an axiom preserves the logical equivalence to the original goal. As long as there exists an axiom in the current goal that can be triggered, then triggering is guaranteed. Thus, termination is in general not guaranteed in the presence of (mutually) recursive axioms. Note that, unlike in term rewrite systems, there is no notion of term orderings or well-defined customizable strategies (at least not in the current version of Z3) that could be used to guide the triggering process of the axioms.

#### 3.2 Axioms over lists

For each sort  $\sigma$  there is a built-in *list sort*  $\mathbb{L}\langle\sigma\rangle$  and a corresponding subuniverse  $\mathscr{U}^{\mathbb{L}\langle\sigma\rangle}$ . (In Z3, lists are provided as built-in algebraic datatypes and are associated with standard constructors and accessors.) For a given element sort  $\sigma$  there is an empty list nil (of sort  $\mathbb{L}\langle\sigma\rangle$ ) and if e is an element of sort  $\sigma$  and e is a list of sort  $\mathbb{L}\langle\sigma\rangle$  then cons(e,l) is a list of sort  $\mathbb{L}\langle\sigma\rangle$ . The accessors are, as usual, e (head) and e (tail). In the following consider a fixed element sort  $\sigma$ . Observe that one can define a well-ordering such that,

in all of the recursive cases of the axioms, the right-hand-side decreases with respect to that ordering, which guarantees that triggering terminates and implies that the axioms are well-defined. In all of the cases, the use of the list constructors in the patterns is fundamental. In most cases one can provide more compact and logically equivalent definitions of the axioms where the right-hand-sides are combined in a disjunction, but where the pattern is too general and may cause nontermination of axiom triggering in an SMT solver.

#### **3.2.1** Filter

Let  $\varphi$  be a formula with a single free variable  $x_0$ :  $\sigma$ . Declare the function symbol  $Filter[\varphi]$ :  $\mathbb{L}\langle \sigma \rangle \to \mathbb{L}\langle \sigma \rangle$  and define the following axioms:

$$Filter[\varphi](nil) = nil$$

$$\forall x_0 x_1 (Filter[\varphi](cons(x_0, x_1)) = Ite(\varphi, cons(x_0, Filter[\varphi](x_1)), Filter[\varphi](x_1)))$$

The Ite-term Ite( $\phi$ ,  $t_1$ ,  $t_2$ ) equals  $t_1$ , if  $\phi$  is true; it equals  $t_2$ , otherwise. Ite is a built-in function.

### 3.2.2 Map

Let  $t:\rho$  be a term with a single free variable  $x_0:\sigma$ . Declare the function symbol  $Map[t]:\mathbb{L}\langle\sigma\rangle\to\mathbb{L}\langle\rho\rangle$  and define:

$$Map[t](nil) = nil$$
  
$$\forall x_0 x_1 (Map[t](cons(x_0, x_1)) = cons(t, Map[t](x_1)))$$

#### **3.2.3** Reduce

Let  $t : \rho$  be a term with two free variables  $x_0 : \sigma$  and  $x_1 : \rho$ . Declare the function symbol  $Reduce[t] : \mathbb{L}\langle \sigma \rangle \times \rho \to \rho$  and define:

$$\forall x (Reduce[t](nil,x) = x)$$
  
$$\forall x_0 x_1 x_2 (Reduce[t](cons(x_0,x_2),x_1) = Reduce[t](x_2,t))$$

For example, if  $l: \mathbb{L}\langle \mathbb{Z} \rangle$  is a list of integers, then  $Reduce[x_0 + x_1](l, 0)$  is equal to the sum of the integers in l, or 0 if l is empty (in any model that satisfies the corresponding Reduce[]-axioms).

#### 3.2.4 Cross product

Declare the function symbols  $Cross: \mathbb{L}\langle \sigma \rangle \times \mathbb{L}\langle \rho \rangle \to \mathbb{L}\langle \mathbb{T}\langle \sigma, \rho \rangle \rangle$  and  $Cr: \sigma \times \mathbb{L}\langle \sigma \rangle \times \mathbb{L}\langle \rho \rangle \to \mathbb{L}\langle \rho \rangle \to \mathbb{L}\langle \sigma, \rho \rangle$ , and define

$$\forall x (Cross(nil,x) = nil)$$

$$\forall x (Cross(x,nil) = nil)$$

$$\forall \bar{x} (Cross(cons(x_0,x_1),cons(x_2,x_3)) = Cr(x_0,x_1,cons(x_2,x_3),cons(x_2,x_3)))$$

$$\forall \bar{x} (Cr(x_0,x_1,nil,x_2) = Cross(x_1,x_2))$$

$$\forall \bar{x} (Cr(x_0,x_1,cons(x_2,x_3),x_4) = cons(T(x_0,x_2),Cr(x_0,x_1,x_3,x_4)))$$

