ABSTRACT

Though inevitable for effective cost-based query rewriting, the derivation of meaningful cardinality estimates has remained a notoriously hard problem in the context of XQuery. By basing the estimation on a relational representation of the XQuery syntax, we show how existing cardinality estimation techniques for XPath and proven relational estimation machinery can play together to yield dependable forecasts for arbitrary XQuery (sub)expressions. Our approach benefits from a light-weight form of data flow analysis. Abstract domain identifiers guide our query analyzer through the estimation process and allow for informed decisions even in case of deeply nested XQuery expressions. A variant of projection paths [14] provides a versatile interface into which existing techniques for XPath cardinality estimation can be plugged in seamlessly. We demonstrate an implementation of this interface based on data guides. Experiments show how our approach can equally cope with both, structure- and value-based queries. It is robust with respect to intermediate estimation errors, from which we typically found our implementation to recover gracefully.

1. INTRODUCTION

Modern database implementations derive much of their performance from sophisticated optimizer components that transform incoming queries into efficient execution plans. To properly select access paths, join order, or materialization strategies, optimizers heavily depend on accurate predictions of the value distribution and cardinality of individual query sub-results.

Such cardinality forecasts have been notoriously hard to make in the context of XQuery, where the absence of a strict database schema, the expressiveness of the XQuery language, and the dualism between structural and value-based querying all add to the complexity of the estimation problem. In this work, we show how relational plan equivalents for XQuery—originally developed to enable scalable XQuery processing on relational back-ends—can be used to determine dependable cardinality forecasts for XQuery. By faithfully keeping the connection between the relational plan and the original query, we make sure these forecasts are valuable even if the evaluation strategy of the actual back-end is not relational.

Consider the following XQuery query against weather.com forecast data for New Zealand (which we hope takes the else branch more often than the then branch during VLDB 2008):

```sql
for $d in //forecast.xml//descendant::day
let $day := $d/@t
let $ppcp := data ($d/descendant::ppcp)
return
if ($ppcp > 50)

then
equal chance of precipitation: "$ppcp"
else "no rain on", $day

Q1
```

Although existing techniques (e.g., [1, 6, 15]) could well estimate the cardinality of the rooted path expression `doc ()/descendant::day`, the remaining expression kinds in this query (for loops, conditionals, sequence construction, and implicit existential quantification), let alone the arbitrary nesting of such clauses, are beyond the capabilities of existing work. It is our goal to derive accurate cardinality estimates for any subexpression in this query, and we will illustrate our approach for the ones marked 1 to 4.

Interlude: The importance of cardinality forecasts.

To pinpoint the impact of such fine-grained cardinality forecasts, we used the Pathfinder relational XQuery compiler [10] to generate a SQL formulation of the XQuery expression `doc("forecast...")//descendant::day//descendant::ppcp`

For two predicates $p_1, p_2$ in this SQL query we injected annotations `SELECTIVITY` $s$ that forced IBM DB2 to assume that the $p_1$ have selectivity 0% ≤ $s$ ≤ 5%.

$p_1$, a predicate emitted by the compiler to extract the document node of the particular document `forecast.xml` from Pathfinder’s tabular XML node encoding, and $p_2$, a predicate that selects the XML elements that are reachable by the subsequent `descendant::day` XPath location step.

The assumed selectivities led DB2 to yield nine different execution plans as documented by Figure 1 (inspired by Haritsa’s Picasso optimizer visualizer [16]). The actual selectivities of $p_1$ and $p_2$ are about 0% and 1.1%, respectively. Equipped with this information, DB2 finds an execution plan that runs in three orders of magnitude less the exe-
execution time of the worst plan. Clearly, there is something to be gained from cardinality forecasts at the XQuery subexpression level.

Expressions like Query $Q_1$ are easily handled by the approach we pursue here. We compile the input query into an equivalent relational representation. Existing techniques for relational plan analysis can then be used to reason over plans that originate from XQuery expressions. The characteristics of the relational plans are simple enough to compute accurate size estimates using a clear and succinct inference procedure. The procedure is carefully designed to interoperate with a wide range of the existing estimation techniques for XPath and, conversely, to make the outcome of the plan analysis accessible to any XQuery processor, whether it is based on a relational back-end or not.

The most effective component of our inference procedure turns out to be the introduction of abstract domain identifiers as an approximation of the value space that individual query subexpressions take at runtime. An inferred inclusion property between value domains, together with an approximation of the size of each domain capture enough information to estimate the cardinality of relational XQuery plans.

We will present our approach as follows. Section 2 recapitulates all relevant aspects of relational XQuery processing, followed by the principles of relational XQuery cardinality estimation in Section 3. In Section 4, we add support for structural (XPath-) and value-based queries and illustrate the cardinality inference process for Query $Q_1$ in Section 5. Sections 6 and 7 discuss related work and wrap up.

## 2. RELATIONAL XQUERY

We map XQuery syntax to relational plans via loop lifting [11], a compilation technique—originally developed for the XQuery compiler Pathfinder [10]—that derives algebraic queries from the compositional XQuery dialect shown in Table 1. The compiler’s target language is a table algebra (Table 2) that has been designed to ease query analysis—the focus in this work—as well as efficient execution on modern SQL-style database engines [11].

To these ends, we work with rather restricted operator variants: selection $\sigma_a$ does not accept a predicate argument but merely a Boolean column $a$, all joins $\delta$ are equi-joins, and the argument tables of $\cup$ are always guaranteed to be disjoint. Duplicate row elimination is explicit in terms of $\delta$. The primitive $\sigma_a(b_1,\ldots,b_n):c$ groups its input table by column $c$ and then attaches new column $a$ holding unique row numbers in $b_1,\ldots,b_n$ order (this mimics the SQL:1999 clause $\text{RANK()}$ OVER ($\text{PARTITION BY}$ $c$ $\text{ORDER BY}$ $b_1,\ldots,b_n$) AS $a$). The non-textbook operators $\cup$, $\delta$, $\nabla$, $\varrho$, $\text{doc}$, $\varepsilon$, $\tau$ reflect specific aspects of the XQuery semantics and are discussed in Section 4.

