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Declarative Semantics and Query Core for the Xcerpt Query Language

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Abstract

This article introduces a preliminary declarative semantics for a subset of the language Xcerpt (so-called *grouping-stratifiable programs*) in form of a classical (Tarski style) model theory, adapted to the specific requirements of Xcerpt's constructs (e.g. the various aspects of incompleteness in query terms, grouping constructs in rule heads, etc.). Most importantly, the model theory uses *term simulation* as a replacement for term equality to handle incomplete term specifications, and an extended notion of substitutions in order to properly convey the semantics of grouping constructs. Based upon this model theory, a fixpoint semantics is also described, leading to a first notion of forward chaining evaluation of Xcerpt programs.

In a second part of this deliverable, syntax, semantics, complexity, and evaluation for the query core of Xcerpt (and many other Web query languages such as XQuery and SPARQL) is introduced and discussed.

Keyword List

reasoning, query language, Semantic Web, model theory, semantics, declarative semantics

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Declarative Semantics and Query Core for the Xcerpt Query Language

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Contents

1 Introduction

This article introduces a declarative semantics for a restricted form of Xcerpt programs (so-called *grouping-stratifiable programs* without negation). Although a short introduction to Xcerpt is given in Section 2, this article does not cover the language in much detail; interested readers can find a more thorough description of Xcerpt in e.g. [SB04] and [Sch04]. The aim of the declarative semantics introduced here is to describe the semantics of Xcerpt programs in a precise and formal, yet intuitive and straightforward, manner without referring to a concrete implementation of the language. This description should serve as a reference for verifying the correctness and completeness of language implementations and as a formal specification for users seeking to get a precise understanding of the language.

The declarative semantics is given as a model theory in the style of *Tarski* (i.e. recursively defined over the formula structure). It follows the semantics for first order logic rather closely but needs to take into account the particularities of Xcerpt terms and programs (e.g. the various aspects of incompleteness in query terms, grouping constructs in rule heads, etc.). Intuitively, the definition of interpretations and models is straightforward: an interpretation is a set of data terms and specifies what data terms exist; a model is then simply an interpretation that consists of the terms that are "produced" by the rules in a program.

Section 2 briefly recapitulates the language Xcerpt and introduces several formalisms and denotations used in the remainder of this article. Section 3 introduces so-called *term formulas* that can be composed of Xcerpt terms and logical connectives like $\wedge$ or $\vee$. Term formulas depart form first order logic in that they do not distinguish between predicate and term symbols, because the Web consists of "data", not "statements". Next, a notion of *substitution sets* is described in Section 4. Substitution sets take the role of substitutions in first order logic and logic programming and are required to properly convey the meaning of Xcerpt's grouping constructs `all` and `some`. Section 5 defines *ground query term simulation* as a relation between terms that properly conveys the meaning of incomplete term specifications (e.g. unordered or partial). This definition is further used in Section 6, where interpretations and the satisfaction of term formulas is defined. In Section 7, a fixpoint semantics for stratifiable Xcerpt programs is suggested, first for programs without negation, and then for arbitrary Xcerpt programs. Finally, Section 8 contains some concluding remarks and perspectives for further refinement of the semantics. Note that this article mostly follows the semantics described in [Sch04].

2 Preliminaries

2.1 Xcerpt: A versatile Web Query Language

An Xcerpt [SB04, Sch04] program consists of at least one *goal* and some (possibly zero) *rules*. Rules and goals contain query and construction patterns, called *terms*. Terms represent tree-like (or graph-like) structures. The children of a node may either be *ordered*, i.e. the order of occurrence is relevant (e.g. in an XML document representing a book), or *unordered*, i.e. the order of occurrence is irrelevant and may be chosen by the storage system (as is common in database systems). In the term syntax, an *ordered term specification* is denoted by square brackets `[ ]`, an *unordered term specification* by curly braces `{ }`.

Likewise, terms may use *partial term specifications* for representing incomplete query patterns and *total term specifications* for representing complete query patterns (or data items). A term t using a partial term specification for its subterms matches with all such terms that (1) contain matching subterms for all subterms of t and that (2) might contain further subterms without corresponding subterms in t. Partial term specification is denoted by *double* square brackets `[[ ]]` or curly braces `{{ }}`. In contrast, a term t using a total term specification does not match with terms that contain additional subterms without corresponding subterms in t. Total term specification is expressed using *single* square brackets `[ ]` or curly braces `{ }`. Matching is formally defined later in this article using so-called *term simulation*.

Furthermore, terms may contain the *reference constructs* `^id` (*referring occurrence of the identifier* `id`) and `id @ t` (*defining occurrence of the identifier* `id`). Using reference constructs, terms can form cyclic (but rooted) graph structures.

2.1.1 Data Terms

Data terms represent XML documents and the data items of a semistructured database, and may thus only contain total term specifications (i.e. single square brackets or curly braces). They are similar to *ground* functional programming expressions and logical atoms. A *database* is a (multi-)set of data terms (e.g. the Web). A non-XML syntax has been chosen for Xcerpt to improve readability, but there is a one-to-one correspondence between an XML document and a data term. Example 1 on the facing page gives an impression of the Xcerpt term syntax.

2.1.2 Query Terms

Query terms are (possibly incomplete) patterns matched against Web resources represented by data terms. They are similar to the latter, but may contain *partial* as well as *total* term specifications, are augmented by *variables* for selecting data items, possibly with *variable restrictions* using the → construct (read *as*), which restricts the admissible bindings to those subterms that are matched by the restriction pattern, and may contain additional query constructs like *position matching* (keyword `position`), *subterm negation* (keyword `without`), *optional subterm specification* (keyword `optional`), and *descendant* (keyword `desc`).

Query terms are "matched" with data or construct terms by a non-standard unification method called *simulation unification* that is based on a relation called *simulation* (cf. Section 5). In contrast to Robinson's unification (as e.g. used in Prolog), simulation unification is capable of determining substitutions also for incomplete and unordered query terms. Since incompleteness usually allows many different alternative bindings for the variables, the result of simulation unification is not only a single substitution, but a (finite) *set of substitutions*, each of which yielding ground instances of the unified terms such that the one ground term matches with the other. Whenever a term t_1 simulates into another term t_2, this shall be denoted by $t_1 \preceq t_2$.

2.1.3 Construct Terms

Construct terms serve to reassemble variables (the bindings of which are specified in query terms) so as to construct new data terms. Again, they are similar to the latter, but augmented by *variables* (acting as place holders for data selected in a query) and the *grouping construct* `all` (which serves to collect all instances that result from different variable bindings). Occurrences of `all` may be accompanied by an optional sorting specification.

Example 2
Left: A query term retrieving departure and arrival stations for a train in the train document. Partial term specifications (partial curly braces) are used since the train document might contain additional information irrelevant to the query. *Right:* A construct term creating a summarised representation of trains grouped inside a `trains` term. Note the use of the `all` construct to collect all instances of the `train` subterm that can be created from substitutions in the substitution set resulting from the query on the left.

Example 1
The following two data terms represent a train timetable (from `http://railways.com`) and a hotel reservation offer (from `http://hotels.net`).

At site `http://railways.com`:

```
travel {
  last-changes-on { "2004-04-30" },
  currency { "EUR" },
  train {
    departure {
      station { "Munich" },
      date { "2004-05-03" },
      time { "15:25" }
    },
    arrival {
      station { "Vienna" },
      date { "2004-05-03" },
      time { "19:50" }
    },
    price { "75" }
  },
  train {
    departure {
      station { "Munich" },
      date { "2004-05-03" },
      time { "13:20" }
    },
    arrival {
      station { "Salzburg" },
      date { "2004-05-03" },
      time { "14:50" }
    },
    price { "25" }
  },
  train {
    departure {
      station { "Salzburg" },
      date { "2004-05-03" },
      time { "15:20" }
    },
    arrival {
      station { "Vienna" },
      date { "2004-05-03" },
      time { "18:10" }
    }
  }
  ...
}
```

At site `http://hotels.net`:

```
voyage {
  currency { "EUR" },
  hotels {
    city { "Vienna" },
    country { "Austria" },
    hotel {
      name { "Comfort␣Blautal" },
      category { "3␣stars" },
      price-per-room { "55" },
      phone { "+43␣1␣88␣8219␣213" },
      no-pets {}
     },
    hotel {
      name { "InterCity" },
      category { "3␣stars" },
      price-per-room { "57" },
      phone { "+43␣1␣82␣8156␣135" }
     },
    hotel {
      name { "Opera" },
      category { "4␣stars" },
      price-per-room { "106" },
      phone { "+43␣1␣77␣8123␣414" }
     },
   ...
  },
...
}
```

```
travel {{
  train {{
    departure {{
      station { var From } }},
    arrival {{
      station { var To }   }}
  }}
}}
```

```
trains {
  all train {
    from { var From },
    to   { var To }
  }
}
```

2.1.4 Construct-Query Rules

Construct-query rules (short: rules) relate a construct term to a query consisting of AND and/or OR connected query terms. They have the form

`CONSTRUCT` *`Construct Term`* `FROM` *`Query`* `END`

Rules can be seen as "views" specifying how to obtain documents shaped in the form of the construct term by evaluating the query against Web resources (e.g. an XML document or a database). Queries or parts of a query may be further restricted by arithmetic constraints in a so-called condition box, beginning with the keyword `where`.

Example 3
The following Xcerpt rule is used to gather information about the hotels in Vienna where a single room costs less than 70 Euro per night and where pets are allowed (specified using the `without` construct).

```
CONSTRUCT
  answer [ all var H ordered by [ P ] ascending ]
FROM
  in {
    resource { "http://hotels.net" },
    voyage {{
      hotels {{
        city { "Vienna" },
        desc var H Žľő hotel {{
          price-per-room { var P },
          without no-pets {}
        }}
      }}
    }}
   } where var P < 70
END
```

An Xcerpt query may contain one or several references to *resources*. Xcerpt rules may furthermore be *chained* like active or deductive database rules to form complex query programs, i.e. rules may query the results of other rules. Recursive chaining of rules is possible (but note that the declarative semantics described here requires certain restrictions on recursion, cf. Section 2.2). In contrast to the inherent structural recursion used e.g. in XSLT, which is essentially limited to the tree structure of the input document, recursion in Xcerpt is always explicit and free in the sense that any kind of recursion can be implemented. Applications of recursion on the Web are manifold:

- structural recursion over the input tree (like in XSLT) is necessary to perform transformations that preserve the overall document structure and change only certain things in arbitrary documents (e.g. replacing all `em` elements in HTML documents by `strong` elements).
- recursion over the conceptual structure of the input data (e.g. over a sequence of elements) is used to iteratively compute data (e.g. create a hierarchical representation from flat structures with references).
- recursion over references to external resources (hyperlinks) is desirable in applications like Web crawlers that recursively visit Web pages.

Example 4

The following scenario illustrates the usage of a "conceptual" recursion to find train connections, including train changes, from Munich to Vienna.

The `train` relation (more precisely the XML element representing this relation) is defined as a "view" on the train database (more precisely on the XML document seen as a database on trains):

```
CONSTRUCT
  train [ from [ var From ], to [ var To ] ]
FROM
  in {
    resource { "file:travel.xml" },
    travel {{
      train {{
        departure {{ station { var From } }},
        arrival   {{ station { var To }   }}
      }}
    }}
  }
END
```

A recursive rule implements the transitive closure `train-connection` of the relation `train`. If the connection is not direct (recursive case), then all intermediate stations are collected in the subterm `via` of the result. Otherwise, `via` is empty (base case).

```
CONSTRUCT
  train-connection [
    from [ var From ],
    to   [ var To ],
    via  [ var Via, all optional var OtherVia ]
  ]
FROM
  and {
    train [ from [ var From ], to [ var Via ] ],
    train-connection [
      from [ var Via ],
      to   [ var To  ],
      via  [[ optional var OtherVia ]]
    ]
  }
END
```

```
CONSTRUCT
  train-connection [
    from [ var From ],
    to   [ var To ],
    via  [ ]
  ]
FROM
  train [ from [ var From ], to [ var To ] ]
END
```

Based on the "generic" transitive closure defined above, the following rule retrieves only connections between Munich and Vienna.

```
GOAL
  connections {
    all var Conn
  }
FROM
  var Conn Žľő train-connection [[ from { "Munich" } , to { "Vienna" } ]]
END
```

2.2 Range Restrictedness and Stratification

The declarative semantics described in this article assumes certain restrictions on Xcerpt programs: *range restrictedness*, *negation stratification*, and *grouping stratification*. Range restrictedness restricts the occurrences of variables in rules and grouping and negation stratification restricts the way recursion is used in Xcerpt programs. Note that for all three kinds of restrictions, there exist examples where a relaxation might be desirable.

2.2.1 Range Restrictedness

Range restrictedness (often referred to as *safe-ness*) means that a variable occurring in a rule head also must occur at least once in every disjunctive part in the rule body. This requirement simplifies the definition of the declarative semantics of Xcerpt, as it allows to assume that all query terms are unified with data terms instead of construct terms (i.e. variable-free and grouping-free terms). Without this restriction, it is necessary to consider undefined or infinite sets of variable bindings, which would be a difficult obstacle for a forward chaining evaluation. Besides this technical reason, range restricted programs are also usually more intuitive, as they disallow variables in the head that are not justified somewhere in the body.

Range restrictedness can be verified by assigning "polarities" to every term and all its subterms in a rule such that all terms in the query part initially have negative polarity while the construct term initially has positive polarity (cf. [Sch04]). A variable occurrence with *positive* polarity represents a *consuming* occurrence of that variable, a variable occurrence with *negative* polarity represents a *defining* occurrence of that variable. Polarities may switch if the query contains negation constructs like `not` or `without`. Range restrictedness requires that every variable occurring positively (i.e. as a consuming occurrence) also must occur negatively (i.e. as a defining occurrence) in each disjunctive part of a rule.

Example 5
Consider the following Xcerpt program:

```
CONSTRUCT
  f{var X, var Y}
FROM
  or {
    g{var X, var Y, var Z},
    and {
      h{var X, var Y},
      not k{var X, var Z}
    }
  }
END
```

Because of the `or`-construct in the rule body, this rule contains two disjuncts. In the first disjunct, the variables `X`, `Y`, and `Z` occur with negative polarity (because they are part of the query), and the variables `X` and `Y` also occur with positive polarity (because they occur in the rule head). This part of the rule would thus be range restricted. However, in the second disjunct, only the variables `X` and `Y` occur positively, while `X`, `Y`, and `Z` occur negatively (note that `Z` is contained within a `not`-negation). Thus, this part is not range restricted.

2.2.2 Stratification

Stratification is a technique to define a class of logic programs where non-monotonic features like Xcerpt's grouping constructs or negation can be defined in a declarative manner. The principal idea of stratification is to disallow programs with a recursion over negated queries ("*negation stratification*") or grouping constructs ("*grouping stratification*") and thereby preclude undesirable programs that have a non-intuitive semantics. While this requirement is very strict, its advantages are that it is straightforward to understand and can be verified by purely syntactical means without considering terms that are not part of the program (as is required by more elaborate techniques like *stable models*).

Several refinements over stratification have been proposed, e.g. *local stratification* [Prz88] that allow certain kinds of recursion, but these usually require more "knowledge" of the program or the queried resources. This section only gives an intuition over grouping and negation stratification; stratification of Xcerpt programs is described in detail in [Sch04].

Grouping Stratification The grouping constructs `all` and `some` are powerful constructs that are justified by many practical applications. However, using them in recursive rules allows to define programs with no useful meaning. Consider for example the program

$$\begin{array}{l} f\{all\ var\ X\} \leftarrow f\{\{var\ X\}\} \\ f\{a\} \end{array}$$

The meaning of such programs is unclear and probably unintended by the program author. The solution is to disallow recursion of rules with grouping constructs, and to require that all rules on which a rule with grouping constructs depends can be evaluated first. Programs that fulfill this propertiy are called *grouping stratifiable*.

Negation Stratification Xcerpt's `not`-construct is evaluated as *negation as failure (NaF)*, i.e. a negated query succeeds if the query itself fails finitely (i.e. can be proven to be not provable). NaF is desirable for a Web query language, because it is close to the intuitive understanding of negation: for instance, it is natural to assume that a train not listed in a train timetable does not exist, instead of requiring that every non-existent train is explicitly listed in the timetable.

Although NaF has a purely operational meaning, it is desirable to provide a declarative semantics as well, because the latter is usually easier to understand than the evaluation algorithm. Unfortunately, like recursion over grouping constructs, negation as failure allows for programs whose meaning is unclear. Consider for instance the following Xcerpt program:

$$f\{a\} \leftarrow not\ f\{a\}$$

Backward chaining evaluation of this rule does not terminate: for proving $f\{a\}$, it is necessary to show (in an auxiliary computation) that $f\{a\}$ does not hold, which again requires to evaluate the rule, and so on.

Declaratively, the meaning of this rule is problematic. When representing rules by implication as in traditional logic programming, this rule is simply equivalent to $f\{a\} \vee \neg\neg f\{a\}$, which simplifies to $f\{a\}$. This interpretation does not reflect the operational behaviour (which is the definition for negation as failure) described in the previous paragraph. Other approaches have been considered (like Clarke's completion or default negation) that interpret the symbol $\leftarrow$ differently, but all of these have similar problems.

Xcerpt programs are therefore assumed to be also *negation stratifiable*, a syntactic restriction that excludes such programs that involve problematic use of negation as in the example above. Negation stratification in Xcerpt programs is defined in the usual manner (as e.g. in [ABW88]). In stratifiable programs, both recursion and negation are allowed, but a recursion "through negation" is disallowed.

2.3 Ground Query Terms and Ground Query Term Graphs

Let T^q be the set of all query terms.

Definition 6 (Ground Query Term)

1. A query term is called *ground*, if it does not contain (subterm, label, namespace, or positional) variables.
2. $T^g \subset T^q$ denotes the set of all ground query terms, and $T^d \subset T^g$ denotes the set of all data terms.

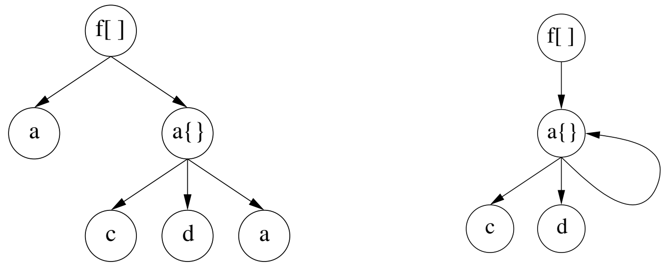
In the following, we differentiate between the ground query term itself and the graphs induced by a ground query term. Whereas the term itself contains subterms of the form `^id` and `id@t`, all references are dereferenced in the graph induced by the ground query term. By the *position* of a subterm in a ground query term, we mean the position in the list of children of that term. For example, in `f{a,b,c}`, *c* is the subterm at position 3. Likewise, in `f{id@a,^id}`, `id@a` is the subterm at position 1, and `^id` is the subterm at position 2. The position of subterms in the graph induced by a ground query term is defined differently: in the last example, the subterm *a* has both the position 1 and the position 2. For this reason, we will usually speak about *successors* when referring to the graph induced by a ground query term, and about *subterms*, when referring to the syntactical representation of a ground query term.