where  $T: \sigma \times \rho \to \mathbb{T}\langle \sigma, \rho \rangle$  is the built-in tuple constructor (for the given sorts). For example, the term Cross(cons(1, cons(2, nil)), cons(3, cons(4, nil))) is equal to the term

$$cons(T(1,3), cons(T(1,4), cons(T(2,3), cons(T(2,4), nil)))).$$

### 3.2.5 Remove duplicates

The function *RemoveDuplicates* is used to remove duplicates from a list. The definition makes use of built-in sets and set operations; the set sort of element sort  $\sigma$  is denoted  $\mathbb{S}\langle\sigma\rangle$ .

Declare: *RemoveDuplicates* :  $\mathbb{L}\langle\sigma\rangle \to \mathbb{L}\langle\sigma\rangle$ , Rd :  $\mathbb{L}\langle\sigma\rangle \times \mathbb{S}\langle\sigma\rangle \to \mathbb{L}\langle\sigma\rangle$ . Define:

```
\forall x (RemoveDuplicates(x) = Rd(x,\emptyset))
\forall x (Rd(nil,x) = nil)
\forall \bar{x} (Rd(cons(x_0,x_1),x_2) = Ite(x_0 \in x_2, Rd(x_1,x_2), cons(x_0, Rd(x_1,\{x_0\} \cup x_2))))
```

## 4 From SQL to formulas

In this section we show how we translate an SQL query q into a set of axioms Th(q) that is suitable as an input soft theory to an SMT solver. The translation makes use of the list axioms discussed in Section 3. We omit full details of the translation and illustrate it through examples and templates, which should be adequate for understanding how the general case works. The focus is on the purely relational subset of SQL (without side-effects). We start by describing how tables are represented.

#### 4.1 Tables and table constraints

Tables are represented by lists of rows where each row is a tuple. The sorts of the elements in the tuple are derived from the types of the corresponding columns that are given in the database schema. The currently supported column types in Qex are: BigInt, Int, SmallInt, TinyInt, Bit, and Char. The first four types are mapped to  $\mathbb{Z}$  (and associated with a corresponding range constraint, e.g., between 0 and 255 for TinyInt). Bit is mapped to  $\mathbb{B}$ . Char (that in SQL stands for a sequence of characters) is mapped to the *string sort* (or *word sort*)  $\mathbb{W} = \mathbb{L}\langle \mathbb{C} \rangle$ , where  $\mathbb{C}$  is the built-in sort of *n*-bitvectors for some fixed *n* that depends on the character range: UTF-16 (n = 16), basic ASCII (n = 7), extended ASCII (n = 8).

The order of rows in a table is irrelevant regarding the evaluation semantics of queries. The number of times the same row occurs in a table is the *multiplicity* of the row. In general, duplicate rows are allowed in tables so the multiplicity may be more than one. However, in most cases input tables have primary keys that disallow duplicates. Tables may also be associated with other constraints such as foreign key constraints and restrictions on the values in the columns. In Qex, these constraints are translated into corresponding formulas on the list elements. The following example illustrates that aspect of Qex.

**Example 1.** Consider the following schema for a school database.

```
CREATE TABLE [School]. [Scores]
(StudentID tinyint not null FOREIGN KEY REFERENCES Students(StudentNr),
CourseID tinyint not null CHECK(1 <= CourseID and CourseID <= 100),
Points tinyint not null CHECK(Points <= 10),
PRIMARY KEY (StudentID, CourseID),
CHECK(NOT(1 <= CourseID and CourseID <= 10) or Points < 6));

CREATE TABLE [School]. [Students]
(StudentNr tinyint not null PRIMARY KEY,
StudentName char(100) not null);
```

The (primary) key of the Scores table is the pair containing a student id and a course id and each row provides the number of points the student has received for the given course. The additional constraints

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are that the course ids go from 1 to 100, no course gives more than 10 points and courses 1 through 10 give a maximum of 5 points.

Qex declares the table variables  $Scores: \mathbb{L}\langle \mathbb{T}\langle \mathbb{Z}, \mathbb{Z}, \mathbb{Z}\rangle \rangle$  and  $Students: \mathbb{L}\langle \mathbb{T}\langle \mathbb{Z}, \mathbb{W}\rangle \rangle$ . There is a given bound k on the number of rows in each table. (In general there is a separate bound per table and the bounds are increased during model generation discussed in Section 5.) The following equalities are generated:

```
Scores = cons(Scores_0,...,cons(Scores_{k-1},nil))

Students = cons(Students_0,...,cons(Students_{k-1},nil))
```

where  $Scores_i: \mathbb{T}\langle \mathbb{Z}, \mathbb{Z}, \mathbb{Z} \rangle$  and  $Students_i: \mathbb{T}\langle \mathbb{Z}, \mathbb{W} \rangle$  for i < k. For the primary key constraints, the following formulas are generated. The distinctness predicate and the projections functions  $\pi_i$  on tuples are built-in. We use t.i to abbreviate the term  $\pi_i(t)$ .

```
Distinct(T(Scores_0.0, Scores_0.1), \dots, T(Scores_{k-1}.0, Scores_{k-1}.1))
Distinct(Students_0.0, \dots, Students_{k-1}.0)
```