In the loop-lifting compiler, the XQuery for clause is the core language construct: any expression $e$ is considered to be in the scope of its innermost enclosing for iteration. For each such $e$, the compiler emits two algebraic plan pieces which jointly compute a tabular encoding of $e$’s result:

1. loop, a unary table with single column iter that holds value $i$ if $e$ is evaluated in the $i$th iteration of its enclosing for loop, and
2. $q_e$, a ternary table iter|pos|item in which a row $[i,p,v]$ indicates that, in iteration $i$, $e$ evaluates to an item sequence in which $v$ (an atomic value or XML node identifier) occurs at position $p$.

To illustrate, consider the subexpression $\text{q}_e$ in the following slightly contrived XQuery Query $Q_2$ which evaluates to $(<\text{gust}>80 \text{ mph}</\text{gust}>,<\text{gust} />, <\text{gust}>95 \text{ mph}</\text{gust}>)$:

1Around a top-level expression $e$ we assume the void loop for $\text{$_\text{1}$ in } (0)$ return $e$ where $\text{$_\text{1}$}$ does not occur free in $e$. 

<table>
<thead>
<tr>
<th>literal values</th>
<th>document order ($e_1$ $\ll$ $e_2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>sequences ($e_1, e_2$)</td>
<td>node identity ($e_1$ is $e_2$)</td>
</tr>
<tr>
<td>variables ($$v$)</td>
<td>arithmetics ($+$, $-$, ...)</td>
</tr>
<tr>
<td>let $$v := e_1$ return $e_2$</td>
<td>comparisons ($\text{eq}$, $\text{lt}$, ...)</td>
</tr>
<tr>
<td>for $$v$ in $e_1$ return $e_2$</td>
<td>Boolean ops ($\text{and}$, or, ...)</td>
</tr>
<tr>
<td>if ($e_1$) then $e_2$ else $e_3$</td>
<td>$\text{fn:doc}(e)$</td>
</tr>
<tr>
<td>typeswitch clauses</td>
<td>$\text{fn:root}(e)$</td>
</tr>
<tr>
<td>text ${ e }$</td>
<td>$\text{fn:data}(e)$</td>
</tr>
</tbody>
</table>
| element $\{ e_1 \}$ $\{ e_2 \}$ | $\text{fn:count}(e)$, $\text{fn:sum}(e)$, ...
| XPath $(e/ax::nt)$ | $\text{fn:empty}(e)$ |
| user-defined functions | $\text{fn:position}(), \text{fn:last}()$ |

| Table 1: Supported XQuery subset (excerpt). |
|----------------|---------------------------------|
| $\pi_{\text{...}|\text{b}_{\text{a}}}|$ | column projection, renaming ($\text{a}$ into $\text{b}$) |
| $\sigma_{\text{a}}$ | selection (select rows with $\text{a} = \text{true}$) |
| $\cup_{\text{a} = \text{b}, \text{x}}$ | equi-join, Cartesian product |
| $\setminus_{\text{a}}$ | disjoint union (append), difference |
| $\delta$ | duplicate row elimination |
| $\sigma_{\text{a}}(b_1,\ldots,b_n):c$ | row numbering (grouped by $c$) |
| $\otimes_{\text{a}}(b_1, b_2)$ | arithmetic/comparison operator $\ast$ |
| $\text{fn:doc}(e)$ | XPath step operator ($a = b/ax::nt$) |
| $\text{doc}_{\text{a:b}}$ | XQuery atomization ($a = \text{fn:data}(b)$) |
| $\varepsilon, \tau$ | XML document access ($a = \text{fn:doc}(b)$) |
| $\text{agg} \in \{ \text{count}, \text{sum}, \text{max}, \ldots \}$ | element/text node construction |

| Table 2: Table algebra used for cardinality estimation ($\text{agg} \in \{ \text{count}, \text{sum}, \text{max}, \ldots \}$). |
known constants, too (as shown, e.g., in Rule Const-3). Rule Const-2 propagates constant column information after column renaming. Further inference rules for const(·) are explained in [8].

In the remainder of this text, we will also use the property $cobs(·)$ to access the column schema of its table argument, such that $cobs(q_k) = \{\text{iter, pos, item}\}$ according to compilation invariant (2), for example.

3. CARDINALITY INFERENCE

The ultimate goal of this work is to infer an additional property $|q|$ for each sub-plan $q$, the estimated number of rows after sub-plan evaluation. For a large class of algebra operators, we can directly turn their definition into an inference rule for $|·|$. Most of the unary operators, e.g., preserve the cardinality of their input, as captured by Rule CARD-1:

$$\sigma(a) \in \mathbb{N} \implies |\sigma(a)| = |a|$$

The binary operators $\cup$ and $\times$ are other examples where the operator definition straightforwardly translates into a cardinality inference rule (recall that $\cup$ preserves duplicates):

$$|a \cup b| = |a| + |b| \quad (CARD-2) \quad |a \times b| = |a| \cdot |b| \quad (CARD-3)$$

In relational XQuery evaluation plans, operator $\cup$ is used, e.g., to combine the subexpressions of the then and else branches of an if conditional (sub-plan $q_2$ in Figure 3) or to implement sequence construction (remaining $\cup$ operators in Figure 3).