The *graph induced by a ground query term* (or short: *ground query term graph*) is defined in a straightforward manner as follows.

Definition 7 (Graph Induced by a Ground Query Term)
Given a ground query term t. The *graph induced by t* is a tuple $G_t = (V, E, r)$, with:

1. a set of *vertices* (or *nodes*) V defined as the set of all (immediate and indirect) subterms of t (including t itself).

Figure 1 Graphs induced by $f[a, a[c, d, a]]$ and $f[[\&1 \mathbin{@} a\{\{c, d, \uparrow \&1\}\}]]$



2. a set of *edges* $E \subseteq V \times V \times \mathbb{N}$ characterised as follows:
   - for all terms $t_1, t_2, t_3 \in V$: if t_2 is the subexpression of t_1 at position i and of the form `^oid` (a referring occurrence), and t_3 is of the form `oid @ t'` (a defining occurrence), with `oid` an identifier and `t'` a term ($\in V$), then $(t_1, t_3, i) \in E$.
   - for all terms $t_1, t_2 \in V$: if t_2 is the subexpression of t_1 at position i and *not* of the form `^oid`, then $(t_1, t_2, i) \in E$.
3. a distinguished vertex $r \in V$ called the *root node* with $r = t$.

The *label* of a vertex is either the label, the string value, or the regular expression of the subterm it represents.

Representing vertices as complete subterms and edges with positions is necessary for the definition of the simulation relation as it conveys information about ordered/unordered and partial/total term specifications and the respective positions of subterms in a term. Figure 1 illustrates this definition on two ground query terms. Note that for space reasons, the vertices in both graphs do not contain the subterms, but only the term labels and specifications.

The following additional terminology from graph theory is used below. Let $G = (V, E, r)$ be the graph induced by a ground query term. For any two nodes $v_1 \in V$ and $v_2 \in V$, if $(v_1, v_2, i) \in E$ for some integer i (i.e. there is an edge from v_1 to v_2), v_1 and v_2 are called *adjacent*, v_2 is the i^{th} *successor* of v_1, and v_1 is a *predecessor* of v_2.

2.4 Term Sequences and Successors

The following sections use the notion of (finite) *term sequences* to represent the (immediate) successors of a term. Note that sequences of subterms are used regardless of the kind of subterm specification: in case of unordered term specifications, there is still a sequence of subterms given by the syntactical representation of the term.

Recall in the following that a function $f : N \to M$ can be seen as a (binary) relation $f \subseteq N \times M$ such that for every two different pairs $(n_1, m_1) \in f$ and $(n_2, m_2) \in f$ holds that $n_1 \neq n_2$. Considering a function as a relation is more convenient for the representation of sequences. A function $f : N \to M$ is furthermore called *total*, if f is defined for every element of N.

Definition 8 (Term Sequence)

1. Let X be a set of terms and let $N = \{1, \ldots, n\}$ ($n \geq 0$) be a set of non-negative integers. A *term sequence* is a total function $S \subseteq N \times X$ mapping integers to terms.

Instead of writing $S = \{(1,a),(2,b),\dots\}$, term sequences are often denoted by $S = \langle a,b,\dots\rangle$.

2. Let S be a term sequence, and let $s = (i,t)$ be an element in S.
   - the *index* of s is defined as $index(s) = i$ (projection on the first element)
   - the *term* of s is defined as $term(s) = x$ (projection on the second element)

If $S = \langle \dots, a, \dots\rangle$ is a term sequence, i.e. $S = \{\dots,(a,i),\dots\}$, then $term((a,i)) = a$. Since using $term((a,i))$ is very inconvenient, we shall often write a instead of (a,i) and e.g. use $a \in S$ instead of $(a,i) \in S$. Accordingly, we use the notion $index(a)$ to represent the position of the subterm a in the term sequence, unless we have to distinguish multiple occurrences of a in S.

Note that empty term sequences are not precluded by the definition, and term sequences are always finite, because they serve to represent the (immediate) successors of a term. Instead of *term sequence*, we shall often simply write *sequence* as other sequences are not considered in this work. The *index* of an element can also be called the *position* of that element. However, the notion *index* is preferred to better distinguish between the `position` construct in a query term and the position in the sequence.

Sequences allow for multiple occurrences of the same term. For example, both $S = \langle a,b,a\rangle = \{(1,a),(2,b),(3,a)\}$ and $T = \langle a,a,b\rangle = \{(1,a),(2,a),(3,b)\}$ are term sequences of a and b.

Based on the graph induced by a ground query term, the definition of the sequence of successors is as expected:

Definition 9 (Sequence of Successors)
Let t be a ground query term, let $G_t = (V,E,t)$ be the graph induced by t, and let $v \in V$ be a node in G_t (i.e. subterm of t). The *sequence of successors* of v, denoted $Succ(v)$, is defined as

$$Succ(v) = \left\{(i,v') \mid (v,v',i) \in E\right\}$$

Note that $Succ(v)$ may be the empty sequence $\langle\ \rangle$, if v does not have successors.

Consider the term $t_1 = f\{a,a,b\}$. The sequence of successors of t_1 is $Succ(t_1) = \langle a,a,b\rangle = \{(1,a),(2,a),(3,b)\}$. Consider furthermore $t_2 = o1@f[a,\uparrow o1,b]$. The sequence of successors of t_2 is $Succ(t_2) = \langle a, o1@f[a,\uparrow o1,b], b\rangle = \{(1,a),(2,o1@f[a,\uparrow o1,b]),(3,b)\}$. Note that the reference in t_2 is dereferenced (one level).

Mostly, the sequence of successors and the sequence of (immediate) subterms of a term coincide. The most significant difference is that the sequence of successors is already dereferenced, i.e. all references are "replaced" by the subterms they refer to. For this reason, the remainder of this Section uses the term *successors* instead of *subterms*. Although it is somewhat imprecise, the notion *subterm* is often added in parentheses to emphasise the coincidence of the two sequences in most cases.

In Section 4, the following additional notions of subsequences and concatenation of sequences are needed. Both definitions are straightforward. In order to distinguish subsequences from subsets, we usually write $S' \sqsubseteq S$.

Definition 10 (Subsequences, Concatenation of Sequences)
Let $S = \langle s_1,\dots,s_m\rangle$ and $T = \langle t_1,\dots,t_n\rangle$ be term sequences.

1. T is called a *subsequence* of S, denoted $T \sqsubseteq S$, if there exists a strictly monotonic mapping π such that for each $(i,x) \in T$ there exists $(\pi(i),x) \in S$.

2. The *concatenation* of S and T, denoted $S \circ T$, is defined as

$$S \circ T = \langle s_1,\dots,s_m,t_1,\dots,t_n\rangle$$

Consider for example the sequences $S_1 = \langle a, b\rangle = \{(1,a),(2,b)\}$ and $S_2 = \langle a, a, b\rangle = \{(1,a),(2,a),(3,b)\}$. S_1 is a subsequence of S_2 with $\pi(1) = 1, \pi(2) = 3$ or with $\pi(1) = 2, \pi(2) = 3$. The concatenation of S_1 and S_2 yields

$$S_1 \circ S_2 = \langle a, b, a, a, b\rangle = \{(1,a),(2,b),(3,a),(4,a),(5,b)\}$$

2.5 Substitutions and Substitution Sets

In principle, the usual notion of substitutions is also used for Xcerpt terms. However, variable restrictions occurring in query terms have to be taken into account. As a variable might be restricted, not every substitution is applicable to every query term.

Also, Xcerpt construct terms extend the usual terms by grouping constructs that group several substitutions within a single ground instance by using the constructs `all` and `some`. For instance, given a construct term $f\{all\ var\ X\}$ and three alternative substitutions $\{X \mapsto a\}$, $\{X \mapsto b\}$ and $\{X \mapsto c\}$, the resulting data term is $f\{a, b, c\}$.

In order to define such groupings, it is therefore necessary to provide a construct that represents all possible alternatives and can be applied to a construct term. This is called a *substitution set* below. Since the application of substitution sets to query and construct terms involves some complexity, it is described separately in Section 4. Substitution sets are then used in Section 6 which defines satisfaction for Xcerpt term formulas. In the following, substitutions are denoted by lowercase greek letters (like σ or π), while substitution sets are denoted by uppercase greek letters (like Σ or Π).

2.5.1 Substitutions

A *substitution* is a mapping from the set of (all) variables to the set of (all) construct terms. In the following, lower case greek letters (like σ or τ) are usually used to denote substitutions. As usual in mathematics, a substitution is a mapping of infinite sets. Of course, finite representations are usually used, as the number of variables occurring in a term is finite. Substitutions are often conveniently denoted as sets of variable assignments instead of as functions. For example, we write $\{X \mapsto a, Y \mapsto b\}$ to denote a substitution that maps the variable X to a and the variable Y to b, and any other variable to arbitrary values. In general, a substitution provides assignments for all variables, but "irrelevant" variables are not given in the description of substitutions.

If a substitution is *applied* to a query term t^q, all occurrences of variables for which the substitution provides assignments are replaced by the respective assignments (see Section 4.1 below). The resulting term is called an *instance* of t^q and the substitution. Not every substitution can be applied to every query term: variable assignments in the substitution have to respect variable restrictions occurring in the pattern for a substitution to be applicable (see also 4.1). If a substitution σ respects the variable restrictions in a query term t^q, it is said to be *a substitution for* t^q. For example, the substitution $\{X \mapsto f\{a\}\}$ is a substitution for $var\ X \rightsquigarrow f\{\{\}\}$, but not for $var\ X \rightsquigarrow g\{\{\}\}$. Note that a substitution cannot be applied to a construct term, because construct terms may contain grouping constructs that group several instances of subterms together. Instead, substitution sets are used for this purpose (see below).

A substitution σ is called a *grounding substitution* for a term t, if $\sigma(t)$ is a ground query term. Consequently, a grounding substitution is always a mapping from the set of variable names to the set of data terms (i.e. ground construct terms). A substitution σ is called an *all-grounding substitution*, if it maps every variable to a data term. Naturally, every all-grounding substitution is a grounding substitution for every query term to which it is applicable. Note that the reverse does not hold: a grounding substitution is grounding wrt. some term t and does not necessarily assign ground terms to variables not occurring in t.

A substitution σ_1 is a *subset* of a substitution σ_2 (i.e. $\sigma_1 \subseteq \sigma_2$), if $\sigma_1(X) \cong \sigma_2(X)$ for every variable name X with $\sigma_1(X) \neq X$ (i.e. σ_1 does not map X to itself), where $\cong$ denotes simulation equivalence (i.e. mutual simulation, cf. Section 5.3). Correspondingly, two substitutions σ_1 and σ_2 are considered to be *equal* (i.e. $\sigma_1 = \sigma_2$), if $\sigma_1 \subseteq \sigma_2$ and $\sigma_2 \subseteq \sigma_1$. For example, $\{X \mapsto f\{a,b\}\}$ and $\{X \mapsto f\{b,a\}\}$ are equal. This definition is reasonable because the data terms resulting from applying two such substitutions are treated equally in the model theory described below.

The *composition* of two substitutions σ_1 and σ_2, denoted by $\sigma_1 \circ \sigma_2$ is defined as $(\sigma_1 \circ \sigma_2)(t) = \sigma_1(\sigma_2(t))$ for every query term t. Note that the assignments in σ_2 take precedence, because σ_2 is applied first. Consider for example $\sigma_1 = \{X \mapsto a, Y \mapsto b\}$ and $\sigma_2 = \{X \mapsto c\}$, and a term $t = f\{var\ X, var\ Y\}$. Applying the composition $\sigma_1 \circ \sigma_2$ to t yields $(\sigma_1 \circ \sigma_2)(t) = f\{c,b\}$.

The *restriction* of a substitution σ to a set of variable names V, denoted by $\sigma_{|V}$, is the mapping that agrees with σ on V and with the identical mapping on the other variables.

2.5.2 Substitution Sets

A *substitution set* is simply a set containing substitutions. In the following, upper case greek letters (like Σ and Φ) are usually used to denote substitution sets.

Substitution sets can be *applied* to a query *or* construct term (cf. Sections 4.1 and 4.2). The result of this application is in general a set of terms called the *instances* of the substitution set and the term. A substitution set Σ is only applicable to a query term t^q, if all substitutions in Σ are applicable to t^q. In this case, Σ is called *a substitution set for* t^q. Since construct terms do not contain variable restrictions, every substitution set except for the empty set is a substitution set for a construct term. There exists no query or construct term t such that the empty substitution set $\{\}$ is a substitution set for t.

A substitution set Σ for a term t is called a *grounding substitution set*, if all instances of t and Σ are ground query terms or data terms. A substitution set Σ is called an *all-grounding substitution set*, if all $\sigma \in \Sigma$ are all-grounding substitutions.

The *composition* of two substitution sets Σ_1 and Σ_2, denoted as $\Sigma_1 \circ \Sigma_2$, is defined as

$$\Sigma_1 \circ \Sigma_2 = \left\{\sigma_1 \circ \sigma_2 \mid \sigma_1 \in \Sigma_1, \sigma_2 \in \Sigma_2\right\}$$

Consider for example the substitution sets $\Sigma_1 = \left\{\{X \mapsto a\}\right\}$ and $\Sigma_2 = \left\{\{Y \mapsto b\}, \{Y \mapsto c\}\right\}$. Then $\Sigma_1 \circ \Sigma_2 = \left\{\{X \mapsto a, Y \mapsto b\}, \{X \mapsto a, Y \mapsto c\}\right\}$.

The *restriction* of a substitution set Σ to a set of variables V, denoted by $\Sigma_{|V}$, is the set of substitutions in Σ restricted to V.

Similarly, the *extension* of a substitution set Σ restricted to a set of variables V to a set of variables V' with $V \subseteq V'$, extends every substitution σ in Σ to substitutions σ' by adding all possible assignments of variables in $V' \setminus V$ to data terms. For example, the extension of the restricted substitution set $\left\{\{X \mapsto a\}\right\}$ to the set of variables $\{X, Y\}$ is the (infinite) set $\left\{\{X \mapsto a, Y \mapsto a\}, \{X \mapsto a, Y \mapsto b\}, \dots\right\}$

Note that in practice, it would be desirable to define substitution sets as *multi-sets* that may contain duplicate elements: if an XML document contains two persons named "Donald Duck", then it should be assumed that these are different persons with the same name. Providing a proper formalisation with multi-sets is, however, not in the scope of this article, as subsequent definitions and proofs would be much more complicated without adding an interesting aspect to the formalisation.

2.5.3 Maximal Substitution Sets

So as to properly convey the meaning of `all`, it is not sufficient to consider arbitrary substitution sets. The interesting substitution sets are those that are *maximal* for the satisfaction of the query part Q of a rule. As satisfaction is not yet formally defined, this property shall for now simply be called P.

Intuitively, the definition of maximal substitution sets is straightforward: a substitution set Σ satisfying P is a maximal substitution set, if there exists no substitution set Φ satisfying P such that Σ is a proper subset of Φ. However, this informal definition does not take into account that there might be substitution sets that differ only in that some substitutions contain bindings that are irrelevant because they do not occur in the considered term formula Q. Maximal substitution sets are therefore formally defined as follows:

Definition 11 (Maximal Substitution Set)
Let Q be a quantifier free query term formula with set of variables V, let P be a property, and let Σ be a set of substitutions such that P holds for Σ. Σ is called a *maximal substitution set wrt. P and Q*, if there exists no substitution set Φ such that P holds for Φ and $\Sigma_{|V}$ is a proper subset of $\Phi_{|V}$ (i.e. $\Sigma_{|V} \subset \Phi_{|V}$).

3 Terms as Formulas

Classical logic distinguishes between

- terms, which are composed of function symbols and serve as data structures representing objects of the application domain at hand, and
- atomic formulas, which are composed of relation symbols and terms and represent statements about objects of the application domain.

Statements represented by formulas have truth values, objects represented by terms have no truth value. In contrast, XML and Web data does not need this distinction, because it has no (formal) semantics and merely holds semistructured data. Therefore, Xcerpt terms (corresponding to Web data) are considered as being atomic formulas representing the statement that the respective terms "exist". A salient aspect of this representation is the possibility to specify integrity constraints for data terms. These are, however, not covered in depth in this article.

3.1 Term Formulas

Atomic formulas are composed of Xcerpt query, construct, and data terms, and of the two special terms $\bot$ and $\top$ (denoting falsity and truth). As an intuition, such atomic formulas are statements about the existence or satisfiability of a term. Compound formulas can be constructed in the usual manner using the binary connectives $\vee$, $\wedge$, $\Rightarrow$, and $\Leftrightarrow$, the unary connective $\neg$, the zero-ary connectives $\top$ and $\bot$, and the quantifiers $\forall$ and $\exists$. Instead of quantifying each variable separately, the construct $\forall^*$ may be used to universally quantify all free variables in a formula. Also, instead of writing $F_1 \vee \cdots \vee F_n$, we sometimes write $\bigvee_{1 \leq i \leq n} F_i$, and instead of writing $F_1 \wedge \cdots \wedge F_n$, we sometimes write $\bigwedge_{1 \leq i \leq n} F_i$.

In the following, formulas built in this manner shall be called *Xcerpt term formulas*, or simply *term formulas*. If a term formula consists only of query terms, it is also called *query term formula*, if it consists only of construct terms, it is called *construct term formula*.

Example 12
The following example shows a term formula built up from query terms, implications and quantifiers. It represents an integrity constraint that requires all books in the `bib.xml` document to have at least one author:

```
∀ B . bib{{ var B → book{{ }} }} ⇒
    ∃ A . bib{{ var B → book{{ authors{{ var A }} }} }}
```

3.2 Xcerpt Programs as Formulas

Like in traditional logic programming, rules in Xcerpt are implications. However, Xcerpt rules with grouping constructs have a particular semantics that cannot be represented as implications in the usual manner. We therefore keep the denotation $t^c \leftarrow Q$ to represent rules.

In addition to the usual quantifiers $\forall$ and $\exists$, the grouping constructs `all` and `some` that may be part of a construct term may bind variables in a formula within a specific scope, usually the head and body of a rule. As these constructs are contained within the term structure, their scope is not immediately apparent. It is thus useful to introduce new symbols $\ll \cdot \gg$ that are used to indicate the scope of *all* the grouping constructs contained in them. In practice, it is neither desirable nor useful to have scopes extending over different subformulas for the grouping constructs contained in a single construct term, thus a single scope for all grouping constructs suffices. The grouping constructs of a construct term always refer to the variables of a single rule and thus all have the same scope.

Example 13
Consider for example the program (in formula notation)

```
g{a,b,c}
f{all var X} ← g{{var X}}
```

The scope of the `all` construct in the rule head is made explicit using $\ll \cdot \gg$ in the following manner:

```
g{a,b,c} ∧ ≪f{all var X} ← g{{var X}}  ≫
```

As usual, formulas representing programs are always considered to be universally closed, even if quantifiers are not explicitly given.