For expressing the foreign key constraint, Qex uses the built-in sets and the subset predicate:

$$\{Scores_i.0\}_{i < k} \subseteq \{Students_i.0\}_{i < k}$$

The remaining constraints are conjunctions of check-constraints on individual rows, e.g.,

$$\bigwedge_{i < k} (\neg (1 \leq Scores_i.1 \land Scores_i.1 \leq 10) \lor Scores_i.2 < 6)$$

asserts that courses 1 through 10 give a maximum of 5 points.

#### 4.2 Null values

If a column in a table is optional, it may contain a null value as a placeholder for an unknown value. Any column in SQL (other than a primary key column) is optional unless a not null type constraint is associated with the column type. Algebraic datatypes provide a convenient mechanism to represent optional values through *lifted sorts*. Let  $\sigma$  be any sort. Declare the datatype  $?\langle \sigma \rangle$  with the constructors  $NotNull: \sigma \to ?\langle \sigma \rangle$ ,  $Null: ?\langle \sigma \rangle$ , the accessor  $Value: ?\langle \sigma \rangle \to \sigma$  (that maps any value NotNull(a) to a), and the testers  $IsNotNull: ?\langle \sigma \rangle \to \mathbb{B}$ ,  $IsNull: ?\langle \sigma \rangle \to \mathbb{B}$ . Declaring such datatypes is directly supported in Z3.

When an SQL expression e is encoded as a term [e], it is assumed that e is well-formed. Operations using optional values are assumed to occur in a context where the value is known to be not null. SQL includes particular predicates IS NULL and IS NOT NULL for this purpose. In the translation the corresponding testers are used and the *Value* accessor is applied to cast the optional value to its underlying sort.

Note that, formally, there is a distinct null value for each lifted sort. This does not cause a semantic discrepency with SQL, since it is not possible in SQL to compare null values with comparison operators.

### 4.3 Formulas for queries

As the concrete input of queries, Qex uses a subset of the abstract syntax of the TSQL [1] grammar. It is not feasible to fit the full details of the translation from queries to formulas into the paper, instead, we look at a collection of representative samples that illustrate the core ideas behind the translation. In the samples, we reuse the schema from Example 1. We denote the formula resulting from a query q by [q].

#### 4.3.1 SELECT clauses

The main component of a query is a *select clause*. A select clause refers to a particular selection of columns from a given table by using a *select list*. The table is often a derived table, as the result of a join operation. Consider the query q:

```
SELECT StudentName, Points
FROM Students JOIN Scores ON Scores.StudentID = Students.StudentNr
WHERE Scores.CourseID = 10 AND Scores.Points > 0
```

The formula [q] is:

$$Map[T(x.0.1,x.1.2)](Filter[x.1.1 = 10 \land x.1.2 > 0](Filter[x.0.0 = x.1.0](Cross(Students, Scores))))$$

where  $x: \mathbb{T}\langle \mathbb{T}\langle \mathbb{Z}, \mathbb{W}\rangle, \mathbb{T}\langle \mathbb{Z}, \mathbb{Z}, \mathbb{Z}\rangle\rangle$ . Such formulas get human-unreadable very quickly. During the process of creating  $[\![q]\!]$ , usually several list axioms are created. This set of axioms is referred to as Th(q). In particular, in this case Th(q) includes the axioms for the map, filter, and cross product function symbols that occur in  $[\![q]\!]$ .

### 4.3.2 Aggregates

Aggregates are used to combine values from all the rows in a table. The most common aggregates are MIN, MAX, SUM, and COUNT. For example, the following query  $q_1$  selects the maximum points from the Scores table.

```
SELECT DISTINCT MAX(Points) from Scores
```

Depending on the use of  $q_1$ , the translation  $[q_1]$  is either the singleton list:

$$cons(T(Reduce[Ite(x_0.2 \ge x_1, x_0.2, x_1)](Scores, -\infty)), nil)$$

or just the *Reduce*[]-term:

$$Reduce[Ite(x_0.2 \ge x_1, x_0.2, x_1)](Scores, -\infty)$$

The first case applies if  $q_1$  is used as a top-level query, the second case applies if  $q_1$  is used as a *subquery* expression. The second case applies in the following query  $q_2$  that also uses the MAX aggregate in the top level select list in combination with GROUP BY that eliminates duplicates from the resulting table:

```
SELECT StudentID, MAX(Points) FROM Scores GROUP BY StudentID HAVING MAX(Points) = (SELECT DISTINCT MAX(Points) from Scores)
```