The traditional approach to estimate the cardinality of the selection $\sigma_a$ and equi-join operators $b_4 \sigma_{a=b}$ operators in relational databases is the one taken in System R [19]. Rules CARD-4 and CARD-5 implement the heuristic “10%” rule of System R:

$$|\sigma_a(q)| = |q| \cdot 1/10 \quad (CARD-4) \quad |q_1 \cup q_2| = |q_1| \cdot |q_2| \cdot 1/10 \quad (CARD-5)$$

Both rules implement rather crude estimates, since the System R optimizer assumes that persistent indexes are typically present to provide statistics for the argument relations $q_1$ and $q_2$. Unfortunately, this assumption is met only rarely in plans generated from XQuery. Nested XQuery expressions more often lead to selections and joins over computed sub-results, instead of input from persistent storage. A peephole-style implementation of data flow analysis in our estimator remedies this situation, as we discuss next. Our actual plan analyzer uses Rules CARD-4 and CARD-5 as a last resort only if no useful information can be inferred about the input relations computed by $q_1$ and $q_2$. Only rarely did we see them being applied to real-world queries by our prototype.
3.1 Abstract Domain Identifiers

The selectivities involved in the evaluation of the $\sigma$ or $\bowtie$ operators could be estimated more accurately with knowledge about the active domain of any column $c$ in the operand relations, i.e., the actual values taken by $c$ at runtime. Obviously, the actual value space of any column is not yet known during static query analysis. Instead, we introduce abstract domain identifiers, denoted by Greek letters $\alpha$, $\beta$, $\gamma$ in this text, to represent the runtime domains. We infer just as much information about value domains as necessary to compute reliable cardinality estimates. A similar device has been used in $[8]$ to aid the algebraic optimization of XQuery joins.

Fresh value domains are usually introduced by operators that establish new table columns, such as, e.g., the row-numbering operator $\rho_{a}((b_{1},\ldots,b_{n}))$. We write $a^\alpha \in \text{dom}(q)$ to indicate that in the result relation computed by $q$ the active domain of column $a$ is $\alpha$ (for a fresh identifier $\alpha$, not used before):

$$\text{dom} \left( \rho_{a}((b_{1},\ldots,b_{n}))(q) \right) \supseteq \text{dom}(q) \cup \{a^\alpha\}.$$  

In our example plan (Figure 3), other instances of operators that introduce fresh domains are projection operators that set up constant columns ($\pi_{\neq a}$), the comparison operator $\ominus_{\text{res.}(\text{item1})}$, or the XPath-related operators $\text{doc}$, $\text{item.attribute}:[\text{item}]$, $\text{item.descendant}:[\text{ppcp} \text{item}]$.

![Figure 3: Complete plan DAG for XQuery expression $Q_1$ (see text for annotations).](image)

3.1.1 Domain Sizes

For each newly established value domain, our plan analyzer also tries to infer additional information that is valuable for our aim, the inference of table cardinalities. Towards this end, we estimate the size of each domain, written as $\|\alpha\|$. $\|\alpha\|$ denotes the number of distinct values in the value domain $\alpha$.

Domain sizes and table cardinalities often interact. Operator $\rho_{a}((b_{1},\ldots,b_{n}))(q)$, e.g., establishes a new key column $a$ over the input relation $q$. The size of $a$'s value domain, hence, coincides with the cardinality of $q$, as reflected in Rule Dom-1 of our inference rule set (this is a refinement of the above inference):

$$\text{dom} \left( \rho_{a}((b_{1},\ldots,b_{n}))(q) \right) \supseteq \text{dom}(q) \cup \{a^\alpha\}.$$  

(Dom-1)

The notation $\|\alpha\| \equiv |q|$ indicates that we are inferring the domain size of $\alpha$ to be the cardinality of $q$ here (rather than deriving it from a domain size inferred earlier).

Conversely, the size of a domain determines the cardinality of aggregates:

$$b^{\beta} \in \text{dom}(q) \quad \left[ \text{agg}_{b}^{\beta}(q) = \|\beta\| \right].$$  

(CARD-6)
or the output of the duplicate elimination operator \( \delta \) for single-column inputs:

\[
cols(q) = \{a\} \quad a^\alpha \in \text{dom}(q) \\
\{\delta(q)\} = \|a\|
\]

(CARD-7)

Further examples of domain usage and inference are shown in Figure 4. The size of a constant-column domain is trivially 1 (Rule Dom-2). The output domain of operators with a Boolean result is the two-item set \{true, false\} (Rule Dom-3). Rules Dom-4 to Dom-6 propagate domain information bottom-up through the inference process.

Rule Dom-7 shows the domain inference for the row-numbering operator \( \varrho_{1, (b_1, \ldots, b_n)} \in c \) in the presence of a grouping column \( c \). The operator creates \( \|\gamma\| \) groups, where \( \gamma \) is the domain associated with \( c \). Assuming equi-sized groups, the average group size is \( \|a\|/\|\gamma\| \). Since \( \gamma \) produces numbers between 1 and the group size, this is also the domain size we estimate for the new column \( a \). Rule Dom-8 is the dual to the aforementioned cardinality inference rule for \( agg_{\text{all}} \).

In our example plan (Figure 3), we use domain sizes, \( \varepsilon \), to infer the cardinalities of the loop \( \bigcirc \) and loop \( Q \) relations, which correspond to the number of times the then and else branches are taken in the original query \( Q_1 \), respectively.

### 3.1.2 Domain Inclusion

So far we have only considered algebraic operators that strictly propagate all values (\( i.e. \), the full value domain) from one column to the operator output. Operators such as selection (\( \sigma_{\alpha} \)), equi join (\( \bowtie_{a=b} \)), or difference (\( \setminus \)), by contrast, typically compute a restriction of their input domains.

The domain inference for the selection operator \( \sigma_{\alpha} \) (see Rule Dom-9, Figure 4) uses the expression

\[
\|\gamma_2\| = \|\gamma_1\| \cdot \left( 1 - (1 - \frac{1}{10})^{\|a\|/\|\gamma_1\|} \right)
\]

(1)

to compute the domain sizes for all output domains. The factor \( \frac{1}{10} \) is the System R 10% heuristic for the general selection operator. Details about the remaining terms in Expression 1 are beyond our current discussion. Interested readers may find them in Appendix A.

Restricting domains also leads to an inclusion relationship between the input and output domains. Domain \( \alpha \) is a subdomain of \( \beta (\alpha \subseteq \beta) \) if all values in \( \alpha \) are also a member of \( \beta \). The values in \( \sigma_{\alpha}(q) \), \( \varepsilon \), are a subset of those in \( q \), hence the inference of \( \gamma_2 \subseteq \gamma_1 \) in Rule Dom-9. Domain inclusion is transitive (\( \alpha \subseteq \beta \wedge \beta \subseteq \gamma \Rightarrow \alpha \subseteq \gamma \)) and reflexive (\( \alpha \subseteq \alpha \)).