Example 14
Consider the following Xcerpt program (in the notation introduced in Section 2 and with internalised resources):

```
f{all var X, var Y} ← and{ g{{var X}}, h{{ e{var X,var Y} }} }
g[ var X ]          ← h{{ e[var X] }}
h[ e[a,1], e[b,1], e[c,1], e[d,2] ]
```

The formula representation of this program is as follows:

```
∀ Y ≪f{all var X, var Y} ← g{{var X}} ∧ h{{ e{var X,var Y} }} ≫ ∧
∀ X ≪g[ var X ]  ← h{{ e[var X] }} ≫ ∧
h[ e[a,1], e[b,1], e[c,1], e[d,2] ]
```

The variable `X` in the first rule is in the scope of the `all` construct in the rule head, while the variable `Y` is in the scope of the universal quantification represented by $\forall Y$. Note that the scope of the `all` is restricted to the first rule and the occurrences of `X` in the second rule are not affected (thus $\forall X$ in the second rule).

4 Application of Substitutions to Xcerpt Terms

4.1 Application to Query Terms

Since query terms do not contain the grouping constructs *all* and *some*, applying substitutions and substitution sets is straightforward. Application of a single substitution yields a *single* term where some variable occurrences are substituted, while application of a substitution set yields a *set* of terms where some variables are substituted.

Definition 15 (Substitutions: Application to Query Terms)
Let t^q be a query term.

1. The application of a *substitution* σ to t^q, written $\sigma(t^q)$ is recursively defined as follows:

   - $\sigma(var\ X) = t'$ if $(X \mapsto t') \in \sigma$
   - $\sigma(var\ X \rightsquigarrow s) = t'$ if $(X \mapsto t') \in \sigma$ and $\sigma(s) \preceq t'$
   - $\sigma(f\{t_1, \dots, t_n\}) = \sigma(f)\{\sigma(t_1), \dots, \sigma(t_n)\}$
   - $\sigma(f[t_1, \dots, t_n]) = \sigma(f)[\sigma(t_1), \dots, \sigma(t_n)]$
   - $\sigma(f\{\{t_1, \dots, t_n\}\}) = \sigma(f)\{\{\sigma(t_1), \dots, \sigma(t_n)\}\}$
   - $\sigma(f[[t_1, \dots, t_n]]) = \sigma(f)[[\sigma(t_1), \dots, \sigma(t_n)]]$
   - $\sigma(without\ t) = without\ \sigma(t)$
   - $\sigma(optional\ t) = optional\ \sigma(t)$

   for some $n \geq 0$.

2. The application of a *substitution set* Σ to t^q is defined as follows:

$$\Sigma(t^q) = \left\{\sigma(t^q) \mid \sigma \in \Sigma\right\}$$

Note that not every substitution can be applied to a query term t^q. If a variable in t^q is restricted as in $var\ X \rightsquigarrow s$, then a substitution can only be applied if it provides bindings for X that are compatible to this restriction. Likewise, a substitution set is only applicable to a query term t^q, if all its substitutions are applicable to t^q.

Since query terms never contain grouping constructs, the cardinality of $\Sigma(t)$ always equals the cardinality of Σ. In particular, if $\Sigma = \emptyset$, then $\Sigma(t) = \emptyset$, even if t is a ground query term. Since an interpretation with an empty substitution set would be a model for any formula, substitution sets in the following are considered to be non-empty. In case no variables are bound, substitution sets are usually defined as $\Sigma = \{\emptyset\}$.

4.2 Application to Construct Terms

Applying a single substitution to a construct term is not reasonable as the meaning of the grouping constructs *all* and *some* is unclear in such cases. In the following, the application is thus only defined for substitution sets. On substitution sets, the grouping constructs group such substitutions that have the same assignment on the *free variables* of a construct term. For each such group, the application of the substitution Σ yields a different construct term. A variable is considered *free* in a construct term if it is not in the scope of a grouping construct. The set of free variables of a construct term t^c is denoted by $FV(t^c)$. The relation $\cong$ denotes simulation equivalence between two ground terms and is defined later in this article.

Definition 16 (Grouping of a Substitution Set)
Given a substitution set Σ and a set of variables $V = \{X_1, \dots, X_n\}$ such that all $\sigma \in \Sigma$ have bindings for all $X_i, 1 \leq i \leq n$.

- The equivalence relation $\simeq_V \subseteq \Sigma \times \Sigma$ is defined as: $\sigma_1 \simeq_V \sigma_2$ iff $\sigma_1(X) \cong \sigma_2(X)$ for all $X \in V$.
- The set of equivalence classes $\Sigma/_{\simeq_V}$ with respect to $\simeq_V$ is called the *grouping of* Σ *on* V.
- Each of the equivalence classes $[\![\sigma]\!] \in \Sigma/_{\simeq_V}$ is accordingly defined as $[\![\sigma]\!] = \{ \tau \in \Sigma \mid \tau \simeq_V \sigma \}$.

Informally, each equivalence class $[\![\sigma]\!] \in \Sigma/_{\simeq_V}$ contains such substitutions that have the same assignment for each of the variables in V.

Example 17
Given the substitution set $\Sigma = \{\sigma_1, \sigma_2, \sigma_3\}$ with

$$\sigma_1 = \{X_1 \mapsto a, X_2 \mapsto b\}, \sigma_2 = \{X_1 \mapsto a, X_2 \mapsto c\}, \text{ and } \sigma_3 = \{X_1 \mapsto c, X_2 \mapsto b\}$$

The grouping of Σ on $V = \{X_1\}$ is

- $[\![\sigma_1]\!] = [\![\sigma_2]\!] = \{\{X_1 \mapsto a, X_2 \mapsto b\}, \{X_1 \mapsto a, X_2 \mapsto c\}\}$
- $[\![\sigma_3]\!] = \{\{X_1 \mapsto c, X_2 \mapsto b\}\}$

The application of a substitution set to a construct term (possibly containing grouping constructs) is defined in terms of this grouping. Given a substitution set Σ, the application $\Sigma(t^c)$ to a construct term t^c with free variables $FV(t^c)$ yields exactly $|\Sigma/_{\simeq_{FV(t^c)}}|$ results, one for each different binding of the free variables in t^c.

Example 18
Given a term $t = f\{X_1, g\{all\ X_2\}\}$, i.e. $FV(t) = \{X_1\}$. Consider again

$$\Sigma = \{\{X_1 \mapsto a, X_2 \mapsto b\}, \{X_1 \mapsto a, X_2 \mapsto c\}, \{X_1 \mapsto c, X_2 \mapsto b\}\}$$

from Example 17. The result of applying Σ to t is

$$\Sigma(t) = \{f\{a, g\{b, c\}\}, f\{c, g\{b\}\}\}$$

The following definition specifies how a substitution set is applied to a construct term t^c. The definition is divided into two parts: In the first part, it is assumed that all substitutions in the substitution set Σ contain the same assignments for the free variables of t^c (variables occurring within the scope of grouping constructs are unrestricted). As the quotient $\Sigma/_{\simeq_{FV(t^c)}}$ in this case obviously only contains a single equivalence class, the application of this restricted Σ to t^c yields only a single term, which simplifies the recursive definition. In the second part of Definition 19, this restriction is lifted.

Since the construction of data terms requires to construct new lists of subterms, the following definition(s) use the notion of *term sequences* introduced in Section 2.4. Recall that a sequence is a binary relation between a set of integers and a set of terms, and usually denoted by $S = \langle x_1, \ldots, x_n \rangle$ for some n and terms x_i. Recall furthermore the definitions of *subsequences* and *concatenation* (Definition 10 on page 10).

Defining the semantics of `order by` furthermore requires a function $sort_{f(V)}(\cdot,\cdot)$, where V is a sequence of variables, that takes as arguments a grouping of a substitution set on V and returns a sequence of substitution sets ordered according to $f(V)$ and the variables in V. $f(V)$ is a total ordering on the set of substitution sets that assign ground terms to the variables in V comparing variable bindings for the variables in V. [1]

[1] As the substitution set is grouped on V, all substitutions in $[\![\sigma]\!]$ (respectively $[\![\tau]\!]$) provide identical bindings for variables in V.

Definition 19 (Substitutions: Application to Construct Terms)

1. Let Σ be a substitution set and let t^c be a construct term such that all free variables of t^c have the same assignment in all substitutions of Σ, i.e. $\Sigma/_{\simeq_{FV(t^c)}} = \{[\![\sigma]\!]\}$. The restricted application of Σ to t^c, written $[\![\sigma]\!](t^c)$, is recursively defined as follows:

   - $[\![\sigma]\!](var\ V) = \langle\sigma(V)\rangle$[2]
   - $[\![\sigma]\!](f\{t_1,\ldots,t_n\}) = \langle[\![\sigma]\!](f)\{[\![\sigma]\!](t_1)\circ\cdots\circ[\![\sigma]\!](t_n)\}\rangle$ for some $n \geq 0$
   - $[\![\sigma]\!](f[t_1,\ldots,t_n]) = \langle[\![\sigma]\!](f)[[\![\sigma]\!](t_1)\circ\cdots\circ[\![\sigma]\!](t_n)]\rangle$ for some $n \geq 0$
   - $[\![\sigma]\!](all\ t) = [\![\tau_1]\!](t)\circ\cdots\circ[\![\tau_k]\!](t)$ where $\{[\![\tau_1]\!],\ldots,[\![\tau_k]\!]\} = [\![\sigma]\!]/_{\simeq_{FV(t)}}$
   - $[\![\sigma]\!](all\ t\ group\ by\ V) = [\![\tau_1]\!](t)\circ\cdots\circ[\![\tau_k]\!](t)$ where $\{[\![\tau_1]\!],\ldots,[\![\tau_k]\!]\} = [\![\sigma]\!]/_{\simeq_{FV(t)\cup V}}$
   - $[\![\sigma]\!](all\ t\ order\ by\ f\ V) = [\![\tau_1]\!](t)\circ\cdots\circ[\![\tau_k]\!](t)$
     where $\langle[\![\tau_1]\!],\ldots,[\![\tau_k]\!]\rangle = sort(f(V),[\![\sigma]\!]/_{\simeq_{FV(t)\cup V}})$
   - $[\![\sigma]\!](some\ k\ t) = [\![\tau_1]\!](t)\circ\cdots\circ[\![\tau_k]\!](t)$ where $\{[\![\tau_1]\!],\ldots,[\![\tau_k]\!]\} \subseteq [\![\sigma]\!]/_{\simeq_{FV(t)}}$
   - $[\![\sigma]\!](some\ k\ t\ group\ by\ V) = [\![\tau_1]\!](t)\circ\cdots\circ[\![\tau_k]\!](t)$ where $\{[\![\tau_1]\!],\ldots,[\![\tau_k]\!]\} \subseteq [\![\sigma]\!]/_{\simeq_{FV(t)\cup V}}$
   - $[\![\sigma]\!](some\ k\ t\ order\ by\ f\ V) = [\![\tau_1]\!](t)\circ\cdots\circ[\![\tau_k]\!](t)$
     where $\langle[\![\tau_1]\!],\ldots,[\![\tau_k]\!]\rangle \sqsubseteq sort(f(V),[\![\sigma]\!]/_{\simeq_{FV(t)\cup V}})$

   where $[\![\tau]\!]1,\ldots,[\![\tau]\!]k$ are pairwise different substitution sets.

2. Let t^c be a term, and let $FV(t^c)$ be the free variables in t^c. The application of a *substitution set* Σ to t^c is defined as follows:

$$\Sigma(t) = \left\{t^{c'} \mid [\![\sigma]\!] \in \Sigma/_{\simeq_{FV(t^c)}} \ \wedge\ \langle t^{c'}\rangle = [\![\sigma]\!](t^c)\right\}$$

Although not explicitly defined above, integrating aggregations and functions in this definition is straightforward.

Example 20
Consider the substitution set

$$\Sigma = \left\{\{X \mapsto f\{a\}, Y \mapsto g\{a\}\},\ \{X \mapsto f\{a\}, Y \mapsto g\{b\}\},\ \{X \mapsto f\{b\}, Y \mapsto g\{a\}\}\right\}$$

and the construct terms $t_1 = h\{all\ var\ X, var\ Y\}$ and $t_2 = h\{var\ X, all\ var\ Y\}$. Grouping Σ according to the free variables $FV(t_1) = \{Y\}$ in t_1 and $FV(t_2) = \{X\}$ in t_2 yields

$$\begin{array}{rcl}
\Sigma/_{\simeq_{FV(t_1)}} & = & \left\{\left\{\{X \mapsto f\{a\}, Y \mapsto g\{a\}\},\{X \mapsto f\{b\}, Y \mapsto g\{a\}\}\right\},\ \left\{\{X \mapsto f\{a\}, Y \mapsto g\{b\}\}\right\}\right\} \\
\Sigma/_{\simeq_{FV(t_2)}} & = & \left\{\left\{\{X \mapsto f\{a\}, Y \mapsto g\{a\}\},\{X \mapsto f\{a\}, Y \mapsto g\{b\}\}\right\},\ \left\{\{X \mapsto f\{b\}, Y \mapsto g\{a\}\}\right\}\right\}
\end{array}$$

The ground instances of t_1 and t_2 by Σ are thus

$$\begin{array}{rcl}
\Sigma(t_1) & = & \left\{\ h\{f\{a\},f\{b\},g\{a\}\},\ h\{f\{a\},g\{b\}\}\ \right\} \\
\Sigma(t_2) & = & \left\{\ h\{f\{a\},g\{a\},g\{b\}\},\ h\{f\{a\},g\{b\}\}\ \right\}
\end{array}$$

[2] Note that σ is the representative of the equivalence class $[\![\sigma]\!]$

4.3 Application to Query Term Formulas

In the following, it is often interesting to study ground instances not only of terms but also of compound formulas. The following definition defines the application of substitution sets to formulas consisting only of query terms (so-called *query term formulas*); construct terms are problematic, as they group several substitutions and thus do not behave “synchronously” with query terms in the same formula. Fortunately, the formalisation of Xcerpt programs does not need to consider formulas containing construct terms. The only exception are program rules, which are treated separately anyway.

Applying a substitution set to a query term formula is straightforward: as each substitution in a substitution set represents a different alternative, the application of the substitution set to a query term formula simply yields a conjunction of all different instances.

Definition 21 (Substitutions: Application to Query Term Formulas)
Let F be a quantifier-free term formula where all atoms are query terms (a *query term formula*).

1. The application of a *substitution* σ to F, written $\sigma(F)$, is recursively defined as follows:
   - $\sigma(F_1 \wedge F_2) = \sigma(F_1) \wedge \sigma(F_2)$
   - $\sigma(F_1 \vee F_2) = \sigma(F_1) \vee \sigma(F_2)$
   - $\sigma(\neg F') = \neg\sigma(F')$
   - $\sigma(\neg F') = \neg\sigma(F')$
2. The application of a *substitution set* Σ to F, written $\Sigma(F)$, is defined as follows:

$$\Sigma(F) = \bigwedge_{\sigma\in\Sigma} \sigma(F)$$

5 Simulation and Simulation Unifiers

Matching query terms with data terms is based on the notion of *rooted graph simulations* [HHK96, Mil71]. Intuitively, a query term matches with a data term, if there exists at least one substitution for the variables in the query term (called *answer substitution* of the query term) such that the corresponding graph induced by the resulting *ground* query term simulates in the graph induced by the data term. Of course, graph simulation needs to be modified to take into account the different term specifications, descendant construct, optional subterms, subterm negation, and regular expressions.

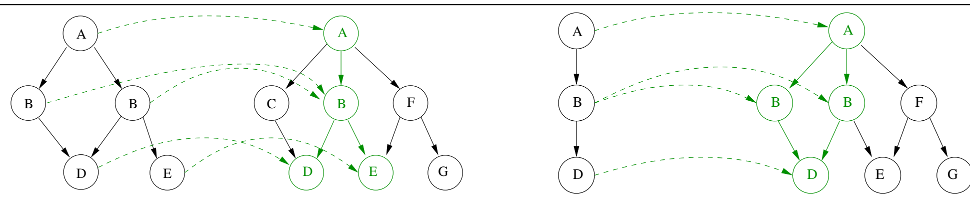
To simplify the formalisation below, it is assumed that strings and regular expressions are represented as compound terms with the string or regular expression as label, no subterms, and a total term specification. For example, the string `"Hello, World"` is represented as the term `"Hello, World"{}`.

5.1 Rooted Graph Simulation

Pattern matching in Xcerpt (and UnQL, for that matter) is based on a similarity relation between the graphs induced by two semistructured expressions, which is called *graph simulation* [HHK96, Mil71]. Graph simulation is a relation very similar to graph homomorphisms, but more general in the sense that it allows to match two nodes in one graph with a single node in the other graph and vice versa.

The following definition is inspired by [HHK96, Mil71] and refines the simulation considered in [BS02]. Recall that a (directed) rooted graph $G = (V, E, r)$ consists in a set V of vertices, a set E of edges (i.e. ordered pairs of vertices), and a vertex r called the root of G such that G contains a path from r to each vertex of G. Note that the initial definition of a rooted graph simulation does not take into

Figure 2 Rooted Graph Simulations (with respect to vertex adornment equality)



account the edge labels of graphs induced by a semistructured expression, it is defined on generic, node labelled and rooted graphs. Note furthermore, that in general, there might be more than one simulation between two graphs, which leads to the notion of *minimal* simulations also defined below.

Definition 22 (Rooted Graph Simulation)
Let $G_1 = (V_1, E_1, r_1)$ and $G_2 = (V_2, E_2, r_2)$ be two rooted graphs and let $\sim \subseteq V_1 \times V_2$ be an order or equivalence relation. A relation $S \subseteq V_1 \times V_2$ is a *rooted simulation* of G_1 in G_2 with respect to ŽÍþ if:

1. $r_1 \; S \; r_2$.

2. If $v_1 \; S \; v_2$, then $v_1 \sim v_2$.

3. If $v_1 \; S \; v_2$ and $(v_1, v_1', i) \in E_1$, then there exists $v_2' \in V_2$ such that $v_1' \; S \; v_2'$ and $(v_2, v_2', j) \in E_2$

A rooted simulation S of G_1 in G_2 with respect to $\sim$ is *minimal* if there are no rooted simulations S' of G_1 in G_2 with respect to $\sim$ such that $S' \subset S$ (and $S \neq S'$).

Definition 22 does not preclude that two distinct vertices v_1 and v_1' of G_1 are simulated by the same vertex v_2 of G_2, i.e. $v_1 \; S \; v_2$ and $v_1' \; S \; v_2$. Figure 2 gives examples of simulations with respect to the equality of vertex adornments. The simulation of the right example is not minimal.

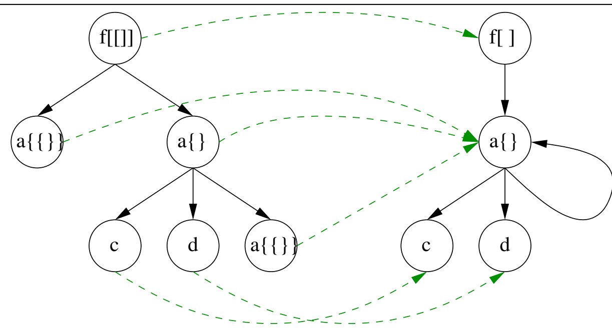
The *existance* of a simulation relation between two graphs (without variables) can be computed efficiently: results presented in [Kil92] give rise to the assumption that such problems can generally be solved in polynomial time and space. However, computation of pattern matching usually requires to compute not only one, but all minimal simulations between two graphs, in which case the complexity increases with the size of the "answer".