The query  $q_2$  selects all students that have the most points at some course. The translation of  $[q_2]$  is as follows where the *Filter*[] application corresponds to the HAVING clause that is applied to the result of the grouping.

$$Filter[x.1 = [q_1]](RemoveDuplicates(Select[x_0.0, MAX(x_0.3)](Scores)))$$

The definition of *Select*[] is technically more complicated but similar to the other recursive list axioms. It collects the maximum points for each student id and uses the built-in *arrays* in Z3 to accumulate the values, see the Appendix.

### 4.3.3 LIKE-patterns

Like-patterns are particular regular expressions that can be used as constraints on strings. A like-pattern r is converted into a *symbolic finite automaton* [23] (SFA)  $A_r$  that is similar to a classical finite automaton except that moves are labeled by formulas denoting *sets* of characters rather than single characters. The automaton  $A_r$  is translated into a theory  $Th(A_r)$ . The theory describes the acceptance condition for words in  $L(A_r)$ . In particular,  $Th(A_r)$  defines a predicate

$$Acc^{A_r}: \mathbb{W} \times \mathbb{N} \to \mathbb{B}$$
.

where  $\mathbb{N}$  is an algebraic datatype for *unary natural numbers* with the constructors  $\overline{0}: \mathbb{N}$  and  $\mathbf{s}: \mathbb{N} \to \mathbb{N}$ . We write  $\overline{k+1}$  for  $\mathbf{s}(\overline{k})$ . We use the following property of the theory of  $A_r$  [23, Theorem 1]:

**Proposition 1.** Let t be a closed term of sort  $\mathbb{W}$ , k a nonnegative integer, and M a model of  $Th(A_r)$ . Then  $M \models Acc^{A_r}(t,\overline{k})$  iff  $t^M \in L(A_r)$  and  $|t^M| \leq k$ .

In column type declarations of SQL database schemas, a maximum string length is associated with the char type (default being 1), e.g., the type char (100) of a column allows strings containing at most 100 characters. In the formula  $Acc^{A_r}(t,\overline{k})$ , where t refers to a column whose values are strings, k is the maximum length of the strings in that column.

**Example 2.** Consider the query q that selects students whose name starts with the letter B followed by any letter between a and n followed by 0 or more additional characters:

SELECT StudentName FROM Students WHERE StudentName like "B[a-n]%"

The SFA A for "B[a-n]%" is (#>=a) where # is a free variable of sort  $\mathbb C$  and each symbolic move  $(i, \varphi[\#], j)$  denotes the set of transitions  $\{(i, a, j) \mid a \in \mathscr{U}^{\mathbb C}, \models \varphi[a]\}$ . For each state SO,SI,S2 of A there are two axioms in Th(A), one for length bound =0 and the other one for length bound >0:

```
\begin{array}{lll} \textit{S0}: & \forall x (Acc(x,\overline{\textbf{0}}) \Leftrightarrow \textit{false}) & \forall x y (Acc(x,\textbf{s}(y)) \Leftrightarrow x \neq \textit{nil} \land \textit{hd}(x) = \texttt{B} \land \textit{Acc}_1(\textit{tl}(x),y)) \\ \textit{S1}: & \forall x (Acc_1(x,\overline{\textbf{0}}) \Leftrightarrow \textit{false}) & \forall x y (Acc_1(x,\textbf{s}(y)) \Leftrightarrow x \neq \textit{nil} \land \textit{hd}(x) \geq \texttt{a} \land \textit{hd}(x) \leq \texttt{n} \land \textit{Acc}_2(\textit{tl}(x),y)) \\ \textit{S2}: & \forall x (Acc_2(x,\overline{\textbf{0}}) \Leftrightarrow x = \textit{nil}) & \forall x y (Acc_2(x,\textbf{s}(y)) \Leftrightarrow x = \textit{nil} \lor (x \neq \textit{nil} \land \textit{Acc}_2(\textit{tl}(x),y))) \end{array}
```

The term [q] is  $Map[T(x_0.1)](Filter[Acc(x_0.1, \overline{100})](Students))$ . Note that  $Th(A) \subseteq Th(q)$ .

The automata based approach opens up several transformation techniques that can be performed in the process of encoding queries and theories of queries that involve like-patterns. These upfront transformations can greatly simplify the formulas. We illustrate this with an example involving the use of *product* of SFAs [23].