System R-style domain inference for joins is covered by Rule Dom-10. However, our plan analyzer can typically avoid the application of this rule and rather derive more fine-grained domain information based on domain inclusion knowledge. Rule Dom-11 presupposes a subdomain relationship \( \alpha \subseteq \beta \) between the value domains \( \alpha \) and \( \beta \), which are associated with the input attributes \( a \) and \( b \) of the input relations \( q_1 \) and \( q_2 \) (respectively). A common instance is the foreign key dependence when column \( a \) of \( q_1 \) references column \( b \) in \( q_2 \).

Under the premise of \( \alpha \subseteq \beta \), all tuples from \( q_1 \) are retained in the join result, hence \( \text{dom}(q_1) \subseteq \text{dom}(q_1 \bowtie_{a=b} q_2) \). Tuples from the right-hand-side relation, by contrast, are filtered depending on the containment of their \( b \) values in domain \( \alpha \). \( \alpha \) has been derived earlier as a restriction of \( \beta \) with a selectivity of \( \|\alpha\|/\|\beta\| \). Rule Dom-11 uses this factor to compute the sizes of those domains that originally come from \( q_2 \). Columns \( a \) and \( b \) are identical in the join result by definition, hence \( b^\alpha \in \text{dom}(q_1 \bowtie_{a=b} q_2) \).

In Figure 3, the input to the \( \bowtie \) operator is a join operation of this kind. The domain associated with the iter column of the right join input is a subdomain of its left-hand-side counterpart here.

More generally, domain inclusion defines a tree-shaped hierarchy of domains. In Rule Dom-12, we consider join operators \( \bowtie_{a=b} \) where \( \alpha \) and \( \beta \), the domains of \( a \) and \( b \), have a subdomain relationship to a common superdomain \( \gamma \) (as illustrated here on the right). Domain \( \alpha \) in join operand \( q_1 \) contains \( \|a\|/\|\gamma\| \) of the values of \( \gamma \). Based on the assumption that \( \alpha \) and \( \beta \) have been derived from \( \gamma \) independently, Rule Dom-12 uses this factor and the domain restriction formula from Appendix A to derive the domain sizes associated with all columns coming from input relation \( q_2 \) (and, vice versa, \( \|a\|/\|\gamma\| \) for column values from \( q_1 \)).

The join operator on top of subexpression \( \bowtie_{0} \) in Figure 3 is an instance of this pattern. The right input of this join contains the iter values of those iterations over \( \text{doc}(\text{"forecast.xml"})/\text{descendant::day} \) that did not satisfy \( \text{ppcp} > 50 \) (\( i.e. \), the iterations that belong to the else branch). The left-hand side contains information only for iterations for which a \( \text{et} \) attribute could be found. The domain established by \( \text{domin} [\text{iter门外}] \) (in the bottom part of the plan) is a common superdomain of both join attributes.

Note that Rule Dom-11 actually is a special instance of Rule Dom-12.

Rule Dom-13 introduces a System R-like 10% factor for domains that result from the relational difference operator \( \setminus \). In Pathfinder-generated plans, operator \( \setminus \) is predominantly used to work over single-column tables.² Virtually all cases thus benefit from more specific domain inference rules such as the ones shown in Rule Dom-14 and Dom-15. The former covers the situation that we also see in Figure 3: the value domain of the single-column relation \( \bowtie_{Q} \) is a subset of the values in \( \bowtie_{Q} \). Hence, subtraction of the two input domain sizes \( \|\alpha\| \) and \( \|\beta\| \) yields the domain size of the output domain \( \gamma \), \( \|\gamma\| = \|\alpha\| - \|\beta\| \) (see Rule Dom-14). Rule Dom-15 is the complimentary rule that decides \( \|\gamma\| = 0 \) based on \( \alpha \subseteq \beta \).

### 3.2 Table Cardinalities

The collected domain information can now be used to compute meaningful cardinalities for subexpressions in the relational plan. Figure 5 lists the missing inference rules that correspond to the plan situations discussed earlier.

Rules Card-8 and Card-9 correspond to Rules Dom-11 and Dom-12 in Figure 4, respectively. Domain sizes are used here to estimate the selectivity of the join predicate \( a = b \). In Rule Card-8, the result contains \( \|a\| \) distinct

²The last premise in Rule Dom-12 ensures that \( \gamma \) is the smallest common subdomain of \( \alpha \) and \( \beta \).

³Pathfinder uses \( \setminus \) operators over single columns, \( \varepsilon \), to compute the \( \bowtie \) relation of an XQuery else branch (as shown in Figure 3) or to handle empty sequences (which are encoded as the absence of their iter value in the loop-lifted sequence encoding). Multi-column differences are, in fact, only needed to evaluate the XQuery except operator.
that depend on XPath navigation or improve the estimation
cussed in the previous section (Rule
Card-11
data.

values in the join attribute. Each of these finds $|\alpha|/|\gamma|$ tuples from the left- and right-hand-side of the join,
respectively, such that the cardinality can be estimated to
$|\alpha|/|\gamma|$.

The domain size of the join attribute in the result

The latter two rules, CARD-10 and CARD-11, implement
cardinality estimation for the general case of the relational
difference (Rule CARD-10) and for the special case we
discussed in the previous section (Rule CARD-11).

Still, our rules do not yet cover the estimation of sub-plans
that depend on XPath navigation or improve the estimation
accuracy for the selection operator $\sigma_a$. Both tasks require
access to statistical information about the underlying (XML)
data.

4. INTERFACING WITH XPATH

Access to XML documents is made explicit in our rela-
tional algebra (Table 2) in terms of the $\langle \cdot \rangle$, doc, and $\left\langle \cdot \right\rangle$ operators. These operators may be backed by system-dependent
implementations for the respective XQuery functionality. In
a purely relational XQuery setup, all three operators are
to look up the document nodes of XML in-

Given node identifiers $\gamma$ stored in a column $b$, the step
operator $\langle \cdot \rangle_{ax::nt}(b)$ evaluates the location step $ax::nt$
for each node in $b$ and populates a new column $a$ with the node
identifiers of the result nodes. Figure 6 illustrates this for
the step child::* and a five-node XML instance.