5.2 Ground Query Term Simulation

Using the graphs induced by ground query terms (cf. Definition 7), the notion of rooted simulation almost immediately extends to all ground query terms: intuitively, there exists a simulation of a ground query term t_1 in a ground query term t_2 if the labels and the structure of (the graph induced by) t_1 can be found in (the graph induced by) t_2 (see Figure 3). So as to define an ordering on the set of all ground query terms, ground query term simulation is designed to be transitive and reflexive.

Naturally, the simulation on ground query terms has to respect the different kinds of term specification: if t_1 has a *total* specification, it is not allowed that there exist successors (i.e. subterms) of t_2 that do not simulate successors of t_1; if t_1 has an *ordered* specification, then the successors of t_2 have to appear in the same order as their partners in t_1 (but there might be additional successors between them if the specification is also partial).

Figure 3 Minimal simulation of $f[[\ a\{\{\ \}\}, a\{\{c, d, a\{\{\ \}\}\ \}\}\ ]]$ in $f[\&1 \mathbin{@} a\{c, d, \uparrow \&1\}]$



The definition of *ground query term simulation* is characterised using a mapping between the sequences of successors (i.e. subterms) of two ground terms with one or more of the following properties, depending on the kinds of subterm specifications and occurrences of the constructs `without` and `optional`. Recall that a mapping is called total if it is defined on all elements of a set and partial if it is defined on some elements of a set.

Definition 23
Given two term sequences $M = \langle s_1, \ldots, s_m \rangle$ and $N = \langle t_1, \ldots, t_n \rangle$.
A partial or total mapping $\pi : M \to N$ is called

- *index injective*, if for all $s_i, s_j \in M$ with $index(s_i) \neq index(s_j)$ holds that $index(\pi(s_i)) \neq index(\pi(s_j))$
- *index monotonic*, if for all $s_i, s_j \in M$ with $index(s_i) < index(s_j)$ holds that $index(\pi(s_i)) < index(\pi(s_j))$
- *index bijective*, if it is index injective and for all $t_k \in N$ exists an $s_i \in M$ such that $\pi(s_i) = t_k$.
- *position respecting*, if for all $s_i \in M$ such that s_i is of the form `position` $j\ s'_i$ holds that $index(\pi(s_i)) = j$
- *position preserving*, if for all $s_i \in M$ such that s_i is of the form `position` $j\ s'_i$ holds that $\pi(s_i)$ is of the form `position` $l\ t'_k$ and $j = l$.

Index monotonic mappings preserve the order of terms in the two sequences and are used for matching terms with ordered term specifications. *Index bijective* mappings are used for total term specifications.

A *position respecting* mapping maps a term with position specification to a term with the specified position and is required (and only applicable) if the term with the sequence of successors (subterms) N uses total and ordered term specification. E.g. given two terms $f\{\{position\ 2\ b\}\}$ and $f[a, b, b]$, a position respecting mapping maps the subterm $position\ 2\ b$ only to the first b, because its position is 2, but not to the second b, because its position is 3.

A *position preserving* mapping maps a term with position specification to a term with the same position specification; it is applicable in case the sequence of successors of the second term N is incomplete with respect to order or breadth, as the exact position cannot be determined otherwise in these cases. In particular, this ensures the reflexivity and transitivity of the ground query term simulation (see Theorem 28 below). E.g. given the terms $f\{\{position\ 2\ b\}\}$ and $f\{a, b, position\ 2\ b\}$, the subterm $position\ 2\ b$ of the first term needs to be mapped to the subterm $position$ 2 b of the second term, but cannot be mapped to the first b because its position is not "guaranteed".

To summarise, a *position respecting* mapping *respects* the specified position by mapping the subterm only to a subterm at this position. On the other hand, a *position preserving* mapping *preserves* the position by mapping the subterm only to a subterm with the same position specification.

Besides these properties, ground query term simulation needs a notion of *label matches* to allow matching of string labels, regular expressions, or both:

Definition 24 (Label Match)
A term label l_1 matches with a term label l_2, if

- if l_1 and l_2 both are character sequences or both are regular expressions, then $l_1 = l_2$ or
- if l_1 is a regular expression and l_2 is a character sequence, then $l_2 \in L(l_1)$ where $L(l_1)$ is the language induced by the regular expression l_1

l_1 does not match with l_2 in all other cases.

Example 25

1. the labels of the terms $f\{a, b\}$ and $f\{b, a\}$ match
2. the labels of the terms $f\{a, b\}$ and $g\{b, a\}$ do not match
3. the labels of the terms `/.*/` and `"Hello World"` match
4. the labels of the terms `"Hello World"` and `/.*/` do not match

Let $G = (V, E, t)$ be the graph induced by a ground query term t. In the following, $Succ(t')$ denotes the sequence of all successors (i.e. immediate subterms) of t' in G, $Succ^+(t') \subseteq Succ(t')$ denotes the sequence of all successors of a term t' in G that are not of the form `without` t'', and $Succ^-(t)$ denotes the sequence of all successors of a term t' in G that are of the form `without` t'' (i.e. $Succ^+(t') \uplus Succ^-(t') \equiv Succ(t')$). Furthermore, $Succ^!(t') \subseteq Succ(t')$ denotes the sequence of all successors of a term t' in G that are not of the form `optional` t'', and $Succ^?(t') \subseteq Succ(t')$ denotes the sequence of all successors of a term t' that are of the form `optional` t'' (i.e. $Succ^!(t') \uplus Succ^?(t') \equiv Succ(t')$). Note that $Succ^- \subseteq Succ^!$, because a combination of `without` and `optional` is not reasonable.[3]

Definition 26 (Ground Query Term Simulaton)
Let r_1 and r_2 be ground (query) terms, and let $G_1 = (V_1, E_1, r_1)$ and $G_2 = (V_2, E_2, r_2)$ be the graphs induced by r_1 and r_2. A relation $\preceq \subseteq V_1 \times V_2$ on the sets V_1 and V_2 of immediate and indirect subterms of r_1 and r_2 is called a *ground query term simulation*, if and only if:

1. $r_1 \preceq r_2$ (i.e. the roots are in $\preceq$)
2. if $v_1 \preceq v_2$ and neither v_1 nor v_2 are of the form $desc\ t$ nor have successors of the forms `without` t or `optional` t, then the labels l_1 and l_2 of v_1 and v_2 match and there exists a *total, index injective mapping* $\pi : Succ(v_1) \rightarrow Succ(v_2)$ such that for all $s \in Succ(v_1)$ holds that $s \preceq \pi(s)$. Depending on the kinds of subterm specifications of v_1 and v_2, π in addition satisfies the following requirements:

[3] `optional` only has effect on the variable bindings, and `without` may never yield variable bindings

v_1	v_2	it holds that
$l_1[s_1,\ldots,s_m]$	$l_2[t_1,\ldots,t_n]$	π is *index bijective* and *index monotonic*
$l_1\{s_1,\ldots,s_m\}$	$l_2[t_1,\ldots,t_n]$	π is *index bijective* and *position respecting*
	$l_2\{t_1,\ldots,t_n\}$	π is *index bijective* and *position preserving*
$l_1[[s_1,\ldots s_m]]$	$l_2[t_1,\ldots,t_n]$	π is *index monotonic* and *position respecting*
	$l_2[[t_1,\ldots,t_n]]$	π is *index monotonic* and *position preserving*
$l_1\{\{s_1,\ldots s_m\}\}$	$l_2\{t_1,\ldots,t_n\}$	π is *position preserving*
	$l_2[t_1,\ldots,t_n]$	π is *position respecting*
	$l_2\{\{t_1,\ldots,t_n\}\}$	π is *position preserving*
	$l_2[[t_1,\ldots,t_n]]$	π is *position preserving*

3. if $v_1 \preceq v_2$ and v_1 is of the form $desc\ t_1$, then
   - v_2 is of the form $desc\ t_2$ and $t_1 \preceq t_2$ (*descendant preserving*, or
   - $t_1 \preceq v_2$ (*descendant shallow*), or
   - there exists a $v_2' \in SubT(v_2)$ such that $v_1 \preceq v_2'$ (*descendant deep*)

In all other cases (e.g. combinations of subterm specifications not listed above), $\preceq$ is no ground query term simulation. In subsequent parts of this article, the symbol $\preceq$ always refers to relations that are ground query term simulations.

Note that although graph simulation allows to relate two nodes of the one graph with a single node of the other graph, it is desirable to restrict simulations between two ground query terms to *injective* cases, i.e. such cases where no two subterms of t_1 are simulated by the same subterm of t_2. While it makes certain queries more difficult, this restriction turned out to be much easier to comprehend for authors of Xcerpt programs and reflected the intuitive understanding of query patterns.

Example 27
The following comprehensive list of examples illustrates the different requirements for a ground query term simulation. They are grouped in categories, each referring to the relevant requirement in Definition 26.

For illustration purposes, subterms are annotated with their index as subscript. This subscript is not considered to be part of the label. Also, `position` is abbreviated as `pos`, `optional` is abbreviated as `opt`, and `without` is abbreviated as $\neg$ for space reasons.

1. **total ordered term specification (cf. requirement 2)**
   Let $t_1 = f[a_1, b_2, c_3]$, $t_2 = f[a_1, b_2, c_3, d_4]$, $t_3 = f[a_1, c_2, b_3]$, $t_4 = f\{a_1, b_2, c_3\}$, and $t_5 = g[a_1, b_2, c_3]$
   - $t_1 \preceq t_1$: there exists a total, index bijective, and index monotonic mapping π from $\langle a_1, b_2, c_3\rangle$ to $\langle a_1, b_2, c_3\rangle$ with $s \preceq \pi(s)$, mapping each subterm to itself.
   - $t_1 \npreceq t_2$: there exists no index bijective mapping from $\langle a_1, b_2, c_3\rangle$ to $\langle a_1, b_2, c_3, d_4\rangle$, as the two sets have different cardinality.
   - $t_1 \npreceq t_3$: there exists no index monotonic mapping from $\langle a_1, b_2, c_3\rangle$ to $\langle a_1, c_2, b_3\rangle$ with $s \preceq \pi(s)$; the only mapping that would satisfy $s \preceq \pi(s)$, i.e. $\{a_1 \mapsto a_1, b_2 \mapsto b_3, c_3 \mapsto c_2\}$, is not index monotonic.
   - $t_1 \npreceq t_4$: the braces of t_1 and t_4 are incompatible.
   - $t_1 \npreceq t_5$: the labels of t_1 and t_5 do not match.
2. **total unordered term specification (cf. requirement 2)**
   Let $t_1 = f\{a_1, b_2, c_3\}$, $t_2 = f[a_1, b_2, c_3, d_4]$, $t_3 = f[a_1, c_2, b_3]$, $t_4 = f\{a_1, b_2, c_3\}$, and $t_5 = g[a_1, b_2, c_3]$

- $t_1 \preceq t_1$: there exists a total and index bijective mapping π from $\langle a_1, b_2, c_3 \rangle$ to $\langle a_1, b_2, c_3 \rangle$ with $s \preceq \pi(s)$, mapping each subterm to itself, thus being position preserving.
- $t_1 \npreceq t_2$: there exists no index bijective mapping from $\langle a_1, b_2, c_3 \rangle$ to $\langle a_1, b_2, c_3, d_4 \rangle$, as the two sets have different cardinality.
- $t_1 \preceq t_3$: there exists a total and index bijective mapping π from $\langle a_1, b_2, c_3 \rangle$ to $\langle a_1, c_2, b_3 \rangle$ with $s \preceq \pi(s)$, the mapping $\{a_1 \mapsto a_1, b_2 \mapsto b_3, c_3 \mapsto c_2\}$ (it does not need to be index monotonic) and it is trivially position respecting, because t_1 does not contain position subterms.
- $t_1 \preceq t_4$: there exists a total and index bijective mapping π from $\langle a_1, b_2, c_3 \rangle$ to $\langle a_1, b_2, c_3 \rangle$ with $s \preceq \pi(s)$, mapping each subterm to itself, thus being position preserving.
- $t_1 \npreceq t_5$: the labels of t_1 and t_5 do not match

3. **partial ordered term specification (cf. requirement 2)**
   Let $t_1 = f[[b_1, c_2]]$, $t_2 = f[a_1, b_2, c_3, d_4]$, $t_3 = f[a_1, c_2, b_3]$, $t_4 = f\{a_1, b_2, c_3\}$, and $t_5 = f[b_1, a_2, c_3]$
   - $t_1 \preceq t_1$
   - $t_1 \preceq t_2$: there exists a total, index injective, and index monotonic mapping $\pi = \{b_1 \mapsto b_2, c_2 \mapsto c_3\}$ with $s \preceq \pi(s)$. It is trivially position respecting.
   - $t_1 \npreceq t_3$: there exists no mapping π with $s \preceq \pi(s)$ that is also index monotonic, because t_3 does not contain b and c in the right order.
   - $t_1 \npreceq t_4$: the braces of t_1 and t_4 are incompatible.
   - $t_1 \preceq t_5$: there exists a total, index injective, and index monotonic mapping $\pi = \{b_1 \mapsto b_1, c_2 \mapsto c_3\}$ with $s \preceq \pi(s)$. It is trivially position respecting.
4. **partial unordered term specification (cf. requirement 2)**
   Let $t_1 = f\{\{b_1, c_2\}\}$, $t_2 = f[a_1, b_2, c_3, d_4]$, $t_3 = f[a_1, c_2, b_3]$, $t_4 = f\{a_1, b_2, c_3\}$, $t_5 = f[b_1, a_2, c_3]$, and $t_6 = f[a_1, b_2, d_3]$. All mappings π on $Succ(t_1)$ are trivially position respecting and position preserving.
   - $t_1 \preceq t_1$
   - $t_1 \preceq t_2$: there exists a total, index injective mapping $\pi = \{b_1 \mapsto b_2, c_2 \mapsto c_3\}$ with $s \preceq \pi(s)$
   - $t_1 \preceq t_3$: there exists a total, index injective mapping $\pi = \{b_1 \mapsto b_3, c_2 \mapsto c_2\}$ with $s \preceq \pi(s)$
   - $t_1 \preceq t_4$: there exists a total, index injective mapping $\pi = \{b_1 \mapsto b_2, c_2 \mapsto c_3\}$ with $s \preceq \pi(s)$
   - $t_1 \preceq t_5$: there exists a total, index injective mapping $\pi = \{b_1 \mapsto b_1, c_2 \mapsto c_3\}$ with $s \preceq \pi(s)$
   - $t_1 \npreceq t_6$: there exists no total mapping π such that $s \preceq \pi(s)$ holds for all s, as t_6 does not contain a subterm matching with c_2.
5. **position specification (cf. requirement 2)**
   Let $t_1 = f\{\{c_1, \mathrm{pos}\ 2\ b_2\}\}$, $t_2 = f[a_1, b_2, c_3]$, $t_3 = f[b_1, c_2, a_3]$, $t_4 = f[[a_1, b_2, c_3]]$ and $t_5 = f[[a_1, \mathrm{pos}\ 2\ b_2, c_3]]$
   - $t_1 \preceq t_1$: there exists a total, index injective, position preserving mapping $\pi = \{c_1 \mapsto c_1, \mathrm{pos}\ 2\ b_2 \mapsto \mathrm{pos}\ 2\ b_2\}$ with $s \preceq \pi(s)$
   - $t_1 \preceq t_2$: there exists a total, index injective, position respecting mapping $\pi = \{c_1 \mapsto c_3), \mathrm{pos}\ 2\ b_2 \mapsto b_2\}$ with $s \preceq \pi(s)$
   - $t_1 \npreceq t_3$: there exists no position respecting mapping π with $s \preceq \pi(s)$; the only mapping with $s \preceq \pi(s)$ is not position respecting, as it contains $\mathrm{pos}\ 2\ b_2 \mapsto b_1$.
   - $t_1 \npreceq t_4$: there exists no position preserving mapping π with $s \preceq \pi(s)$, because t_4 contains no subterm of the form `pos 2` t'; position *respecting* is not sufficient, as t_4 is incomplete and might match further terms with b at a different position than 2, e.g. the term $f[a_1, d_2, b_3, c_4]$, in which case $\preceq$ would not be transitive.

- $t_1 \preceq t_5$: there exists a total, index injective, position preserving mapping $\pi = \{c_1 \mapsto c_3), \text{pos } 2\ b_2 \mapsto \text{pos } 2\ b_{)}\}$ with $s \preceq \pi(s)$; in contrast to t_4, the term t_5 "preserves transitivity" of $\preceq$.

6. **descendant (cf. requirement 3)**
   Let $t_1 = desc\ f\{a\}$, $t_2 = desc\ f\{a\}$, $t_3 = desc\ f\{\{a, b\}\}$, and $t_4 = g\{f\{a\}, h\{b\}\}$
   - $t_1 \preceq t_2$, because $f\{a\} \preceq f\{a\}$
   - $t_1 \npreceq t_3$, because $f\{a\} \npreceq f\{\{a, b\}\}$
   - $t_1 \preceq t_4$, because t_4 contains a subterm t'_4 such that $f\{a\} \preceq t'_4$.

5.3 Simulation Order and Simulation Equivalence

Ground query term simulation has been designed carefully to be transitive and reflexive, because it is desirable that ground query term simulation is an ordering over the set T^g of ground query terms. This is necessary e.g. for the definition of *Grouping of a Substitution Set* (cf. Definition 16).

Theorem 28 (Transitivity and Reflexivity of $\preceq$ [Sch04])
$\preceq$ is reflexive and transitive.

With this result, the following corollary follows trivially:

Corollary and Definition 29
$\preceq$ defines a preorder[4] on the set of all ground query terms called the *simulation order*.

Note that the simulation order is not antisymmetric (e.g. $f\{a, b\} \preceq f\{b, a\}$ and $f\{b, a\} \preceq f\{a, b\}$, but $f\{a, b\} \neq f\{b, a\}$) and thus does not immediately provide a partial ordering. We therefore define an equivalence relation as follows:

Definition 30 (Simulation Equivalence)
Two ground query terms t_1 and t_2 are said to be *simulation equivalent*, denoted $t_1 \cong t_2$, if $t_1 \preceq t_2$ and $t_2 \preceq t_1$.

The meaning of simulation equivalence is rather intuitive: two terms are considered to be equivalent, if they differ only "insignificantly", e.g. in a different order in the sequence of subterms in unordered term specifications (e.g. $f\{a, b\}$ and $f\{b, a\}$). This is consistent with the intuitive notion of unordered term specifications given above. Note, however, that $f\{a, a\} \ncong f\{a\}$, because the first term contains two a subterms, whereas the second contains only one a subterm, i.e. there cannot exist an index bijective mapping of the successors of the first into the successors of the second term (and vice versa). Simulation equivalence plays an important role later, because it allows to consider terms as "equal" that behave equally.

Simulation equivalence extends to non-ground terms in a straightforward manner: two non-ground query terms t_1 and t_2 are simulation equivalent, if for every grounding substitution σ holds that $\sigma(t_1) \cong \sigma(t_2)$. Note that for any two data terms t_1 and t_2 it holds that if $t_1 \preceq t_2$ then $t_1 \cong t_2$, because data terms do not contain partial term specifications.

Note that simulation equivalence is similar, but not equal to, bisimulation, because bisimulation requires the *same* relation to be a simulation in both directions, whereas simulation equivalence allows two different relations.