**Proposition 2.** Let A and B be SFAs, then  $L(A \otimes B) = L(A) \cap L(B)$ .

**Example 3.** Consider the following query  $q_{LIKE}$  with n+1 occurrences of "\_" in the first like-pattern and n occurrences of "\_" in the second like-pattern:

```
SELECT StudentName FROM Students
WHERE StudentName like "%a____" AND StudentName like "%b____"
```

 $\boxtimes$ 

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The first like-pattern corresponds to the regex  $r_1$ =.\*a.{n+1} and the second like-pattern corresponds to the regex  $r_2$ =.\*b.{n}. The query is essentially an intersection constraint of  $r_1$  and  $r_2$ . In a direct encoding of  $q_{\text{LIKE}}$ ,  $Th(q_{\text{LIKE}})$  includes both the axioms for  $A_{r_1}$  as well as  $A_{r_2}$ . Rather than using  $A_{r_1}$  and  $A_{r_2}$  separately, the product  $A_{r_1} \otimes A_{r_2}$  of  $A_{r_1}$  and  $A_{r_2}$  can be used together with the theory  $Th(A_{r_1} \otimes A_{r_2})$  instead of  $Th(A_{r_1}) \cup Th(A_{r_2})$ . Thus, with *product encoding*,

$$[[q_{LIKE}]] = Map[T(x_0.1)](Filter[Acc^{A_{r_1} \otimes A_{r_2}}(x_0.1, \overline{100})](Students))$$

and with direct encoding,

$$[q_{\text{LIKE}}] = Map[T(x_0.1)](Filter[Acc^{A_{r_1}}(x_0.1, \overline{100}) \land Acc^{A_{r_2}}(x_0.1, \overline{100})](Students))$$

The gain in performance is discussed in Section 6.

Note that correctness of the transformation illustrated in Example 3 follows from Propositions 1 and 2.

# 5 Implementation

Qex uses the SMT solver Z3 [26, 10]. Interaction with Z3 is implemented through its programmatic API rather than using a textual format, such as the smt-lib format [20]. The main reasons for working with the API are: access to built-in datatypes; model generation; working within a given context. The first point is fundamental, since algebraic datatypes are central to the whole approach and are not part of the smt-lib standard.

Besides allowing to check satisfiability, perhaps the most important feature exposed by some SMT solvers (including Z3) for the purposes of test input generation is *generating a model* as a witness of the satisfiability check, i.e., a mapping of the uninterpreted function symbols to their interpretations. Z3 has a separate method for satisfiability checking with model generation. This code snippet illustrates the use of that functionality:

```
Model m;
z3.AssertCnstr(f);
LBool sat = z3.CheckAndGetModel(out m);
Term v = m.Eval(s); ...
```

A *context* includes declarations for a set of symbols, and assertions for a set of formulas. A context is essentially a layering mechanism for signature expansions with related constraints. There is a *current context* and a backtrack stack of previous contexts. Contexts can be saved through *pushing* and restored through *popping*. When a satisfiability check is performed in a given context, the context may become inconsistent. Qex uses contexts during table generation and in SFA algorithms during theory generation for like-patterns.

### 5.1 Incremental table generation

Let q be a fixed query and assume that  $X_1, \ldots, X_n$  are the input table variables. Assume [q]:  $\sigma$  and let  $\varphi[Y]$  be a formula with the free variable Y:  $\sigma$ . Intuitively,  $\varphi$  is a *test condition* on the result of the query, e.g.  $Y \neq nil$ . The following *basic table generation procedure* describes the input table generation for q and  $\varphi$ .

1. Assert Th(q), i.e. add the axioms of q to the current context.

- 2. Let  $\vec{k} = (k_1, \dots, k_n) = (1, \dots, 1)$  be the initial sizes of the input tables. Repeat the following until a model M is found or a timeout occurs.
  - (a) Push the current context, i.e., create a backtrack point.
  - (b) Create constraints for  $X_1, \ldots, X_n$  using  $\vec{k}$  to fix the table sizes.
  - (c) Assert  $\varphi[[q]]$
  - (d) Check and get the model M. If the check fails, increase  $\vec{k}$  systematically and pop the context.
- 3. Get the values of  $X_1, \ldots, X_n$  in M.

There are several possible variations of the basic procedure. The table constraints can be updated incrementally when the table sizes are increased. The table constraints can also be created for *upper* bounds rather than exact bounds on the table sizes. One way to do so is as follows:

$$table = cons(row1, rest1) \land (rest1 = nil \lor (rest1 = cons(row2, rest2) \land \cdots))$$

The size of the overall resulting formula is always polynomial in the size of the original query and  $\vec{k}$ . In practice, Qex uses bounds on  $\vec{k}$  and overall time constraints to guarantee termination, as deciding the satisfiability of queries is undecidable in general [9].