The XML document access operator $\langle \cdot \rangle_{ax::nt}$ uses the URIs
in column $b$ to look up the document nodes of XML inst-
ances. Their node identifiers are populated into the new
column $a$.

Operator $\langle \cdot \rangle_{ax::nt}$ implements XQuery atomization [4], i.e.,
the extraction of simple-typed data from XML node content.
The new column $a$ holds the values obtained from atomizing
the XML nodes referenced by the identifiers in column $b$. In
4.1 XPath Navigation

With all operations on XML data made explicit using distinguished algebra operators, our cardinality estimation procedure remains mostly independent of its XPath estimation subsystem and can play well together with existing XPath estimation techniques proposed in the literature. We have successfully built implementations based on straight line tree grammars [6] and data guides [7].

To facilitate the interaction with the XPath estimation subsystem, we adapt the idea of projection paths [14]. Our query analyzer infers a trace of all XPath navigation steps that have been followed to compute the result of a plan subexpression. Traces (projection paths) are then used to guide the interaction with the XPath estimation subsystem. In [14], similar information was used to pre-filter XML instances at document loading time (and, consequently, reduce the main-memory requirements of the Galax XQuery processor).

4.1.1 Projection Paths

Projection paths are inferred as the path (q) property of a plan operator q. An entry a→p in path(q) indicates that all node identifiers in column a in the output of q have been reached by an XPath navigation along the path p, possibly constrained by additional predicates. The node references in a, therefore, are a subset of those returned by the XPath expression p.

Unlike [14], we allow projection paths composed of arbitrary XPath axes and node tests. Our current plan analyzer does not generate predicative projection paths (i.e., paths of the form π₁(π₂ ...)), since those are normalized into explicit for iterations prior to query compilation [5]. Our setup could easily be modified to generate such paths if an XPath estimation subsystem provides specialized support for predicates, however. Further, we do not label projection paths with any additional flags (such as the # in [14]).

Informally, a new projection path is instantiated for every call to the XQuery built-in function fn:doc (·) (operator docc[ ] in the algebraic plan). As the analyzer processes the plan bottom-up, each occurrence of an XPath navigation step ax::nt (operator δax::nt(b)) is recorded as an appendix to the existing projection path information. The remaining plan operators only propagate projection paths bottom-up.

The process is covered by Inference Rules PATH-1 to PATH-7 in Figure 7. Rule PATH-1 establishes a new projection path for the result column of a of operator docc[ ]. On occurrence of a step operator δax::nt(b), this path is extended by the step ax::nt and annotated to the output column b of the operator (Rule PATH-2).

Otherwise, projection path information is propagated bottom-up. Rules PATH-3 to PATH-7 thereby ensure proper treatment of attribute renaming and projection (Rule PATH-3) and of the semantics of the set operators \ and ∪ (Rules PATH-5 and PATH-7, respectively).

In Figure 3, the output column item of operator docc[ ] (bottom of the plan) is annotated with the projection path fn:doc("forecast.xml"). Operators δitem:ax::nt(item) in the upstream DAG then update the projection path information recorded for column item to read fn:doc("forecast.xml")/attribute::t and fn:doc("forecast.xml")/descendant::ppcp in the left and right branches of the query plan, respectively.

4.1.2 Cardinality Estimation for XPath Steps

XPath navigation also affects table cardinalities, as can be seen in Figure 6. Three rows are contributed to the operator output by the first input tuple (since a has three children in Figure 6(a)). The second tuple disappears during step evaluation (b/child::* is empty), while the last tuple produces one output row.

The effect of operator δax::nt(b) on the table cardinality is determined by the fanout of the node identifiers in column b with respect to the location step ax::nt. In Figure 6, the average fanout of the input nodes (nodes a, b, and d) is

\[ f_{avg} = \frac{3 + 0 + 1}{3} = 4/3 \]

Multiplication with the input cardinality yields the row count of the result:

\[ |\delta_{ax::nt}(b)| = |q| \cdot f_{avg} = 3 \cdot 4/3 = 4 \]

We can estimate the factor f_{avg} involved in determining the cardinality of δax::nt(b) based on the projection path p that has been inferred for the context column b in q (i.e., b→p ⊆ path(q)). We base the estimate for f_{avg} on statistical information about the XML document:

\[ f_{avg} \approx Pr_{ax::nt}(p) := \frac{fn:count(p/ax::nt)}{fn:count(p)} \]

The cardinality of δax::nt(b)(q) can then be approximated as shown in Rule CARD-14 (Figure 7).

The approximation assumes that the nodes referenced in input column b are a random sample of those reachable by p. In particular, they are assumed to be picked from p independently of their fanout with respect to ax::nt. This assumption is met by most real-world queries that we could get hold of in experimental studies.

The fanout function Pr_{ax::nt}(p) is part of our interface to the XPath estimation subsystem. Every XPath estimator that provides Pr_{ax::nt}(p) and the two functions that we define in a moment can seamlessly be plugged into the XQuery estimator described here. In Section 4.3, we illustrate a naive implementation based on Goldman and Widom’s data guides [7].

4.1.3 Domains and XPath Location Steps

With regards to value domains, operator δax::nt(b) acts like a filter on all column values coming from the input relation q. Only tuples for which at least one node can be found along the step ax::nt will appear in the operator result. Since, e.g., in Figure 6, node b has no children
XPath estimation subsystem: selectivity function thus introduce the 2-step is

equation of the domain associated with column $\gamma_0$.

to the operator output. We have already seen how domain information and cardinalities can be inferred for aggregation functions, respectively. The forecasted cardinality, typically the size of the domain associated with column $\text{iter}$, is consistent with the semantics of node construction in XQuery. Consider Query $Q_2$ again: each evaluation of $\text{element gust} \{e\}$ yielded exactly one new element node, regardless of the cardinality of $e$.