$\cong$ partitions T^g into a set of equivalence classes $T^g/_{\cong}$. On this set, $\preceq$ is a partial ordering. Given two equivalence classes $\tilde{t}_1 \in T^g/_{\cong}$ and $\tilde{t}_2 \in T^g/_{\cong}$, we shall write $\tilde{t}_1 \preceq \tilde{t}_2$ iff $t_1 \preceq t_2$.

[4] a preorder is defined as a transitive, reflexive relation

Corollary 31
$\preceq$ is a partial ordering on $T^g/_{\cong}$.

In this partial ordering, it even holds that given two terms t_1 and t_2 such that there exists a least upper bound t_3, then t_3 is unique except for terms t_3' that are equivalent wrt. $\cong$.

5.4 Simulation Unifiers

In Classical Logic, a unifier is a substitution for two terms t_1 and t_2 that, applied to t_1 and t_2, makes the two terms identical. The *simulation unifiers* introduced here follow this basic scheme, with two extensions: instead of equality, simulation unifiers are based on the (asymmetric) simulation relation of Section 5 and instead of a single substitution, substitution sets are considered. Both extensions are necessary for handling the special Xcerpt constructs all and $some$ and incomplete term specifications.

Informally, a *simulation unifier* for a query term t^q and a construct term t^c is a set of substitutions Σ, such that each ground instance $t^{q'}$ of t^q in Σ simulates into a ground instance $t^{c'}$ of t^c in Σ. This restriction is too weak for fully describing the semantics of the evaluation algorithm. For example, consider a substitution set $\Sigma = \big\{\{X \mapsto a, Y \mapsto b\}, \{X \mapsto b, Y \mapsto a\}$, a query term $t^q = f\{var\ X\}$ and a construct term $t^c = f\{var\ Y\}$. With the informal description above, Σ would be a simulation unifier of t^q in t^c, but this is not reasonable. We therefore also require that the substitution $\sigma \in \Sigma$ that yields $t^{q'}$ also is "used" by $t^{c'}$. This can be expressed by grouping the substitutions according to the free variables in t^c (cf. Definition 16 on page 15).

Definition 32 (Simulation Unifier)
Let t^q be a query term, let t^c be a construct term with the set of free variables $FV(t^c)$, and let Σ be an all-grounding substitution set. Σ is called a *simulation unifier* of t^q in t^c, if for each $[\![\sigma]\!] \in \Sigma/_{\simeq_{FV(t^c)}}$ holds that

$$\forall t^{q'} \in [\![\sigma]\!](t^q) \quad t^{q'} \preceq [\![\sigma]\!](t^c)$$

Recall from Section 4 that all substitutions in an all-grounding substitution set assign data terms to each variable. Intuitively, it is sufficient to only consider grounding substitutions for t^q and t^c. However, all-grounding substitution sets simplify the formalisation of most general simulation unifiers below.

Example 33 (Simulation Unifiers)

1. Let $t^q = f\{\{var\ X, b\}\}$ and let $t^c = f\{a, var\ Y, c\}$. A simulation unifier of t^q in t^c is the (all-grounding) substitution set

$$\Sigma_1 = \big\{\{X \mapsto a, Y \mapsto b\}, \{X \mapsto c, Y \mapsto b\}\big\}$$

2. Let $t^q = f\{\{var\ X\}\}$ and let $t^c = f\{all\ var\ Y\}$. A simulation unifier of t^q in t^c is the (all-grounding) substitution set

$$\Sigma_2 = \big\{\{X \mapsto a, Y \mapsto b\}, \{X \mapsto a, Y \mapsto a\}\big\}$$

Assignments for variables not occurring in the terms t^q and t^c are not given in the substitutions above.

Simulation unifiers are required to be *grounding* substitution sets, because otherwise the simulation relation cannot be established. Also, only grounding substitution sets can be applied to construct terms containing grouping constructs, because a grouping is not possible otherwise. This restriction is less significant than it might appear: as rules in Xcerpt are range restricted, the evaluation algorithm always determines bindings for the variables in t^c, so that it is always possible to extend the solutions determined by the simulation unification algorithm to a grounding substitution set by merging with these bindings.

Usually, there are infinitely many unifiers for a query term and a construct term. Traditional logic programming therefore considers the most general unifier (mgu), i.e. the unifier that subsumes all other unifiers. Since simulation unifiers are always grounding substitution sets, such a definition is not possible for simulation unifiers. Instead, we define the *most general simulation unifier* (mgsu) as the smallest superset of all other simulation unifiers. Note that the notion *most general simulation unifier* is – although different in presentation – indeed similar to the traditional notion of most general unifiers, because a most general simulation unifier subsumes all other simulation unifiers.

Definition 34 (Most General Simulation Unifier)
Let t^q be a query term and let t^c be a construct term without grouping constructs such that there exists at least one simulation unifier of t^q in t^c. The *most general simulation unifier* (mgsu) of t^q in t^c is defined as the union of all simulation unifiers of t^q in t^c.

Note that the most general simulation unifier is indeed always a simulation unifier if t^c does not contain grouping constructs. This is easy to see because the union of two simulation unifiers simply adds ground instances of t^q and t^c where for every ground instance $t^{q'}$ of t^q there exists a ground instance $t^{c'}$ of t^c such that $t^{q'} \preceq t^{c'}$. This does in general not hold for construct terms with grouping.

6 Interpretations and Entailment

The definition of satisfaction of Xcerpt term formulas, and in particular of Xcerpt programs, is similar to the approach taken in classical first order logic, but differs in several important aspects: term formulas do not differentiate between relations and terms, and the incompleteness of query terms and the grouping constructs in construct terms have to be taken into account. Section 6.1 gives an intuitive meaning of interpretations for Xcerpt term formulas. Satisfaction is then defined in Section 6.2 in terms of the *simulation relation* introduced earlier in Section 5. Based on this definition of satisfaction, entailment between formulas can be defined in the classical manner.

6.1 Interpretations

As terms are considered to be formulas themselves, interpretations – informally – convey whether "a term exists" or "a term does not exist". Thus, a first approximation defines an interpretation as a set of data terms (which are also ground query terms). A ground atom (i.e. a ground query term) is then satisfied if it is contained in the set, or it simulates into a term that is contained in the set. Since Xcerpt data terms represent Web pages, this definition is natural and close to the application, and thus well suited for reasoning on the Web. Such a definition may be unusual from a Classical Logic perspective, but is rather common in logic programming for it is close to Herbrand interpretations.

Furthermore, an interpretation provides a grounding substitution set which provides assignments to all free variables in the formulas considered. Interpretations are thus formally defined as follows:

Definition 35 (Interpretation)
An *interpretation* M is a tuple $M = (I, \Sigma)$ where I is a set of data terms and $\Sigma \neq \varnothing$ is a grounding substitution set.

The set of data terms I conveys what data terms (Web pages) are considered to exist. The substitution set Σ is necessary to properly treat formulas containing free variables, and allows to provide a recursive definition of satisfaction below. As formulas are usually always (explicitly or implicitly) universally closed, Σ can be seen as a mere technicality of the definition and is irrelevant for the general notion of satisfaction.

For this reason, the following Sections often somewhat imprecisely equate interpretations with the set of data terms I.

Note that $\Sigma \neq \varnothing$. Otherwise, $\Sigma(t)$ would yield an empty set of terms even in case t is a ground query term. As the application of a substitution set to a query term formula yields a conjunction over all substitutions, application of $\varnothing$ would yield an empty conjunction, i.e. $\top$. To define a substitution set that merely maps each term to itself it has to be specified as $\Sigma = \left\{ \varnothing \right\}$, where the empty substitution σ corresponds to the identity function.

It is important to note that the interpretations considered here are very specific in that they only consider *terms* as objects, instead of arbitrary objects. They are thus similar to Herbrand interpretations in traditional model theory. However, this restriction is reasonable, as term formulas do not intend to represent arbitrary objects.

6.2 Satisfaction and Models

Although similar to the definition of satisfaction in classical logic, satisfaction for Xcerpt term formulas differs in several important aspects, in particular the satisfaction of atoms (i.e. terms) and of program rules. A term (atomic formula) is considered to be satisfied if (and only if) its ground instance simulates in some term of the interpretation. Considering the Web as an interpretation, this means that a query term "succeeds" (is satisfied) if there exists a Web page (data term) such that the ground instance of the query term simulates into this data term.

Unlike in traditional logic programs, rules in Xcerpt are not treated as (classical) implications ($\Rightarrow$ below), because the grouping constructs `all` and `some` require that the query part of a rule is not only satisfied, but that it is also satisfied in the maximal manner, i.e. the substitution set yielding the ground instance of the construct term must include all possible substitutions for which the query part is satisfied. Otherwise, interpretations would include answer terms for a rule that differ from the intuitive understanding of the constructs `all` and `some` (see Example 38 below). The definition of satisfaction for Xcerpt rules uses the notion of maximal substitution sets defined above in Definition 11.

With the exception of term and rule satisfaction, the following definition follows the classical definition of satisfaction. Note in particular, that the negation used in this definition is *classical* negation and not negation as failure (as the query negation in Xcerpt programs).

Definition 36 (Satisfaction, Model)

1. Let $M = (I, \Sigma)$ be an interpretation (i.e. a set of data terms I and a substitution set Σ), and let t be a construct or query term.

   The satisfaction of a term formula F in M, denoted by $M \vDash F$, is defined recursively over the structure of F:

$M \models \top$		holds
$M \models \bot$		does not hold
$M \models t$	iff	for all $t' \in \Sigma(t)$ there exists a term $t^d \in I$ such that $t' \preceq t^d$
$M \models \neg F$	iff	$M \not\models F$
$M \models F_1 \wedge \cdots \wedge F_n$	iff	$M \models F_1$ and ... and $M \models F_n$
$M \models F_1 \vee \cdots \vee F_n$	iff	$M \models F_1$ or ... or $M \models F_n$
$M \models F \Rightarrow G$	iff	$M \models \neg F \vee G$
$M \models \forall x.F$	iff	for all $t \in I$ holds that $M' = (I, \Sigma') \models F$, where $\Sigma' = \{\sigma \circ \{x \mapsto t\} \mid \sigma \in \Sigma\}$
$M \models \exists x.F$	iff	there exists a $t \in I$ such that $M' = (I, \Sigma') \models F$, where $\Sigma' = \{\sigma \circ \{x \mapsto t\} \mid \sigma \in \Sigma\}$
$M \models \forall^* \ll t^c \leftarrow Q \gg$	iff	$M' = (I, \Sigma') \models t^c$ for a maximal grounding substitution set Σ' for Q with $M' \models Q$

2. If a formula F is satisfied in an interpretation $\mathcal{M}$, i.e. $\mathcal{M} \models F$, then $\mathcal{M}$ is called a *model* of F.

Note that the maximality requirement in the last part of (1) refers to the satisfaction of Q in M and ensures that grouping constructs in the head of the rule are substituted properly.

As instances of Xcerpt rules are variable disjoint (so-called *standardisation apart*), it is possible to replace Σ by Σ' in the model definition for $\forall^* \ll t \leftarrow Q \gg$. Otherwise, the substitutions in Σ and Σ' would have to be merged to $\Sigma \circ \Sigma'$.

Example 37 (Satisfaction of Term Formulas)
Let $M = (I, \Sigma)$ be an interpretation with

$$\begin{array}{lcl} I & := & \{f[a,b], f[a,c], b\} \\ \Sigma & := & \{\{X \mapsto a,\ Y \mapsto b\}, \{X \mapsto a,\ Y \mapsto c\}\} \end{array}$$

The following statements hold for M:

1. $M \models f[a,b]$, because for each $t \in \Sigma(f[a,b]) = \{f[a,b]\}$ exists a $t' \in I$ with $t \preceq t'$
2. $M \not\models f[a,d]$, because for $t = f[a,d] \in \Sigma(f[a,d]) = \{f[a,d]\}$ does not exist a $t' \in I$ with $t \preceq t'$.
3. $M \models f\{a,b\}$, because for each $t \in \Sigma(f\{a,b\}) = \{f\{a,b\}\}$ exists a $t' \in I$ with $t \preceq t'$
4. $M \models f\{\{var\ X, var\ Y\}\}$, because
   - $\sigma_1 = \{X \mapsto a,\ Y \mapsto b\}$ and $\sigma_1(f\{\{var\ X, var\ Y\}\}) \preceq f[a,b]$, and
   - $\sigma_2 = \{X \mapsto a,\ Y \mapsto c\}$ and $\sigma_2(f\{\{var\ X, var\ Y\}\}) \preceq f[a,c]$
5. $M \models \exists Z.f\{\{var\ Z\}\}$, because $M' = (I, \Sigma')$ with
   $\Sigma' = \{\{X \mapsto a,\ Y \mapsto b,\ Z \mapsto a\}, \{X \mapsto a,\ Y \mapsto c,\ Z \mapsto a\}\}$
   is a model for $f\{\{var\ Z\}\}$
6. $M \not\models \forall Z.f\{\{var\ Z\}\}$, because there exists a term $f[a,b]$ as substitution for Z such that $M \not\models f\{\{f[a,b]\}\}$
7. $M \models \forall Z.var\ Z$, because for all $t \in I$ holds that $M' = (I, \Sigma')$ with $\Sigma' = \{\{X \mapsto a,\ Y \mapsto b,\ Z \mapsto t\}, \{X \mapsto a,\ Y \mapsto c,\ Z \mapsto t\}\}$
   is a model for $var\ Z$[5]

[5] This result might be surprising from a classical perspective, but it is self-evident when considering terms as formulas: universal quantification quantifies over all existing terms, and obviously all these are satisfied in any interpretation.

For a program P, a model is intuitively an interpretation that contains all the data terms that are "produced" by P (and possibly also further data terms unrelated to P).

Example 38 (Satisfaction of Xcerpt Programs)
Let P be the following Xcerpt program (in compact notation):

```
p{all var X} ← q{{var X}}
q{a,b,c}
```

- the interpretation $M_1 = (I_1, \{\emptyset\})$ with $I_1 = \left\{q\{a, b, c\}, p\{a, b, c\}\right\}$ is a model for P, i.e. $M_1 \models P$.
- the interpretation $M_2 = (I_2, \{\emptyset\})$ with $I_1 = \left\{q\{a, b, c\}, p\{a, b\}\right\}$ is no model for P, i.e. $M_1 \not\models P$, because $p\{a, b\}$ is not the ground instance of $p\{all\ var\ X\}$ by the *maximal* substitution set for which $q\{\{var\ X\}\}$ is satisfied
- the interpretation $M_3 = (I_3, \{\emptyset\})$ with $I_3 = \left\{q\{a, b, c\}, p\{a, b, c\}, p\{a, b\}\right\}$ is a model for P, i.e. $M_3 \models P$, because $p\{a, b, c\} \in I$; the additional $p\{a, b\}$ is not produced by P, but irrelevant for the satisfaction of P in M_3.

Note that "terms" with infinite breadth are precluded by the definition of terms and can thus never appear in an interpretation. Programs where a rule "defines" such terms do not have a model. For example, the program

$$
\begin{array}{l}
f\{all\ var\ X\} \leftarrow g\{var\ X\} \\
g\{g\{var\ Y\}\} \leftarrow g\{var\ Y\} \\
g\{a\}
\end{array}
$$

does not have a model, because the first rule defines a "term" of the form $f\{a, g\{a\}, g\{g\{a\}\}, \ldots\}$. To avoid non-terminating evaluation of such programs, it is desirable to find sufficient requirements to preclude such programs syntactically. This is however out of the scope of this article.

7 Fixpoint Semantics

A classical approach to describing the semantics of logic programs is the so-called *fixpoint semantics*, first proposed by Van Emden and Kowalski [vEK76]. In the fixpoint semantics, a model is constructed by iteratively trying to apply program rules (using an operator called T_P) to a set of data terms and adding their results until a fixpoint is reached, i.e. no new data terms can be added. This smallest fixpoint is then a model of the program (assuming that programs do not contain negation).

Example 39
Consider again the program

$$
\begin{array}{l}
f\{all\ var\ X\} \leftarrow g\{\{var\ X\}\} \\
g\{a\}
\end{array}
$$

By definition, the starting point is always $I_0 = \emptyset$. In the first iteration, no rules are applicable, but the data terms are added to the set. Thus,

$$I_1 = T_P(\emptyset) = \left\{g\{a\}\right\}$$

The next iteration allows to apply the program rule. Thus,

$$I_2 = T_P(I_1) = \left\{g\{a\}, f\{a\}\right\}$$

Further application of rules does not add new terms, thus I_2 is the smallest fixpoint. It is easy to see that I_2 is also a "reasonable" model of the program. Note that there are other fixpoints besides I_2, e.g. $\{g\{a\}, f\{a\}, f\{b\}\}$, all of them supersets of I_2.

The following section proposes a fixpoint semantics for Xcerpt programs with grouping constructs but without negation, and shows that the fixpoint of the program is also a model of a program. Since the fixpoint semantics is the most precise characterisation of Xcerpt programs available, it is also used as the reference for the verification of the backward chaining algorithm. Programs with negation are not considered in this article, but their treatment should be very similar to the treatment of negation in other logic programming languages. Since Xcerpt programs are negation stratifiable, a similar approach to the approach taken by Apt, Blair, and Walker [ABW88] appears promising.

This article slightly diverges from the traditional definition of the fixpoint operator T_P in that it defines T_P as a function whose result contains not only the new terms but also those given as argument. Thus, it is sufficient to simply let T_P saturate in iterative applications instead of using a complex notion of powers of the form $T_P \uparrow n$. Arguably, this approach is more straightforward, because it reflects the intuitive understanding of program evaluation.

Recall that ω denotes the first ordinal number, i.e. the smallest number that is larger than any natural number. Thus, T_P^ω denotes the application of T_P "until a fixpoint is reached" (whether it be finite or infinite). The fixpoint operator is defined as follows:

Definition 40 (Fixpoint Operator T_P, Fixpoint Interpretation)
Let P be an Xcerpt program.

1. The fixpoint operator T_P is defined as follows:

$$T_P(I) = I \cup \left\{ t^d \mid \begin{array}{l} \text{there exists a rule } t^c \leftarrow Q \text{ in } P \text{ and substitution set } \Sigma \\ \text{such that } \Sigma \text{ is the maximal set with } (I,\Sigma) \vDash Q \text{ and } t^d \in \Sigma(t^c), \\ \text{or } t^d \text{ is a data term in } P \end{array} \right\}$$

2. The fixpoint of T_P is denoted by $M_P = T_P^\omega(\emptyset)$ and called the fixpoint interpretation of P.

A problem with this first definition is that it can yield interpretations that contain unjustified terms in case the program contains grouping constructs, because rules with grouping constructs require the rule body to be satisfied maximally, but not all required information might be available in the iteration of T_P where the rule is applied.