### 5.2 Symmetry breaking formulas

The translation of a query q into a formula  $[\![q]\!]$  together with Th(q) and the additional table constraints looks very much like a "functional program with constraints". This intuition is correct as far as the logical meaning of the translation is concerned. There are, however, no mechanisms to control the evaluation order of patterns (such as, "outermost first") and no notion of term orderings. The search space for  $[\![q]\!]$  is typically vast.

Recall that although Qex uses lists to encode tables, the order of rows is not relevant according to the SQL semantics. We can therefore assert predicates that constrain the input tables to be *ordered* (thus eliminating all symmetrical models where the ordering does not hold). Consider a table  $cons(row_0, cons(row_1, \cdots cons(row_n, nil)))$  of sort  $\mathbb{L}\langle\sigma\rangle$ . Define a lexicographic order predicate  $\preceq : \sigma \times \sigma \to \mathbb{B}$ . The definition of  $\preceq$  on integers is just the built-in order  $\leq$ , similarly for bitvectors. For tuples, it is the standard lexicographic order defined in terms of the orders of the respective element sorts. For strings (lists of bitvectors) the order predicate can be defined using recursion over lists. Assert the *symmetry breaking formula* 

$$\bigwedge_{i < n-1} row_i \leq row_{i+1}$$

In some situations the symmetry breaking formula can be strengthened. For example, when the table has a primary key then the formula can be strengthened by using the strict order  $\prec$  instead of  $\leq$ . Moreover, if all of the columns are part of the primary key then the primary key constraint itself becomes redundant.

Using symmetry breaking over lists in this way improves the performance by orders of magnitude over the previous approach [24] using bags.

# 6 Experiments

We provide some performance evaluation results of Qex on a collection of sample queries.<sup>1</sup> In the first set of experiments we look at the performance of the basic table generation procedure. In these experiments

<sup>&</sup>lt;sup>1</sup>The experiments were run on a Lenovo T61 laptop with Intel dual core T7500 2.2GHz processor.

Table 2: Sample queries.

#	Query	t[ms]	k
1	DECLARE @x as tinyint; SELECT DISTINCT Scores.StudentID, SUM(Scores.Points) FROM Scores WHERE Scores.Points > 2 HAVING SUM(Scores.Points) >= @x AND @x > 5	20	1
2	SELECT Scores.StudentID, MAX(Scores.Points) FROM Scores GROUP BY Scores.StudentID HAVING MAX(Scores.Points) = (SELECT MAX(Scores.Points) FROM Scores)	20	1
3	DECLARE @x as tinyint; SELECT DISTINCT COUNT(S.StudentName) FROM Students as S WHERE S.StudentName LIKE "%Mar[gkc]us%" AND S.StudentNr > @x HAVING COUNT(S.StudentName) > @x AND @x > 2	1200	4
4	DECLARE @x as tinyint;  SELECT Students.StudentName, SUM(Points)  FROM Scores JOIN Students ON Scores.StudentID = Students.StudentNr  WHERE Scores.Points > 2 AND Students.StudentName LIKE "John%"  GROUP BY Students.StudentName  HAVING SUM(Points) >= @x AND @x > 15	130	2
5	SELECT Students.StudentName, Scores.Points FROM Students JOIN Scores ON Scores.StudentID = Students.StudentNr WHERE Scores.CourseID = 10 AND Scores.Points > 0	30	1
6	SELECT Students.StudentName, Courses.CourseName, Scores.Points FROM Scores JOIN Students ON Scores.StudentID = Students.StudentNr JOIN Courses ON Courses.CourseNr = Scores.CourseID WHERE Scores.Points > 2 AND Students.StudentName LIKE "%bob%" AND Courses.CourseName LIKE "AI%"	160	1

we use the same bound k for both tables. The test condition used here is that the result is nonempty. Table 2 summarizes the overall time t (in ms) for each query q, which includes the parsing time, the generation time of Th(q), and the model generation time. The column k shows the number of rows generated for the input tables. Some of the queries include parameters, indicated with  $\mathfrak Q$ , the values of parameters are also generated. (The actual data that was generated is not shown here.) We reuse the schema introduced in Example 1. The last query uses an additional table called Courses.

The total size of the query seems to have very little effect on the time t. The key factor is the use of *aggregates* and the constraints they introduce that cause the input tables to grow, thus, causing backtracking during model generation, that is clearly seen for query #3. Consider the following experiment. Take query #3 and replace the constant 2 in it with the constant n for  $n = 1, \ldots, 15$ . Figure 1 shows the time t in seconds as a function of n; k is always n + 2.