More valuable than the projected size of the node construction result may be information about the cardinality of the constructor’s input. Since we infer $\{e\}$ for any subexpression $e$, such information is readily available to, e.g., allocate enough memory to hold the content of the new tree fragment below element $\text{gust}$.

4.2 Value-Based Predicates

The reliance on functions $Pr(\cdot)$ to access statistical information about XPath navigation enables data-dependent cardinality estimation only for the structural aspects of XML document access. To judge the selectivity of the predicate $\text{ppcp} > 50$ in Query $Q_1$, we also need to have information about the distribution of values in $\text{forecast.xml}$.

4.2.1 Typed Value Histograms

Our estimator assumes the availability of such information in terms of typed value histograms, which can be set up by the database administrator for frequently queried values in the XML document catalog. A histogram created with, for example,

```
create typed value histogram H1
on '/descendant::day/descendant::ppcp'
validate as xs:integer
```

can be used to judge the selectivity of the predicate in Query $Q_1$. Typed value histograms of this kind are readily provided by, e.g., the XML data indices in IBM DB2 9 [12].

We leave histogram maintenance up to the XPath subsystem and remain fully agnostic with respect to its concrete implementation here. The only assumption we make is that the histogram for path $p$, if available, is accessible from the XPath estimation subsystem via the interface function $\text{Hist}(p)$.

4.2.2 Trading Paths for Histograms

In XQuery, access to typed value information requires atomization of the respective XML tree nodes. Calls to the XQuery built-in function $\text{fn: data}()$ make this process ex-
explicit in the query after normalization to XQuery Core [5]. In relational XQuery evaluation plans, the atomization operator $\mathcal{P} \sigma_\text{a}$ marks this situation where the query engine trades nodes for values.

It is the same spot where our plan analyzer trades projection path annotations for typed value histograms. In Rule Hist-1 (Figure 8), it uses the projection path inferred for the input column $b$ to request the typed value histogram $H$ from the XPath subsystem. The histogram is then recorded as $H_i$ in the $\text{hist}(\cdot)$ annotation of the result expression.

Operations on values (arithmetic computations and value comparisons) are represented explicitly using the $\odot$ operators in our algebra (e.g., $\odot_a(b_1,b_2)$, $\odot_a(b_1,b_2)$, $\odot_a(\text{string}(b_1))$, $\cdots$). To reflect these operations in algebraic histogram annotations, a new histogram is computed for the result column $a$ based on histograms available for the input columns $b_i$. In Rule Hist-2, we used $\oplus(H_1,\ldots,H_n)$ to express arithmetics on histograms. A possible implementation for $\oplus$ is the histogram discretization technique by Benard [3]. Histogram information is propagated bottom-up for the remaining algebra operators (not shown formally).

With histogram information available, the cardinality inference for the selection operator $\sigma_a$ now becomes an educated guess. As shown in Rule CARD-15, the two-bucket (true/false) histogram annotated to column $a$ readily describes the selectivity of $\sigma_a$. In Rule DOM-17, we also use it to infer domain sizes associated with the output of $\sigma_a$.

In Figure 3, a typed value histogram is fetched from the XPath estimator to annotate column item $\text{item}$ of the atomization operator $\mathcal{P}_\text{item}$. After propagation through the join operator $\mathcal{P}_\text{iter}$ and histogram arithmetics in $\oplus(\mathcal{P}_\text{res}(\mathcal{P}_\text{iter})),\mathcal{P}_\text{res}(\mathcal{P}_\text{item})$ this histogram is then used to judge the output cardinality of $\sigma_{\text{res}}$.

### 4.3 An Implementation for $\Pr$: Data Guides

The two interface functions to access fanout, $\Pr_{ax1::nl}$ $(p)$, and selectivity, $\Pr_{ax1::nt}$ $(p)$, in Section 4.1 suggest the use of data guides [7] to maintain statistical information about the underlying document structure. In a nutshell, a data guide is built by reducing element nodes with identical root-to-leaf paths to a single instance in the guide. The outcome is a "skeleton tree" holding all distinct paths (we assume a strong data guide in the sense of [7]) that may be annotated with, e.g., statistical information.

#### 4.3.1 Fanouts and Selectivities

Figure 9 shows the data guide that corresponds to a small collection of weather data for cities in New Zealand that we retrieved from weather.com at the time of this writing. To implement the two XPath interface functions, each edge in the data guide is labeled with a pair of values $[f,s]$ ($f > 0$ and $0 < s \leq 1$), which correspond to the average fanout and selectivity (respectively) along the corresponding axis in the full document. The document contains, e.g., ten day elements below each day, each day contains two parts (day and night). The structure of weather data is more deterministic than the forecast it describes: each edge is guaranteed to be present for corresponding parent nodes in the document, hence $s \equiv 1$ in our example.

Based on these annotations, $\Pr_{ax1::nl}(p)$ and $\Pr_{ax1::nt}(p)$ are straightforward to implement. For named child steps, both pieces of information can directly be read from the annotations. Otherwise, fanout information can be computed by adding horizontally and multiplying vertically along guide edges that qualify for the given step and node test. The aggregation of selectivity values is beyond the scope of this paper and uses similar observations as those that we sketch in Appendix A. Note that data guides do not capture the order between siblings and hence cannot be used to implement $\Pr_{ax1::nl}(p)$ for order-sensitive axes ax such as, e.g., the following or preceding-sibling axes. To support estimation of order-sensitive axes, other synopses can be used, such as [13] or the straight line tree grammars of [6].

#### 4.3.2 Typed Value Histograms

Figure 9 also illustrates how our prototype implements typed value histograms as annotations to nodes in the data guide. Histogram $H_1$, created in Section 4.2.1, is annotated to the pccp data guide node. (If, in $\text{Hist}(p)$, more than one histogram can be found for path $p$, our implementation uses discretization [3] to compute the effective typed value histogram.)