Example 41
Consider the following Xcerpt program:

$$\begin{array}{l} f\{all\ var\ X\} \leftarrow g\{\{var\ X\}\} \\ g\{var\ Y\} \leftarrow h\{\{var\ Y\}\} \\ g\{a\} \\ h\{b\} \end{array}$$

Applying the fixpoint operator T_P yields the following results:

$$\begin{array}{rcrcl} & & T_P^1(\emptyset) & = & \{g\{a\}, h\{b\}\} \\ & & T_P^2(\emptyset) & = & \{g\{a\}, h\{b\}, g\{b\}, f\{a\}\} \\ M_P & = & T_P^3(\emptyset) & = & \{g\{a\}, h\{b\}, g\{b\}, f\{a\}, f\{a,b\}\} \end{array}$$

However, $f\{a\}$ should not occur, because it is not the result of the maximal substitution for $g\{\{var\ X\}\}$. Obviously, applying the first rule already in T_P^2 is too early.

Therefore, we refine the notion of fixpoint interpretations to fixpoint interpretations for stratifiable programs. Constructing fixpoints for Xcerpt programs containing grouping constructs is based on the grouping stratification of such programs and simply applies the fixpoint operator stratum by stratum, beginning with the lowest stratum and ending with the highest. The following definition follows closely a definition by Apt, Blair, and Walker [ABW88]:

Definition 42 (Fixpoint Interpretation for Stratifiable Programs)
Let P be a program with grouping stratification $P = P_1 \uplus \cdots \uplus P_n$ $(n \geq 1)$. The fixpoint interpretation M_P is defined by

$$\begin{array}{lcl} M_1 & = & T^{\omega}_{P_1}(\varnothing) \\ M_2 & = & T^{\omega}_{P_2}(M_1) \\ \vdots & & \\ M_n & = & T^{\omega}_{P_n}(M_{n-1}) \end{array}$$

with $M_P = M_n$.

Note that this definition of M_P is in principle applicable to all kinds of stratification, i.e. grouping stratification, negation stratification, and full stratification.

Example 43
Consider the following Xcerpt program stratifiable into two strata P_1 and P_2:

P_2	$f\{all\ var\ X\} \leftarrow g\{\{var\ X\}\}$
P_1	$g\{var\ Y\} \leftarrow h\{\{var\ Y\}\}$
	$g\{a\}$
	$h\{b\}$

Applying the fixpoint operator T_{P_1} for the stratum P_1 yields the following sets:

$$\begin{array}{lcccl} & & T^1_{P_1}(\varnothing) & = & \{g\{a\}, h\{b\}\} \\ M_1 & = & T^2_{P_1}(\varnothing) & = & \{g\{a\}, h\{b\}, g\{b\}\} \end{array}$$

$M_1 = T^2_{P_1}$ is a fixpoint for this stratum. Further application of the fixpoint operator T_{P_2} for the stratum P_2 to this set then results in:

$$M_2 \quad = \quad T^1_{P_2}(M_1) \quad = \quad \{g\{a\}, h\{b\}, g\{b\}, f\{a, b\}\}$$

it is easy to see that $M_2 = T^1_{P_2}(M_1)$ is a model of P, and that M_2 does not contain unjustified terms.

We now show that the fixpoint of a program is also a model. Note, however, that the inverse statement does not hold:

Theorem 44
Let P be a grouping stratified program without negation. Then the fixpoint M_P of P is a model of P.

Proof. Suppose M_P is not a model of P. Then there exists a term t not in M_P that is required by M_P and P. There are two cases for this:

- t is a data term in P. By definition of T_P, t is then in M_P. $\lightning$
- t is a ground instance of a rule in P, i.e. there exists a rule $t^c \leftarrow Q$ in P and a substitution set Σ that is a maximal substitution with $M_P \models \Sigma(Q)$ such that $t \in \Sigma(t^c)$. By definition of T_P, it holds that $\Sigma(t^c) \subseteq M_P$. $\lightning$

8 Outlook and Future Work

The semantics described in this article is unsatisfactory in that it only covers a limited set of Xcerpt programs (namely those that are grouping stratifiable), does not cover negation (as failure), and does not provide a theory of minimal model as is usually done in traditional logic programming. The following sections briefly suggest refinements that might be addressed in future work.

8.1 Semantics of Advanced Xcerpt Constructs

Some more advanced Xcerpt constructs are not covered by the model-theoretic semantics described in this article. This section gives a brief outline over possible approaches for these constructs. More elaborated proposals can be found in [Sch04].

Arithmetic Expressions and Aggregation Functions. Xcerpt construct terms may contain arithmetic expressions (like `+`, `-`, string concatenation, etc.) and aggregation functions (like `count`, `sum`, etc., usually in conjunction with grouping constructs). In general, both arithmetic expressions and aggregation functions are applied to a number of data terms (i.e. ground construct terms) and yield a new data term (for example, `sum` can be applied to the three data terms `3`, `4`, and `5`, and yields the data term `12`). Extending the model-theoretic semantics to convey their meaning can be achieved by a simple modification of the *application of substitution sets to construct terms* (cf. Section 4.2). Expressions might e.g. be evaluated on the ground instances that are the result of applying a substitution set to a construct term.

Optional Subterms. Xcerpt query and construct terms may contain so-called *optional* subterms preceded by the keyword `optional`. Intuitively, optional subterms have the following meaning:

- *query terms* containing optional subterms may match with data terms even if there exists no corresponding subterm in the data term, i.e. matching does not fail in this case (but does not yield variable bindings). On the other hand, if the data term does contain at least one corresponding subterm, optional subterms are required to match (and possibly yield variable bindings). The semantics of optional subterms in a query term can be formalised by properly adapting the notion of *ground query term simulation* (cf. Section 5). To reflect that optional subterms are required to match if possible, it is furthermore necessary to allow only those substitutions as valid answers for a query term and a data term that provide bindings for a maximal subset of variables.

- optional subterms in *construct terms* may be omitted if a substitution or substitution set does not provide bindings for at least one of the variables contained in the optional subterm (such "incomplete" substitutions might be the result of optional subterms in the query part of a rule). The sematics of optional subterms in a construct term can be formalised by extending the definition of *application of substitution sets to construct terms* (cf. Section 4.2).

Subterm Negation. In query terms, subterm negation (using the keyword `without`) denotes that matching data terms may not contain corresponding subterms that are matched by the negated subterm. For example, `f{{without b}}` matches only with data terms that have a root with label `f` and arbitrary subterms except for such that are matched by *b*. Thus, the data term `f{a,c}` would match, whereas the data term `f{a,b}` would not.

The semantics of subterm negation is best integrated into the *ground query term simulation* defined in Section 5. A first approach following this idea is described in [Sch04].

8.2 (Non-)Monotonicity: Negation and Grouping Constructs

Requiring grouping/negation stratification as in this article is too strict for many applications. Therefore, it would be worthwhile to investigate relaxations of these requirements (like *local stratification* [Prz88]) or even entirely different approaches that have been proposed in the last 20 years (like *stable models* [GL88] or *paraconsistent interpretations* [Bry02]) to non-monotonic constructs in Xcerpt.

8.3 Minimal Models

In traditional logic programming, the fixpoint of a program coincides with its *minimal model*, which is simply the intersection of all models of the program. It is easy to see that this approach is not feasible in the presence of grouping constructs like in Xcerpt. Consider the following simple program P consisting of a single rule and a single data term:

```
CONSTRUCT
  f{all var X}
FROM
  g{var X}
END

CONSTRUCT
  g{a}
END
```

Models for this program are e.g.

- $I_1 = \{g\{a\}, f\{a\}\}$
- $I_2 = \{g\{a\}, g\{b\}, f\{a, b\}\}$
- $I_3 = \{g\{a\}, g\{b\}, g\{c\}, f\{a, b, c\}\}$

Obviously, I_1 is the only "desirable" model, and also the fixpoint of P, i.e. $I_1 = T_P^\omega(\varnothing)$. It is easy to see that the intersection of e.g. I_1 and I_2 is not a model of P, i.e. the minimal model cannot be determined by simple set intersections.

Approaches to this problem could redefine intersection to "look inside terms". In the above example, a solution could be to not only do set intersection but also "term intersection". Thus, the intersection of $f\{a, b\}$ and $f\{a\}$ would be $f\{a\}$. However, several further problems arise with this kind of definition: it is unclear which terms to intersect, one cannot rely on known properties of set operations (if intersection is redefined, how about union?), and the resulting minimal model semantics is no longer as "declarative" as would be desirable.

Regardless of the approach taken, the minimal model semantics needs to be simple, because it is intended to *describe* the meaning of a program without relying on its operational behaviour; if no reasonable, understandable minimal model semantics can be found, it would probably be preferrable to be stick to the operational description given in form of the fixpoint semantics.

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Revision History[6]

Since the publication of I4-D4 two important developments have occured w.r.t. to I4's query language Xcerpt that influence the semantics discussed in this deliverable:

- A revised syntax has been published in I4-D6 that includes an identification of open issues. Several of the open issues are also related to the semantics, most notably the question of the proper data model (infinite regular trees based with extensional identity or graphs with object or surrogate identity) and of parameterizable grouping and aggregation. These issues are expected to be resolved in the coming months leading to a further update to this deliverable.
- A query core of Xcerpt has been defined both syntactically and semantically. Its formal properties have been studied and an efficient evaluation technique has been developed for this query core. The details on the query core are discussed in the appended paper.

[6] Major revisions from deliverable I4-D4.

Efficient Evaluation of n-ary Conjunctive Queries over Trees and Graphs*

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ABSTRACT

Query languages for semi-structured data on the Web in the form of XML or RDF have become an essential part of many applications and services. N-ary conjunctive queries, i.e., queries with any number of answer variables, are the formal core of most Web query languages including XSLT, XQuery, SPARQL, and Xcerpt. Despite a considerable body of research on the optimization of such queries against *tree-shaped* XML data, little attention has been paid so far to efficient access to *graph-shaped* XML, RDF, or Topic Maps. We propose a novel evaluation technique for n-ary conjunctive queries that applies to both tree- and graph-shaped data. It has the same complexity as the best known approaches that are restricted to tree-shaped data only. The core of the evaluation technique is a memoization data structure, called "memoization matrix", which holds (intermediary) results. It can be populated and consumed in different ways. For both, population and consumption, we propose two algorithms, each having its own advantages. The complexity of the algorithms is compared analytically and experimentally.

Categories and Subject Descriptors

E.1 [**Data**]: Data Structures—*Graphs and networks*; H.2.4 [**Information Systems**]: Database Management—*system, query processing*

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Keywords

query evaluation and optimization, conjunctive queries, memoization, semi-structured data, XML, RDF, Topic Maps

1. INTRODUCTION

Semi-structured data in the form of XML or RDF now dominates data representation and exchange on the Web. Accessing such Web data, often from multiple sources and in different formats, is more and more an essential part of many applications, e.g., for bibliography management, news aggregation, information classification, and digital asset management. Web query languages such as XSLT [10], XQuery [4], SPARQL [22], or Xcerpt [24] provide convenient and efficient means to access and process such data, whether it is stored in native XML or RDF databases or accessed via Web service query interfaces. Increasingly, Web applications need access not just to XML data, but also to data in other Web formats such as RDF or Topic Maps, even in the same query.

Efficient evaluation of queries over XML data has received considerable attention in recent years [5, 18, 13], including extensive studies of complexity of query evaluation for XPath [14], XQuery [17], and general conjunctive queries over trees [15].

However, these techniques and results have considered XML data as tree-shaped. For many applications, a *graph view* of XML is preferable, e.g., when links after XLink, (X)HTML, or XML's own ID/IDREF mechanism are considered first class elements of the data model. Furthermore, other semi-structured Web data formats such as RDF or Topic Maps are evidently graph-shaped. Therefore, we propose in this article a novel evaluation algorithm that exhibits on tree data the same worst-case complexity as the best known approaches for tree data, but operates with similar complexity also on graph data.

We formalize queries against semi-structured data, whether tree- or graph-shaped, as *n-ary conjunctive queries over unary and binary relations.* Conjunctive queries against tree data form a common formal basis for the query core of a large set of XML query languages such as UnQL [6], XPath [14], and thus XQuery [4]. Conjunctive queries against graph

	tree query	**graph** query
tree data	$O(q \cdot v^2 + o)$	$O(v^q)$
graph data	$O(q \cdot v \cdot e + o)$	$O(v^q)$

Table 1: Overview of Combined Time Complexity (q: number of query variables; e, v number of edges, vertices resp., in the data; o: size of output)

data form a common query core for RDF query languages such as SPARQL [22] and general semi-structured query languages such as Lorel [2] and Xcerpt [24].

Compared to full semi-structured query languages, the main restrictions of n-ary conjunctive queries are twofold: **(1)** They provide no *result construction*: The result of an n-ary conjunctive query is just a set of tuples of bindings for the n answer variables, each tuple representing one match, whereas full semi-structured query languages allow additional construction including grouping and aggregation on these results. **(2)** They are *composition-free* in the sense of [17], i.e., the query can only access the original input data, but no intermediary results can be constructed or queried, preventing in particular the use of views, rules, or functions. The second restriction is less easy to overcome and dropping it makes the query evaluation far more expensive [17].

An extension of the results presented here that drops the first restriction is straightforward and covers *composition-free core XQuery without negation* [17]. Indeed, the algorithms presented in this paper reaffirm the complexity results from [17] on tree data and extend them to graph data.

For the evaluation of n-ary conjunctive queries, we present two algorithms both founded on a compact data structure, called *"memoization matrix"*, for memoizing intermediary results during the evaluation of an n-ary query. The two algorithms differ only in the way the memoization matrix is filled: The first algorithm uses a bottom-up strategy for filling matrix cells starting with variables in leaf nodes of the query. The second algorithm performs a recursive descent over the query tree populating the matrix top-down from root to leaf query nodes. More involved population strategies are conceivable (e.g., a mix of the two presented algorithms or a pathwise population inspired by [20]), but only briefly outlined in this article.

Both algorithms can be applied in the same manner to tree and graph data, only the computation of the structural relations is affected by the type of data. Unsurprisingly, the shape of the query has a more pronounced effect on the complexity and performance of the evaluation algorithms: Where for path and tree queries the complexity of the evaluation algorithms is polynomial, it requires expontential time for evaluating graph queries. This is unsurprising in light of complexity results in [14, 15] that show that evaluation of graph queries even against tree data is NP-complete.

Two variants of matrix consumption and result generation algorithms are discussed: The first variant provides an in-memory representation of all result tuples that is useful if further processing such as aggregation or grouping is going to take place on the result tuples, the second variant computes the result tuples on the fly (using, e.g., a simple nested loop join) in exponential time but requiring only polynomial space. Both variants are justified and useful, depending on the construction performed on the results, if any.

The remainder of this article is organized along its **contributions**:

1: Based on the formalization of the query core of many semi-structured query languages as n-ary conjunctive queries (Section 2), a memoization technique for the compact representation of intermediary and final results of an n-ary conjunctive query is introduced in Section 3. This "memoization matrix" forms the core of the proposed novel evaluation technique, but allows for variation in two respects: first the population of the matrix and second the consumption of the matrix for result generation.

2: We introduce two algorithms for populating this matrix, one bottom-up in Section 4.1, one top-down in Section 4.2, and compare these algorithms w.r.t. complexity and likely usage scenarios. In an outlook, further population strategies are briefly noted. These algorithms can be used for *both* tree and graph data.

3: We introduce three algorithms for matrix consumption, one for tree queries (Section 5.1), one for graph queries (Section 5.2) which also enforces the remaining non-hierarchical relations that are unconsidered during matrix population, and one based on nested loop joins (Section 5.3). Above this, we show how order restrictions can be enforced using the matrix consumption algorithm for graphs (Section 6).

4: Careful complexity analysis of the algorithms in Sections 4 and Section 5 is complemented by an extensive experimental evaluation (Section 7) that confirms that the proposed algorithms are competitive with the best known evaluation techniques for tree data but also extend to graph data. To the best of the authors' knowledge, it is the first evaluation technique for semi-structured data with this property. This result applies over all three classes of queries considered, viz. n-ary path, tree, and graph queries. A summary of the complexity results for tree and graph queries is given in Table 1.

5: In an outlook further optimizations regarding advanced query constructs such as optional query parts or negation and the relation of the presented technique to relational query planing and constraint solving are briefly outlined (Section 8).

2. PRELIMINARIES

2.1 Graph Data Model

From the perspective of their data model, many Web representation formats such as XML, RDF, and Topic Maps have a lot of commonalities: the data is semi-structured, tree- or graph-shaped, and sometimes ordered, sometimes not (XML elements vs. XML attributes, RDF sequence containers vs. bag containers). In this article, we choose finite **unranked labeled ordered simple directed graphs** as common data model for Web data. Precisely, a query is evaluated against a data graph D over a label alphabet Σ_L and a value alphabet Σ_V. A data graph is represented as a 5-tuple

$$D = (N, E, R, \mathcal{L}, \mathcal{V}),$$

where N is the set of nodes of the graph, $E \subset N \times \mathbb{N} \times N$ the set of edges, $R \subset N$ the set of root vertices, $\mathcal{L} : N \to \Sigma_L$ the labeling function, and $\mathcal{V} : N \to \Sigma_V$ the value assignment function.

D is a *simple directed* graph, i.e., there are neither multi-edges nor loops in the graph (but other, i.e., indirect, cycles are allowed). This restriction is used to simplify the presentation of the algorithms and complexity results below, but is not strictly necessary. Indeed, any directed graph D with

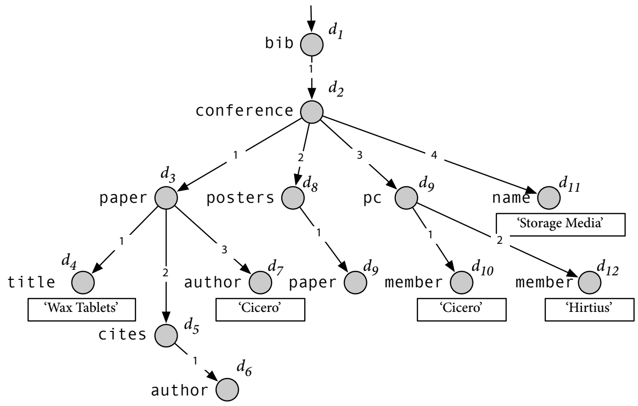

Figure 1: Exemplary Data Graph: Labeled Ordered Simple Directed Graph

multi-edges and loops can be represented as a simple directed graph D' by replacing each edge $(n_1, i, n_2) \in E$ with a new node $n \in N' \backslash N$ and edges (n_1, i, n), $(n, 1, n_2) \in E'$. Obviously, D' has by the number of edges in D more nodes than D: $|N'| = |N| + |E|$ and $|E'| = 2\,|E|$.

D is an *ordered* graph, i.e., the order of the children of a node is significant. Since the order is relative to the parent and a single node can be child of several parents, the order is associated with the edge rather than with the child node. It is assumed, that each child has a unique position in the order of its siblings $(p, i, c), (p, i', c') \in E$: $i = i' \implies c = c'$. On simple graphs this induces a proper order relation among siblings, but only on trees an obvious generalization to an order over all nodes (like document order in XML) exists.

Two *labeling functions* are provided, viz. $\mathcal{L}$ and $\mathcal{V}$. The first associates conventional node labels with each node, the second "content" values. The difference is made to be able to distinguish the cost of comparing two labels vs. two content values. Furthermore, $\mathcal{L}$ is assumed to be total, whereas $\mathcal{V}$ may be undefined for some nodes in the graph. In Figure 1, an exemplary data graph is shown. Labels are denoted to the left of the node, "content" values in boxes under the nodes. A root node is indicated by an incoming arrow.