Given a query q, several optimizations or transformations can be performed on the term  $[\![q]\!]$  as well as the set of axioms Th(q) prior to asserting them to the solver. Figure 2 shows a drastic decrease in model generation time for  $q_{\rm LIKE}$  from Example 3 in Qex when the product construction is used. By performing localized SMT solver queries during product construction of SFAs, the size of the resulting automata can often dramatically decrease.

We also reevaluated the performance of Qex on the benchmarks reported in [24, Table 1] that use a different sample database schema (where strings do not occur). In all of the cases the performance improvement was between 10x and 100x. As we suspected, the eager expansion time reported as  $t_{\rm exp}$  in [24], that was by an order of magnitude larger than the model generation time  $t_{\rm z3}$ , is avoided completely in the new approach. The initial cost of creating [q] is negligable, since the size of [q] is polynomial in the size of [q] in theory, and close to linear in practice. The added overhead during model generation due

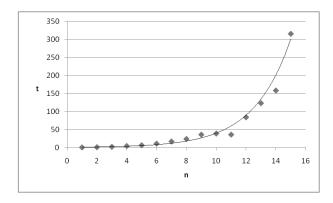


Figure 1: Exploration times (sec) for query #3 in Table 2 when the constant 2 is replaced with n for n = 1, ..., 15.

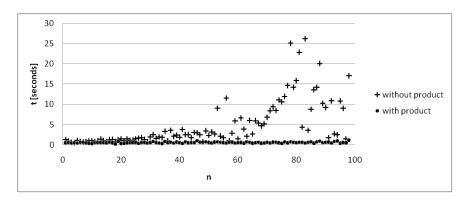


Figure 2: Exploration times (sec) for query  $q_{LIKE}$  without (scattered crosses) and with (solid line of dots at the bottom) product construction for n = 1, ..., 98.

to the use of axioms only marginally increased the model generation time  $t_{z3}$ .

### 7 Related work

The first prototype of Qex was introduced in [24]. The current paper presents a continuation of the Qex project [19], and a redesign of the encoding of queries into formulas based on a lazy axiomatic approach that was briefly mentioned in [24] but required support for algebraic datatypes in the underlying solver. Moreover, Qex now also supports a substantially larger fragment of SQL (such as subquery expressions) and like-patterns on strings, as discussed above.

Deciding satisfiability of SQL queries requires a formal semantics. While we give meaning to SQL queries by an embedding into the theory of an SMT solver, there are other approaches, e.g., defining the semantics in the Extended Three Valued Predicate Calculus [17], or using bags as a foundation [7]. Satisfiability of queries is also related to logic-based approaches to semantic query optimization [5]. The general problem of satisfiability of SQL queries is undecidable and computationally hard for very restricted fragments, e.g., deciding if a query has a nonempty answer is NEXP-hard for nonrecursive range-restricted queries [9].

Several research efforts have considered formal analysis and verification of aspects of database sys-

tems, usually employing a possibly interactive theorem prover. For example, one system [21] checks whether a transaction is guaranteed to maintain integrity constraints in a relational database; the system is based on Boyer and Moore-style theorem proving [4].

There are many existing approaches to generate database tables as test inputs. Most approaches create data in an ad-hoc fashion. Only few consider a target query. Tsai et.al. present an approach for test input generation for relational algebra queries [22]. They do not use lists to represent tables. They propose a translation of queries to a set of systems of linear inequalities, for which they implemented an ad-hoc solving framework which compares favorably to random guessing of solutions. A practical system for testing database transactions is AGENDA [11]. It generates test inputs satisfying a database schema by combining user-provided data, and it supports checking of complex integrity constraints by breaking them into simpler constraints that can be enforced by the database. While this system does not employ a constraint solver, it has been recently refined with the TGQG [6] algorithm: Based on given SQL statements, it generates test generation queries; execution of these queries against a user-provided set of data groups yields test inputs which cover desired properties of the given SQL statements.

Some recent approaches to test input generation for databases employ automated reasoning. The relational logic solver Alloy [14, 15] has been used by Khalek et.al. [16] to generate input data for database queries. Their implementation supports a subset of SQL with a simplified syntax. In queries, they can reason about relational operations on integers, equality operations on strings, and logical operations, but not about nullable values, or grouping with aggregates such as SUM; they also do not reason about duplicates in the query results. QAGen [3] is another approach to query-solving. It first processes a query in an adhoc-way, which requires numerous user-provided "knob" settings as additional inputs. From the query, a propositional logic formula is generated, which is then decided by the Cogent [8] solver to generate the test inputs. In [2] a model-checking based approach, called Reverse Query Processing, is introduced that, given a query and a result table as input, returns a possible database instance that could have produced that result for that query, the approach uses reverse relational algebra. In [25] an intentional approach is presented in which the database states required for testing are specified as constrained queries using a domain specific language. Recently, test input generation of queries has been combined with test input generation of programs that contain embedded queries in the program text [12], using ad-hoc heuristic solvers for some of the arising constraints from the program and the queries.