### 5. FORECASTING IN PRACTICE

With all bits and pieces together, we are now ready to infer plan annotations and cardinalities for the query plan in Figure 3. For space reasons, we only report inferred plan properties for its most interesting sub-plan, illustrated in Figure 10. Towards the end of this section, we also report on empirical results for a realistic set of XQuery expressions, taken from the XMark benchmark [18].

#### 5.1 Zooming in on the Running Example

The input to the sub-plan in Figure 10 is essentially determined by the XPath subexpression result $\text{doc("forecast.xml")/ descendant:: day, whose cardinality we estimated to } 99 \cdot 1 \cdot 10 = 990$, following the fanout annotations in the data guide. This information is propagated bottom-up along operators $\mathcal{P}$ and $\mathcal{C}$. 

Figure 9: Data guide for weather.com weather data. Edges are annotated with pairs $[f,s]$ of fanout $f$ and selectivity $s$. 

Based on these annotations, $\Pr_{ax1::nl}(p)$ and $\Pr_{ax1::nt}(p)$ are straightforward to implement. For named child steps, both pieces of information can directly be read from the annotations. Otherwise, fanout information can be computed by adding horizontally and multiplying vertically along guide edges that qualify for the given step and node test. The aggregation of selectivity values is beyond the scope of this paper and uses similar observations as those that we sketch in Appendix A. Note that data guides do not capture the order between siblings and hence cannot be used to implement $\Pr_{ax1::nl}(p)$ for order-sensitive axes ax such as, e.g., the following or preceding-sibling axes. To support estimation of order-sensitive axes, other synopses can be used, such as [13] or the straight line tree grammars of [6].
Annotations in the right branch of the plan depend on the projection path information available for column item. Using \( \text{P}_{\text{descendant::ppcp}} \) (fn:doc(\( \cdot \cdot \cdot \)/descendant::day) = 2 (fanout annotation in Figure 9), we can infer the cardinality of operator (D) to 1980 (Rule CARD-14), as well as the domain size of \( \alpha_6 \), \( |\alpha_6| = 1980 \) (left part of Rule DOM-16). By contrast, since the selectivity \( \text{P}_{\text{descendant::ppcp}} \) (\( \cdot \cdot \cdot \)) of the step descendant::ppcp is 1, the domain size annotated to column \( \text{iter} \) remains \( |\alpha_5| = 990 \) (right part of Rule DOM-16). The factor \(|\alpha_5|/|\alpha_6| = 2\) stems from the two pppc elements encountered in each iteration over \( \text{doc}(\cdot\cdot\cdot)/\text{descendant::ppcp} \) (Rule Hist-1). The histogram will be accessed later in the plan to judge the selectivity of the predicate \( \text{pppcp} > 50 \).

Operator (F) is an instance of the situation in Rules DOM-11 and CARD-8. Since each tuple in the right branch is guaranteed to find a (single) join partner in the left branch, we expect 1980 tuples to flow upwards the execution plan.

To judge the effect of operators (H) and (I), we access the histogram information for input column item. Together with the \( const(\cdot) \) information available for column item1 (which we interpret as the second input histogram in Rule Hist-2), we compute a two-bucket histogram for column res that reflects the Boolean outcome of the comparison operator (I).

Operator (J) finally performs the selection and we determine its output cardinality based on Rule CARD-15.

After propagation of plan annotations through operator (J), the cardinality estimate for (K) depends on the domain size annotated to column iter. Using Rule CARD-7, we infer 107 as its predicted tuple count. The cardinality of operator (L) then is 883, according to Inference Rule CARD-11.

Recall that operators (K) and (L) correspond to the \text{loop}_{(c)} and \text{loop}_{(f)} relations, i.e., the number of evaluations of the then and else branches of the original query, respectively. A query run over the real data reveals 158 and 832 evaluations of the two branches—the weather in New Zealand is slightly worse than expected. While this may look like an ominous forecast for VILD, the deviation is actually caused by a skewed data distribution around a rain probability of 50% (which meteorologists seem to avoid whenever possible). Substituted back into Q1, we obtain the final forecast output:

```
990 for $d$ in doc("forecast.xml")/descendant::day let $day:=d/@t
let $ppcp :=data($d/*descendant::ppcp
return 2301

if $ppcp > 50$ then "rain likely on", $day,
  "chance of precipitation:", $ppcp
else "no rain on", $day)
```

Figure 10: Full annotations for a sub-plan of Figure 3 (annotations explained in Section 5.1).
Our overall cardinality forecast for Query $Q_1$ is 2301, which is $\approx 6\%$ off the actual result cardinality of 2454.

5.2 A Cardinality Injection for DB2

To assess the advantage of algebraic cardinality estimation in real-world scenarios, we implemented the ideas of this work in a variant of the SQL:1999 code generator of [9]. The new back-end to the Pathfinder XQuery compiler produces SQL code that has been enriched with SELECTIVITY annotations that inform the SQL compiler of DB2 about the table cardinalities inferred for individual sub-expressions.

The generated SQL code operates over a relational encoding of XML documents. For our experiments, we shredded a 100 MB XMark [18] instance into database tables of a DB2 9 server installation (Linux-based, 3.2 GHz Intel Xeon, 8 GB RAM). Prior to loading, we turned XML ID attributes into numerical values, making them susceptible for our histogram implementation. To maintain statistical information, we implemented the data guide of Section 4.3, including histograms for all numerical fields in the loaded document. Data guides are known to be space-efficient for data like XMark: we measured 50 KB for our full statistics collection—a size that remains constant also for larger instances of XMark data.

Based on cardinality information, we injected SELECTIVITY clauses into all 20 XMark benchmark queries to make cardinalities available to the SQL compiler of DB2. Figure 11 reports the speedup that we observed when running these queries, as compared to their un-modified twins. A speedup of 100% in Figure 11 indicates that the annotated query ran twice as fast as before due to cardinality annotation.

Not all of the queries could benefit from the cardinality information the same way. No improvement can be observed, e.g., for Query $X_5$, which DB2 already is able to answer within 4 ms in its non-annotated variant. Query $X_{15}$ constitutes the biggest surprise where performance improved by several orders of magnitude. This is due to a long multi-step path expression that causes the bulk of the work. The path is compiled into a 13-fold self-join over the relational document encoding. Without guidance by cardinality annotations, the DB2 query optimizer gets lost in exploring the possible re-orderings of this join.