The definition allows *multiple root nodes*, e.g., if there are several connected components in the graph. Any node may be a root node. In particular root nodes may, in contrast to usual rooted graph models, have parents. Intuitively, root nodes are simply highlighted "entrance" points into the graph that can be chosen arbitrarily when defining the data graph: If the data graph is a single XML document there will be a single such root node, however this formalization also covers collections of XML documents (as in XQuery) and RDF graphs where, e.g., each subject node can be considered a root node. In the following, we assume without loss of generality that a data graph has a single root and is connected. This ensures that $|E| \geq |N| - 1$, and thus $O(|E| + |N|) = O(|E|)$.

Specificities of XML, RDF, and Topic Maps such as attributes, namespaces, containers, collections, etc. are not provided by the basic data model. Handling these specificities poses no challenge to the evaluation algorithm and complexity analysis in this article and is therefore disregarded here.

2.2 Conjunctive Queries

Conjunctive queries are a convenient and relevant formalization of the query core of many XML and RDF query languages such as XSLT, XQuery, SPARQL, and Xcerpt.

Query syntax. A conjunctive query consists of a query *head* and a query *body*. The query body is a conjunction of atoms, and each atom is a relation over query variables. The domain of the query variables are the nodes N of the data graph D the query is evaluated against. The query head is a list of answer variable bindings which form an answer to the query. All answer variables must also occur in the body of the query. All other variables in the query body are existentially quantified [1].

In this article, only *binary and unary relations* are considered in conjunctive queries (though Section 6 briefly discusses an extension for handling order relations on graph data that uses *ternary* relations). Thus, conjunctive queries follow the following grammar:

$$\langle query \rangle ::= \langle label \rangle \text{ `('} \langle variable \rangle \text{ (`,'} \langle variable \rangle)^* \text{ `)'} \text{ `}\leftarrow\text{'} \langle atom \rangle \text{ (`,'} \langle atom \rangle)^*$$

$$\langle atom \rangle ::= \langle relation \rangle \text{ `('} \langle variable \rangle \text{ (`,'} \langle variable \rangle)? \text{ `)'}$$

Query Relations. Three types of relations may occur in conjunctive queries: unary "property" relations that restrict the valuation to nodes with a certain property, binary "structural" relations that require pairs of nodes to stand in the queried data graph in a certain structural relation, and binary "join" relations that compare nodes based on some property.

The proposed algorithms and complexity considerations apply to arbitrary property, structural, and join relations as long as for given nodes, each property relation can be checked in constant time, each structural relation in $O(|E|)$, and each join relation in at most $O(j(|E|))$ for some polynomial j. Additionally, the enumeration of the structurally related nodes for a given node n must be possible in $O(|E|)$. For join relations, a parameterized complexity is used to allow constant-time value joins based, e.g., on a fixed set of key values as well as deep-equal or "string value" joins as in XPath, that access the entire sub-structure rooted at a node and require in worst-case $O(|E|)$ time to be checked on a pair of nodes.

In the remainder of this article, we use the *property* relation ROOT, which is satisfied only by the root nodes of the queried data graph, as well as label relations LABEL_σ for all $\sigma \in \Sigma_L$ (i.e., for all possible labels) that restrict to nodes v where $\mathcal{L}(v) = \sigma$.

As *structural* relations only CHILD and its closures CHILD^+ and CHILD^* are considered. An extension to regular path expressions (or conditional axes [19]) is straightforward, as a regular path expression can be checked with data complexity $O(|E|)$ for two given nodes. In Section 6, an extension with (ternary) sibling-order relations is briefly outlined.

The *join* relations used are IDENT and VALEQUAL. IDENT is the identity relation, VALEQUAL is defined over the value labeling function $\mathcal{V}$. IDENT can be used to rewrite queries with structural relations that form a graph to queries with structural relations that form a tree but contain additional VALEQUAL atoms.

Figure 2 shows the query graphs for two conjunctive queries. This intuitive representation of graphs is used through-

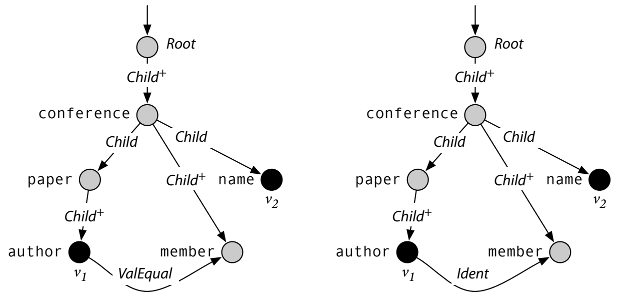

Figure 2: Exemplary Query Graphs (left: Q_1 with value join, right: Q_2 with identity join)

$$
\begin{array}{ll}
[\![q(v_1,\ldots,v_n) \leftarrow atom_1,\ldots,atom_m]\!]^q_D & \\
\quad = \pi_{v_1,\ldots,v_n}([\![atom_1]\!]^q_D \cap \ldots \cap [\![atom_m]\!]^q_D) & \\
[\![unary(x)]\!]^q_D & = \{t \in N^q : t[x] \in [\![unary]\!]_D\} \\
[\![binary(x,x')]\!]^q_D & = \{t \in N^q : (t[x],t[x']) \in [\![binary]\!]_D\} \\
[\![\text{ROOT}]\!]_D & = R \\
[\![\text{LABEL}_\sigma]\!]_D & = \{n \in N : \mathcal{L}(n) = \sigma\} \\
[\![\text{CHILD}]\!]_D & = \{(n,n') \in N^2 : \exists i \in \mathbb{N} : (n,i,n') \in E\} \\
[\![\text{CHILD}^+]\!]_D & = \bigcup_{i>0}([\![\text{CHILD}]\!]_D)^i \\
[\![\text{CHILD}^*]\!]_D & = \bigcup_{i\geq 0}([\![\text{CHILD}]\!]_D)^i \\
[\![\text{IDENT}]\!]_D & = \{(d,d) \in N^2\} \\
[\![\text{VALEQUAL}]\!]_D & = \{(d,d') \in N^2 : \mathcal{V}(d) = \mathcal{V}(d')\}
\end{array}
$$

Table 2: Semantics of n-ary Conjunctive Queries over Data Graphs

out this paper: The representation of labels and values, as well as root nodes is as in data graphs, but edges are annotated with structural or join relations. Answer variables are marked by the name of the variable and a black instead of a gray node.

The two queries both select article authors together with article titles and conference names if the author is also a program committee member at the conference. However, the first one uses a value, the second an identity join. Thus, the first matches also if just the values are the same but different nodes are used for the representation of the article author and the program committee (this is a common way to model such data in XML), the second only matches if identical nodes are used (a common way to model the data in RDF where globally unique identifiers for entities such as persons are available).

In the remainder of this paper, we assume w.l.o.g. that every query node (i.e., variable) is reachable from a root query node by a path of structural relations.

Query semantics. Let D be the data graph the query is evaluated against and q the number of variables occurring in Q, then Table 2 gives the precise semantics of n-ary conjunctive queries over graphs as used in this article. The semantics is defined based on *sets of valuations* for query variables. A valuation t for n variables is an n-ary tuple with one column for each of the variables. We use $t[v]$ to denote the binding of variable v in the valuation t, and $[v_1 : n_1, \ldots v_q : n_q]$ for the construction of a q-ary tuple. We also allow an empty tuple $[]$; the combination of the relation $\{[]\}$ with a relation R by cartesian is defined as $R = \{[]\} \times R$.

Query classes. We distinguish graph, tree, and path queries. Tree queries are queries whose graphs are tree-shaped. Analogously, path queries are queries whose graphs are in fact single paths. In addition to these basic classes, we introduce the class of *structural tree queries*. These are queries where the query without join relations is a tree. There may be additional arbitrary join relations, so that the complete graph may be no tree. Both of the example query graphs from Figure 2 are structural tree queries, but no proper tree queries.

Although it is known that evaluating graph queries is NP-complete even against tree data [15], the need for graph queries is evident. It is not only often necessary to retrieve more than one value but to compare the retrieved values with each other. Whenever the number of binary relations equals or exceeds the number of variables, the query is no tree query, since a tree with q nodes has $q-1$ edges and thus a tree query with n variables has $n-1$ structural relations. Indeed, many queries formulated in XQuery, XLST, or XPath fall into the class of graph queries [7].

Graph-shaped conjunctive queries may have multiple root or source variables, i.e., variables that occur only as source in structural relations, but not as sink. Let $SourceVars(Q)$ be the set of such variables in the query Q. As for data graphs, we assume in the following w.l.o.g. that there is exactly one such variable in each query, i.e., that all query graphs are rooted. We use $FreeVars(Q)$ to reference the answer variables in Q. We write $a \in Q$ to test for the occurrence of an atom a in Q, and $Q \backslash \{a_1,\ldots,a_n\}$ to remove a set of atoms $a_1,\ldots,a_n$ from Q. For brevity, we use if unambiguous in the context also $Q \backslash \{v_1,\ldots,v_n\}$ to indicate the conjunctive query Q' that contains all atoms from Q except those involving variables $v_1,\ldots,v_n$.

Note that (rooted) graph queries can be transformed into structural tree queries by replacing non-tree structural relations with identity joins: First, compute a spanning tree, considering the structural relation edges only. For each non-tree edge representing a structural relation REL between variables x and y, take a fresh variable y'. Replace the edge representing $\text{REL}(x,y)$ by the tree edge $\text{REL}(x,y')$, and add $\text{IDENT}(y,y')$ to the query Q. The size of the query increases by the number of non-tree edges, which is linear in the size of Q, but quadratic in the number of variables in the query.

For a rooted query Q, we denote a spanning tree of Q, consisting of only structural relations, with $T(Q)$. Based on this spanning tree, $JoinVars(Q)$ denotes the set of existentially quantified variables contained in an atom that labels a non-tree edge.

3. MEMOIZATION MATRIX

At the core of the evaluation technique detailed in this paper stands the "memoization matrix". It is a compact data structure holding intermediary results of the evaluation of an n-ary conjunctive query. A memoization matrix associates query nodes (i.e., variables) q with bindings $n \in N$ and *one* sub-matrix, containing for each query child node q' the compatible bindings $n' \in N$ for q' under the binding n for q.

DEFINITION 1. ***Memoization matrix.*** *Given a query Q with variables $Vars(Q)$ and spanning tree $T(Q)$, and a data graph D with nodes N, a memoization matrix for the evaluation of Q against D is a recursive data structure rep-*

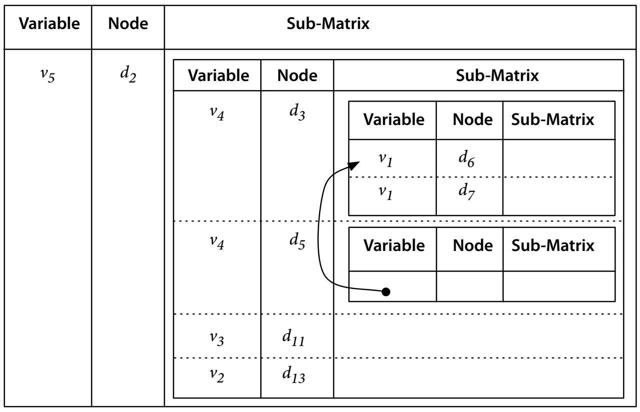

Figure 3: Filled Memoization Matrix (on Data of Figure 1)

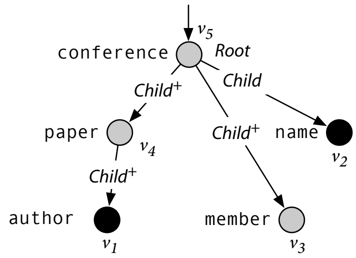

Figure 4: Modified Exemplary Query

resenting all possible *bindings of query variables in Q to nodes from D. The memoization matrix is a relation containing for each* $q_s \in \mathit{SourceVars}(T(Q))$ *and each possible binding* $n \in N$ *for* q_s *that satisfies all property relations on* q_s *one triple* (q_s, n, M') *with* M' *a subset of the memoization sub-matrix for* $Q \backslash \mathit{SourceVars}(T(Q))$ *such that for each tuple* $(q', n', M'') \in M'$ *and each atom* $\mathrm{REL}(q_s, q') \in T(Q)$*, it holds that* $(n, n') \in [\![\mathrm{REL}]\!]_D$.

Intuitively, this definition requires that the bindings for source variables in a sub-matrix M' are structurally compatible with the binding of the source variable in the corresponding tuple of M.

Notice that only the spanning tree of Q, denoted by $T(Q)$, is considered in the memoization matrix. The memoization matrix ensures only consistency w.r.t. relations within $T(Q)$. It does not ensure that the valuations are consistent w.r.t. relations outside $T(Q)$. Exploiting the tree shape of $T(Q)$, this makes a local evaluation of relations possible: A full-match can be incrementally computed from local matches that consider parent and child variables in the tree query in isolation.

The memoization matrix has been proposed first in a variant of which has been proposed first in [23]. Here, we refine this proposal with tuple sharing: To avoid multiple computations of matches in the case of queries where the same data node can be a match for a variable under different constellations of the remaining variable, the memoization matrix shares tuples where possible: Each tuple (q, n, M) exists only once and is referenced if the same tuple may occur in different sub-matrices. Notice that sharing of tuples only occurs between sub-matrices at the same level (i.e., sub-matrices of the same common super-matrix). The following sections show how this property can be ensured during the construction of the memoization matrix. Once more that this property relies on the tree structure of the relations checked in the memoization matrix.

It is furthermore assumed that the matrix is clustered by variables in order to allow linear time access to all entries relating to a variable.

Figure 3 shows the memoization matrix for the evaluation of the query from Figure 4 against the sample data graph from Figure 1.

The algorithms for matrix population discussed in the following section that guarantee a population of the matrix for a given n-ary conjunctive query Q against a data graph D takes at most $O(|\mathit{Vars}(Q)| \cdot |N| \cdot |E|)$ time, where $|\mathit{Vars}(Q)|$ denotes the number of variables in Q, $|N|$ the number of nodes, and $|E|$ the number of edges in the data graph D. Note that in the special case of tree-shaped data, $|E| = |N| - 1$, so that the worst case complexity becomes $O(|\mathit{Vars}(Q)| \cdot |N|^2)$. The size of the memoization matrix is in $O(\mathit{Vars}(Q) \cdot |N|^2)$ independently from the used algorithm, just by assuming sharing of submatrices, as demonstrated in the following.

Lemma 1 (Size of Memoization Matrix). *The size of the memoization matrix M for a query Q and a data graph D with nodes N is bounded by* $(2q - 1) \cdot v^2$*, where* $q = |Vars(Q)|$*, and* $v = |N|$.

Proof. By structural induction over $T(Q)$.
Query leaves: It holds that $q = 1$, and obviously the number of valuations for a single variable is bounded by v. The size of the memoization matrix is $q \cdot v \leq (2q - 1) \cdot v^2$.
Inner query nodes: Let the inner query node i have c children. It holds that the sum of nodes of all child queries is equal to $q - 1 = \sum_{j=1}^{c} q_j \quad (*)$. There are again at most v valuations of i. As tuples are shared over parent matrices, there is at most *one* tuple for each such valuation. The size of the sub-matrix contained in the tuple itself is bounded by $c \cdot v$, as each child has at most v assignments. The size of all tuples for the inner node i (i.e. of the complete sub-matrix of i) is hence $c \cdot v^2$. The overall matrix size is

$$\sum_{j=1}^{c} (2q_i - 1) \cdot v^2 + c \cdot v^2 \overset{(*)}{=} (2(q-1) - c + c) \cdot v^2 \leq (2q-1) \cdot v^2,$$

using the induction hypothesis. □

Based on the populated matrix, the algorithms discussed in Section 5 traverse the memoization matrix, enforce the remaining (non-hierarchical) relations, if there are any, and create the output according to the query semantics introduced above.

4. MATRIX POPULATION

The compact memoization matrix introduced in the last section can be produced bottom-up ($\mathsf{Match}_{\uparrow}$, Section 4.1) or top-down ($\mathsf{Match}_{\downarrow}$, Section 4.2), that is, starting with the root variable and the root data node or with the leaf variables and all data nodes. While both algorithms have the same worst case complexity, experimental evaluation in Section 7 shows that an in-memory implementation of the bottom-up algorithm has an experimental runtime close to the worst case complexity, while the top-down approach displays far better runtime behavior in realistic cases.

4.1 Bottom-Up Approach

The bottom-up approach ($\mathsf{Match}_\uparrow$) is a bulk-processing approach often employed in secondary-storage databases. It starts by matching the leaf variables of $T(Q)$ with all nodes of D, and uses these results to successively fill the domains of variables that have a common structural relation with these leaf variables. This process is repeated iteratively until either a variable domain becomes empty, indicating that the query has no matches, or the root variable of Q is reached, indicating that all matches of the query are found.

Algorithm 1 $\mathsf{Match}_\uparrow(Q, D)$

1: $q \leftarrow |\mathit{Vars}(Q)|$; $V_Q \leftarrow \mathit{Vars}(Q)$; $N \leftarrow \mathit{nodes}(D)$; $\rho \leftarrow \emptyset$
2: $\mathit{root} \in \mathit{SourceVars}(Q)$
3: **while** $\rho(\mathit{root}) = \emptyset$ **do**
4: take $x \in V_Q : \rho(x) = \emptyset \wedge$ $\forall \text{REL}(x, x') \in T(Q) : \rho(x') \neq \emptyset$
5: $M \leftarrow \emptyset$
6: **for all** $n \in N$ **do**
7: **if** $\exists \text{REL}(x) \in Q : n \notin [\![\text{REL}]\!]_D$ **then**
8: **continue** n
9: $M_S \leftarrow \emptyset$
10: **for all** $\text{REL}(x, x') \in T(Q)$ **do**
11: $M_R \leftarrow \emptyset$
12: **for all** $(x', n', M') \in \rho(x')$ **do**
13: **if** $(n, n') \in [\![\text{REL}]\!]_D$ **then**
14: $M_R \leftarrow M_R \cup \{(x', n', M')\}$
15: **if** $M_R = \emptyset$ **then**
16: **continue** n
17: $M_S \leftarrow M_S \cup M_R$
18: $M \leftarrow M \cup \{(x, n, M_S)\}$
19: $\rho(x) \leftarrow M$
20: **if** $\rho(x) = \emptyset$ **then**
21: **return** $\emptyset$
22: **return** $\rho(\mathit{root})$

The algorithm uses a helper function ρ to associate variables with sets of tuples representing bindings for these variables. ρ is initially empty and populated step by step in the outer **while** loop: Starting with the leaf nodes, the algorithm generates the set of tuples $\rho(x)$ (l. 3 and 19) for each variable x, until either no match is found for a variable and thus the query fails (returns an empty set) (l. 20–21) or the root node has been processed (l. 3) and the memoization matrix for the root node is returned (l. 22).