### 8 Conclusion and future work

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The current implementation of the Qex project is still in its early stages, but we were highly encouraged by the performance improvements when switching to the lazy approach and reducing the need for nonlinear constraints through a different representation of tables. There are many more possible optimizations that can be performed as a preprocessing step on formulas generated by Qex, before asserting them to the SMT solver. One such optimization, using automata theory, was illustrated in Example 3 and Figure 2 when multiple like-patterns occur in a query. Systematic preprocessing can also often reveal that a query is trivially false, independent of the size of input tables, e.g., if an '\_' is missed in the first like-pattern in Example 3 then the product automaton would be empty.

For practical usage in an industrial context, where SQL queries are usually embedded in other programs or in store procedures, we are looking at integrating Qex in Pex [18]. For efficient support for regex constraints in Pex, integration of Rex [23] is a first step in that integration.

It is also possible to apply a translation similar to the one described in the paper to LINQ queries, although, unlike in SQL, the semantics of LINQ queries depends on the order of the rows in the tables. This fits well with the list representation of tables but imposes some limitations on the use of certain optimizations (such as the use of symmetry breaking formulas).

A practical limitation of Qex is if queries use multiple joins and aggregates and the input tables need to contain a high number of rows in order to satisfy the test condition. Another limitation is the use nonlinear constraints over unbounded integers, in particular multiplication, that has currently only limited support in Z3. We consider using bitvectors instead. Despite these limitations, the mere size of queries does not seem to be a concern, neither the size of Th(q) for a given query q. The size of Th(q) may easily be in hundreds, in particular when several like-patterns are used, where the number of axioms is proportional to the size of the finite automaton accepting the pattern.

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# **Appendix: Select with grouping and aggregates**

Select clauses with aggregates and grouping are translated into formulas using the following axioms. Let  $t_1:\rho$  be a term with a single free variable  $x_0:\sigma$ . Let  $t_2:\mathbb{Z}$  be a term with a single free variable  $x_0:\sigma$ . Intuitively,  $\sigma$  is a tuple sort, both  $t_1$  and  $t_2$  are projections, and the term  $t_2$  corresponds to some aggregate operation, such as MAX.

We declare the function symbol  $Select[t_1,t_2]: \mathbb{L}\langle \sigma \rangle \to \mathbb{L}\langle \mathbb{T}\langle \rho, \mathbb{Z}\rangle \rangle$  and define a set of recursive axioms for it that for each element in the list collect the maximum value with respect to  $t_2$  and then create a list of pairs that for each projection  $t_1$  provides that maximum value. In order to define these axioms, arrays (mathematical maps) are used.

Given argument sort  $\sigma_1$  and result sort  $\sigma_2$ ,  $\mathbb{A}\langle \sigma_1, \sigma_2 \rangle$  is the corresponding array sort. (In particular  $\mathbb{S}\langle \sigma_1 \rangle$  is synonymous with  $\mathbb{A}\langle \sigma_1, \mathbb{B} \rangle$ .) Declare

```
\begin{split} \textit{Select}[t_1,\mathsf{MAX}(t_2)] & : & \mathbb{L}\langle\sigma\rangle \to \mathbb{L}\langle\mathbb{T}\langle\rho,\mathbb{Z}\rangle\rangle, \\ \textit{Sel1} & : & \mathbb{L}\langle\sigma\rangle \times \mathbb{A}\langle\sigma,\mathbb{Z}\rangle \times \mathbb{L}\langle\sigma\rangle \to \mathbb{L}\langle\sigma\rangle, \\ \textit{Sel2} & : & \mathbb{L}\langle\sigma\rangle \times \mathbb{A}\langle\sigma,\mathbb{Z}\rangle \to \mathbb{L}\langle\sigma\rangle \end{split}
```

and define the axioms, where ArrayRead and ArrayStore are built-in,

```
 \forall x (Select[t_1, \text{MAX}(t_2)](x) = Sel1(x, \{\_\mapsto -\infty\}, x)) 
 \forall \bar{x} (Sel1(cons(x_0, x_1), x_2, x_3) = Sel1(x_1, Ite(ArrayRead(x_2, T(t_1, t_2)) \ge t_2, x_2, ArrayStore(x_2, T(t_1, t_2), t_2)), x_3)) 
 \forall \bar{x} (Sel1(nil, x_0, x_1) = Sel2(x_1, x_0)) 
 \forall \bar{x} (Sel2(cons(x_0, x_1), x_2) = cons(ArrayRead(x_2, T(t_1, t_2)), Sel2(x_1, x_2))) 
 \forall x (Sel2(nil, x) = nil)
```