Queries $X_8$ to $X_{12}$ include value-based joins, using data correlations that our query analyzer cannot (yet) assess. According to Figure 11, the annotations we provided could not really help DB2 figure out better execution plans.

One of the most valuable aspects of relational cardinality assessment often remains hidden in the depths of the relational plans. Even though we frequently saw our plan analyzer mis-estimate fragments of a complex XQuery expression, we typically found it to recover gracefully from such intermediate errors. This can be observed in Query $Q_4$, for example, where the cardinality forecast will report the correct overall result size regardless of any intermediate error made when estimating the subexpressions $X_9$, $X_6$, or $X_7$ in the scope of the element gust constructor.

Language constructs with such a grouping semantics (e.g., node construction, the computation of effective Boolean values, or the existential semantics of comparisons) are pervasive in XQuery and allow the cardinality analysis to reasonable proceed even if the forecast went astray for a specific sub-plan.

6. MORE RELATED WORK

Work on cardinality estimation for semi-structured data has emerged even long before the advent of XML as a syntactical format and XPath/XQuery as a means to query XML data. Goldman and Widom have proposed data guides as a tool to hold statistical information in the Lore database manager [7]. We build on their work to demonstrate a simple implementation for the XPath aspect of our relational approach to XQuery estimation. Later work on XPath estimation (e.g., [1, 6, 13, 15]) was mainly concerned with improved accuracy and the reduction of space. Since we strictly kept the estimation of XPath subexpressions separate in our work, all of them could serve as a drop-in replacement for the data guides in Section 4.3.

The separation of path estimation into fanout and selectivity has also been observed by Balmín et al. [2]. The pureXML query optimizer built into DB2 9 maintains statistics about XML data by means of the same two parameters. Their work also considers “lowest common ancestor” situations in a fashion similar to our domain analysis for tree-shaped domain relationships (Section 3.1.2), remains limited to explicit branches in the XPath surface language (also known as twigs), however.

Other estimation techniques that target XQuery (as opposed to just XPath) are surprisingly rare. Sartiani [17] looked at a restricted form of XQuery for clauses and their cardinalities. It remains unclear, however, whether his approach could be pushed to full XQuery support at all.

In Section 4.1.1, we picked up an idea of Marian and Siméon [14]. In the same way that the Galax XQuery processor analyzes navigation into XML documents, we use traces of XPath step navigation—projection paths—to associate statistical information about value distributions in simple-typed XML nodes to relational plans.

7. WRAP-UP

We have described a framework that fills the gap between the feature richness of the XQuery language and existing work on cardinality estimation for the XPath sub-language.

5For this reason, we forecast the exact overall cardinality for nearly all of the 20 XMark benchmark queries.
Based on a relational representation of the input queries, we can re-use existing machinery from the relational domain to derive cardinality estimates for XQuery subexpressions in arbitrary compositions. Our strategy plays well together with estimation techniques for XPath proposed in earlier work (e.g., [1, 6, 13, 15]), which can be plugged into our setup seamlessly.

To account for the characteristics of relational query plans that originate from XQuery, our work lays a focus on a peephole-style implementation of data flow analysis based on abstract domain identifiers. Abstract domain identifiers approximate the value space taken by individual table columns at runtime. Reasoning over inclusion relationship between domains and their sizes provides just the information that we need to derive cardinality estimates in a dependable manner.

Our setup remains agnostic with respect to the details of XPath location path estimation. A simple data guide-style implementation of this component proved sufficient to compute meaningful XQuery estimates in an experimental assessment.

The estimation procedure is defined in terms of a set of inference rules. As such, it provides a flexible basis for the addition of refined or domain-specific estimation rules. Currently we are looking into first-class support for positional numbers according to the XML document order. A selection (<position number on ID>), an inference rule that originates from XQuery, our work lays a focus on a

\[ \rho \]

... could annotate the output column \( \text{pos} \) with child distribution information. A \( \gamma \) operator of this kind is generated by the compiler for XPath location steps to set up a positional numbering according to the XML document order. A selection on \( \text{pos} \) later implements a positional predicate, whose effect we could judge with the annotated histogram.

Our experiments indicate that a closer look into value-based joins might be valuable for further accuracy and/or performance improvements. A possible approach could be the inspection of XML Schema information, or ID/IDREF(S) constraints in DTDs.

8. REFERENCES


APPENDIX

A. PROBABILITIES AND DOMAIN SIZES

Algebraic operators that discard rows from their input (most prominently the \( \sigma_s \) and \( b_{a \rightarrow b} \) operators) affect the domain sizes associated with columns of the input table. Quantifying this effect requires a brief look into probability theory.

Suppose we apply a filter \( \sigma_c \) of selectivity \( s \) to table \( R \) (see right). Assuming an independence between \( \sigma_c \) and a column \( c \), we can estimate the size of \( c \)'s domain in the output, \( ||\gamma_{out}|| \), based on \( s, ||R||, \) and \( k = ||\gamma_{in}|| \) (the domain size associated with column \( c \) in the input relation \( R \)).

On average, each value \( a_i \in \gamma_{in} \) occurs \( ||R||/||\gamma_{in}|| \) times in relation \( R \). The chance that all of these occurrences are filtered out during \( \sigma_c(R) \) (which means that \( a_i \notin \gamma_{out} \)) is

\[ P_q = (1 - s)^{||R||/||\gamma_{in}||} \]

(2)

(since the chance of losing a single occurrence is \( (1 - s) \)).

The chance that at least one instance of \( a_i \) is retained after \( \sigma_c(R) \) (i.e., \( a_i \in \gamma_{out} \)) is \( (1 - P_q) \), hence,

\[ ||\gamma_{out}|| = ||\gamma_{in}|| \cdot \left( 1 - (1 - s)^{||R||/||\gamma_{in}||} \right) \]

(3)