When processing a variable x (l. 3–21), the algorithm creates an empty memoization matrix for that variable and iterates over each node n in the nodes N of D (l. 6–18) verifying first the unary relations (l. 7–8). If any of the relations fails on n, the next node is tested. If it succeeds, a sub-matrix M_S is initialized (l. 9). For every variable x' related to x via a structural relation in the spanning tree $T(Q)$ (l. 10) only the tuples with nodes n' that actually satisfy the relation with n are included in the sub-matrix (l.12–14). A temporary matrix M_R for each relation is used to test whether there is no matching node pair for that relation. If so, the current data node is skipped (l. 11 and 15–16). Only if the matrix M for x is empty at the end of the processing of x, the query fails as there are no compatible bindings for x in the data.

Notice, that the algorithm does not specify the details of row sharing between matrices at the same level. It is assumed that in l. 14 and l. 18 pointers to M', resp. M are used instead of copies.

Theorem 1 (Complexity of $\mathsf{Match}_\uparrow$). *Let $v = |N|$, $q = |\mathit{Vars}(Q)|$, and $e = |E|$. Then, $\mathsf{Match}_\uparrow$ is in $O(q \cdot v \cdot e)$ combined time complexity and in $O(q \cdot v^2)$ combined space complexity.*

Proof. There are q variables, so that the outer loop (l. 3) is bounded by q. The loop over all nodes (l. 6) is bounded by v. The verification of the property relations takes constant time, as there is a fixed number of such relations in the language and each test (such as a label test) is assumed to be constant (l. 7–8). Since $T(Q)$ is a spanning *tree* there are at most $q-1$ structural relations in that tree that need to be tested in the iteration over all binary relations (l. 10). As each binary relation is visited only once (when the source variable of that relation is processed), the loop body (l. 11–17) is executed $(q-1) \cdot v$ times. Since at most all nodes in the document can match with a variable, the iteration in l. 12 is bounded by v. As the verification of $(n, n') \in [\![\text{REL}]\!]_D$ is required to be in $O(e)$ for structural relations (cf. Section 2), the overall time complexity is in $O(q \cdot v^2 \cdot e)$, if the structural relations are verified for each pair (n, n'). However, we can assume that the structural relations are precomputed in an index structure such as a bit array which provides constant verification of the structural relation at a space cost of $O(v^2)$ and time cost $O(v \cdot e)$. This is an acceptable trade-off as there are usually only a small number of structural relations and as the memoization matrix already requires $O(q \cdot v^2)$ space as discussed above. Under this assumption, the overall combined time complexity becomes $O(q \cdot v \cdot e)$. The overall space complexity is dominated by the size of the memoization matrix $O(q \cdot v^2)$, as the only helper structures are the precomputed relations at $O(v^2)$ and ρ which is bounded by q. $\square$

Even though the bottom-up approach has a nice upper bound of computational complexity, it needs further refinements to be usable in practice as the experimental evaluation in Section 7 demonstrates. To obtain a practically useful performance, the bottom-up algorithm needs efficient index structures on the property relations occurring in the query. Examples of such index structures are so-called streaming schemes [8]. A further performance increase might result from evaluating groups of structural and property relations at once using holistic tree queries, cf. [5, 18]. The benefits of the latter approach are not clear for n-ary graph queries, where most query variables are either answer variables or involved in non-structural joins, preventing large groups of relations that can be evaluated at once using [18] or similar approaches. Further investigation of the use of such holistic schemes for n-ary conjunctive queries with graph-shape is required, but out of the scope of this paper.

4.2 Top-Down Approach

The runtime of the bottom-up approach can be very close to its worst case complexity if the query leafs are not selective enough or if efficient evaluation of property relations through indices is not available. For an in-memory evaluation of n-ary conjunctive queries without indices, the top-down approach matching the query from the root to the leafs and restricting the number of candidate nodes primarily based on query structure presents a feasible and often superior alternative. Furthermore, the top-down algorithm does not need any adjacency index to guarantee a runtime in

$O(q \cdot v \cdot e)$. However, iteration over the range of a structural relation for one data node must be guaranteed in $O(e)$ time. This assumption holds for any structural relation occurring in XPath, XSLT, XQuery, SPARQL, or Xcerpt.

Like the bottom-up algorithm, the top-down algorithm needs an additional helper structure ρ. However, in this case it associates tuples of query variable *and* data node to entire sub-matrices. Constant access is assumed for this structure by basing it on a two-dimensional array. It is assumed that $\rho = \emptyset$ at the first call of the algorithm. Furthermore, an explicit "no match" indicator $\perp$ is used to mark combinations of nodes and variables that are certain not to match. This must be distinguished from the case where the combination has not yet been computed and the case where there is no sub-matrix for the combination (i.e., the variable is a leaf in the query).

Algorithm 2 $\mathsf{Match}_{\downarrow}(x, n)$

1: **if** $\rho(x, n) = \perp$ **then**
2:    **return** $\emptyset$
3: **if** $\rho(x, n)$ defined **then**
4:    **return** $\{(x, n, \rho(x, n))\}$
5: **if** $\exists \text{REL}(x) \in Q : n \notin [\![\text{REL}]\!]_D$ **then**
6:    $\rho(x, n) \leftarrow \perp$
7:    **return** $\emptyset$
8: $M_S \leftarrow \emptyset$
9: **for all** $\text{REL}(x, x') \in T(Q)$ **do**
10:    $M_R \leftarrow \emptyset$
11:    **for all** $n' \in N : (n, n') \in [\![\text{REL}]\!]_D$ **do**
12:       $M_R \leftarrow M_R \cup \mathsf{Match}(x', n')$
13:    **if** $M_R = \emptyset$ **then**
14:       $\rho(x, n) \leftarrow \perp$
15:       **return** $\emptyset$
16:    $M_S \leftarrow M_S \cup M_R$
17: $\rho(x, n) \leftarrow M_S$
18: **return** $\{(x, n, M_S)\}$

The top-down algorithm is a typical recursive descent over the query structure. It has two parameters, a query and a data node, and computes the memoization matrix for these two nodes. If called with the root of the query Q and the root of the data graph D, the result is the memoization matrix for the evaluation of Q against D.

The algorithm $\mathsf{Match}_{\downarrow}$ operates on pairs (x, n) of variables and data nodes, and a matching is computed at most once for each combination of query and data node. Lines 1–4 verify whether a matrix for the given pair of variable and value has already been computed. If this is the case, the call immediately returns. The unary relations of the input variable x are verified on the data node n (l. 5). If any of the unary relations fails, the matching fails, stores the information that the pair is incompatible in ρ and returns (l. 6–7). If n satisfies all unary relations, the sub-matrix M_S of the entry is initialized (l. 8) and $\mathsf{Match}_{\downarrow}$ iterates over all structural relations in the spanning tree $T(Q)$ with x as source variable. It creates a temporary matrix M_R for each such relation (l. 10). M_R is filled with the result of recursive calls to $\mathsf{Match}_{\downarrow}$ (l. 12) with any data node n' that satisfies the structural relation REL together with n. If the matching fails, the result of the recursive call is an empty set, thus leaving M_R unchanged. Again, if for any structural relation in the spanning tree no matching data node is found and thus M_R is still empty in line 13, the matching of x with n fails (l. 13–15). At the end of the loop starting in line 9, the temporary matrix M_R is added to the sub-matrix M_S for x and n. Finally, if all structural relations for x are processed, the resulting matrix M_S is stored in $\rho(x, n)$, and a matrix with a single tuple (x, n, M_S) is returned representing the entry for x and n.

THEOREM 2 (COMPLEXITY OF MATCH$_{\downarrow}$). *Let $v = |N|$, $q = |\mathit{Vars}(Q)|$, and $e = |E|$. Then, $\mathsf{Match}_{\downarrow}$ is in $O(q \cdot v \cdot e)$ combined time complexity and $O(q \cdot v^2)$ combined space complexity.*

PROOF. The use of matrix memoization (l.1–3, 14, 17) guarantees that $\mathsf{Match}_{\downarrow}$ is executed at most once for each combination of variable and data node (x, d). Testing unary predicates takes again constant time as argued in the proof of Theorem 1. As each of the $q - 1$ relations is visited at most once, the loop over all binary relations (l. 9) is visited at most $(q - 1) \cdot v$ times. The enumeration of all values of any structural relation is required to be in $O(e)$ and thus the set initialization of the inner loop (l. 11) takes time in $O(e)$. Since there are at most v elements in the range of any structural relation and the loop body (l. 12) is constant (the recursive call is amortized by memoization), $\mathsf{Match}_{\downarrow}$ is in $O(q \cdot v \cdot e)$ combined time complexity. The space complexity of the memoizatin matrix is $O(q \cdot v^2)$, and the size of ρ is in $O(q \cdot v)$, so that the space complexity of $\mathsf{Match}_{\downarrow}$ is again dominated by the memoizatin matrix. □

As section 7 shows, the algorithm $\mathsf{Match}_{\downarrow}$ is a competitive algorithm, exhibiting a linear time complexity in many real world scenarios, even without any index structures. Streaming schemes [8] and similar techniques could most likely be used to refine the algorithm further and speedup the average runtime. However, such optimizations are beyond the scope of this paper.

5. MATRIX CONSUMPTION

The consumption of a memoization matrix for the evaluation of a query Q against a data graph D creates the extensional representation of the result. That is to say, the compact in-memory result representation in the memoization matrix is *expanded* to a set of valuations for answer variables, i.e. a set of tuples associating answer variables with matching data nodes. This is comparable to the transformation of a non-first-normal-form relation into a flat relation, except for two details: Nested matrices consist of bindings for several relations and must hence be decomposed into partitions before the flattening takes place and a sub-matrix tuple can be referenced by more than one matrix. With the same reasoning as for sharing of sub-matrices, the results of the transformation from matrices to flat valuations must be memoized to avoid their repeated computation.

In contrast to matrix population, the algorithms for matrix consumption, though still agnostic to the shape of the data, have to treat tree and graph *queries* differently. This is necessary, because graph queries contain binary relations that are not verified by the matrix population algorithms. Obviously, there are no such remaining relations in tree queries. This reduces the matrix consumption algorithm to a simple flattening of the nested memoization matrix to produce the output. Since the output size of tree queries is guaranteed to be larger than every intermediate result, the time and space complexity of the consuming algorithm is bounded by the result size. For graph-shaped queries, however, this is not the case: an intermediate result of exponential size can be created and only then be reduced through the remaining binary relations that are not part of the query spanning tree relations. Thus, even if the output size is subexponential, the matrix consumption for graph queries has exponential combined time complexity. To illustrate this, consider the queries from Figure 2: The memoization matrix only enforces the structural relations, but does not consider VALEQUAL and IDENT. These relations may reduce the result size considerably if they are applied.

In the following three sections, we first take a look at the basic matrix consumption for tree queries (Section 5.1) and compare it in a second step (Section 5.2) with the case for arbitrary graph queries. Finally, we outline briefly the benefits and drawbacks of a nested loop join for incremental output generation (Section 5.3).

5.1 Matrix Consumption for Tree Queries

To obtain the set of answers to a query Q against a data graph D according to the semantics of n-ary conjunctive queries in Section 2, the algorithm is called with the memoization matrix resulting from the application of one of the Match algorithms in Section 4. In the following algorithms, we rely on the fact that the memoization matrix for the root variable consists of one single entry, which is guaranteed by the matrix population algorithms. The matrix population algorithms are called with this single tuple (x, n, M) as parameter.

As in the top-down population algorithm, a helper structure ρ for memoizing the flattened relation for each pair of query and data node is used. It is intially assumed to be $\emptyset$.

Algorithm 3 $\mathsf{Output}_T(x, n, M)$

1: **if** $\rho(x, n)$ defined **then**
2:     **return** $\rho(x, n)$
3: **if** $x \in \mathit{FreeVars}(Q)$ **then**
4:     $A \leftarrow \{[x : n]\}$
5: **else**
6:     $A \leftarrow \{[]\}$
7: **for all** $x' \in \pi_1(M)$ **do**
8:     $A_{x'} \leftarrow \emptyset$
9:     **for all** $n', M' : (x', n', M') \in M$ **do**
10:         $A_x \leftarrow A_{x'} \cup \mathsf{Output}_T(x', n', M')$
11:     $A \leftarrow A \times A_{x'}$
12: $\rho(x, n) \leftarrow A$
13: **return** A

The Output_T algorithm unfolds the compact solution representation to a set of valuations, eliminating duplicates (note the set union l. 10). The algorithm returns a set of valuations, each representing a match of the query in the data. Given a triple (x, n, M), it is first verified whether the answers have already been computed and memoized in ρ in an earlier call for (x, n), in which case they are immediately returned (l. 1–2). Otherwise, the answer set A is initialized accordingly to the type of x (l. 3–6). In the case that x is no free variable, bindings for x should not be part of the answer set. Thus the empty tuple is used as initial valuation. Matrix M is partitioned by variables (l. 7–9). Note that since the considered structural relations stem from a spanning tree, the variable x' determines also the structural relation of the partition. The result of each partition is stored into $A_{x'}$. The innermost loop (l. 6) iterates over each pair of data node n, and sub-matrix M' of the current partition. The result of the recursive calls to $\mathsf{Output}_T(x', n', M')$ are collected in $A_{x'}$. The result A is then multiplied by $A_{x'}$ to create the answer (l. 11). The answer set is a relation over the free variables of Q, as required by the semantics (cf. Section 2.2).

PROPOSITION 1 (COMPLEXITY OF OUTPUT_T). *The algorithm Output_T has $O(|Vars(Q)| \cdot |N|^2 + |Q(D)|)$ time complexity where $|Q(D)|$ denotes the result size.*

PROOF SKETCH. Each matrix is transformed to an answer set with result size, and the intermediate sets can only get as large as the final results. The worst case scenario is that each recursive call to Output_T creates an answer set of result size. In this case, the elimination of duplicates takes $O(2 \cdot |Q(D)| \cdot log(2 \cdot |Q(D)|)) = O(|Q(D)| \cdot log\,|Q(D)|)$ using a sort-based elimination, and $O(|Q(D)|)$ using a nondegenerating hash-based duplicate elimination. As the complete matrix structure of size $O(|Vars(Q)| \cdot |N|^2)$ must be traversed to create the output, the worst case complexity becomes $O(|Vars(Q)| \cdot |N|^2 + |Q(D)|)$. $\square$

Duplicate bindings are generated by projection; as existentially quantified variables are dropped, equal bindings of the remaining variables are produced. The problem is the same as duplicate generation in relational databases, and it can be reasonably assumed that the same elimination techniques may be used (such as [3]).

Avoiding duplicate generation when evaluating tree queries against tree data has been studied extensively, e.g., in [16, 21]. Though such techniques are beyond the scope of this paper, Section 8 briefly addresses the support of regular path expressions that can drastically reduce the number of existential variables in a query and thus, in many queries, the need for duplicate elimination.

5.2 Matrix Consumption for Graph Queries

In [15] it is shown that the evaluation of graph-shaped conjunctive queries over the relations *Child* and *Child** is already NP-complete on tree data. Nevertheless, the need for graph-shaped queries is evident, especially when comparison relations such as VALEQUAL and EQUAL are supported. This is evidenced by the fact that queries in all of XSLT, XQuery, SPARQL, and Xcerpt make extensive use of graph-shaped queries and formalizations for graph-shaped queries can cover much larger sub-sets of these languages than those restricted to tree-shaped queries.

The matrix method applies to graph-shaped queries in the following way: First, a spanning tree $T(Q)$ over the structural relations of Q is computed offline. Second, $\mathsf{Match}_\downarrow$ or $\mathsf{Match}_\uparrow$ is applied to create the memoization matrix of the query problem. Finally, this memoization matrix is consumed with a new output algorithm, Output_G.

The new algorithm must verify whether the produced valuations satisfy all relations that are not part of the spanning tree $T(Q)$. To put it another way, the non-tree relations impose additional selection conditions on the produced valuations. These additional selection conditions are distributed over cartesian products that the consumption algorithm for tree queries computes. They are combined into joins, with possibly non-atomic conditions, if more than one relation must be verified in one cartesian product. Due to the nested structure of the memoization matrix, the output algorithm performs $q - 2$ different kinds of cartesian products. As several sub-matrices of a given level share the same structure,

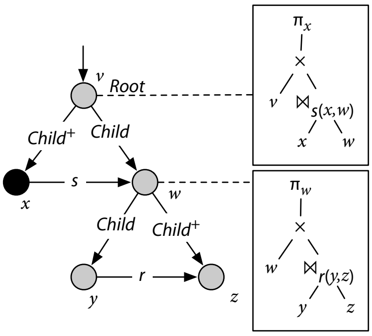

Figure 5: Exemplary Join and Projection Specification

each kind of cartesian product is performed several times for each sub-matrix.

Of course, these additional selections should be applied as soon as possible (i.e., pushed down) to keep intermediate results small. Since existentially quantified variables involved in join conditions must be kept until these joins are performed, it is furthermore necessary to infer the position at which each existentially quantified join variable can be projected away. Hence, a *join and projection specification* $\bowtie$–*Π*–*spec* is associated with each variable. This specification defines which joins and which projections can be performed when outputting the results for x. It furthermore determines the ordering of joins and projections.

Since join order optimization is out of the scope of this paper, the output algorithm abstracts from these topics by assuming the existence of a specification $\bowtie$–*Π*–*spec* for each variable, and of a function that applies these join specification to a set of valuation sets. Using a set of valuations instead of a canonical cartesian product allows to use joins instead of selections, increasing the performance of the output algorithm considerably. The join and projection specification is typically created by the query planner and can be executed by a conventional relational query engine.

Figure 5 shows an example of a join and projection specification. Recall, that $JoinVars(Q)$ is the set of join variables, i.e., the set of variables that are existentially quantified (no answer variables) and occur in at least one binary relation that is not part of $T(Q)$.

Algorithm 4 $\text{Output}_G(x, n, M)$

if $\rho(x,n)$ defined **then**
  return $\rho(x,n)$
if $x \in FreeVars(Q) \cup JoinVars(Q)$ **then**
  $A_S \leftarrow \{\{[x:n]\}\}$
else
  $A_S \leftarrow \{\{[]\}\}$
for all $x' \in \pi_1(M)$ **do**
  $A_{x'} \leftarrow \emptyset$
  for all $n', M' : (x', n', M') \in M$ **do**
    $A_{x'} \leftarrow A_{x'} \cup \text{Output}_T(x', n', M')$
  $A_S \leftarrow A_S \cup \{A_{x'}\}$
$A \leftarrow$apply $\bowtie$–*Π*–*spec*(x) to A_S
$\rho(x,n) \leftarrow A$
return A

The new algorithm however exhibits exponential worst case runtime in that it may perform at worst $q-3$ cartesian products without any selection based on non-tree edges (q being again $q = |Vars(Q)|$). In this case, the size and time complexity are both in $O(|N|^q)$, as the output algorithm keeps the set of valuations in memory.

Furthermore, the cost of value-based joins that are assessed with a cost function $j(|N|)$ must be considered. The worst case estimation is as follows: as every variable can be involved in a join, there are at most $q-1$ value-based joins (as equality is transitive, a query with more than $q-1$ joins can be transformed into an equivalent query with $q-1$ joins). Furthermore, every tuple of an exponential sized intermediate result is joined with each value-based join. As the application of a join reduces the result size by a factor at least linear in $|N|$, the overall runtime can be aproximated as $O(\sum_{i=2}^{q} j(|N|) \cdot |N|^i) = O(j(|N|) \cdot |N|^q)$.

Proposition 2 (Complexity of Output_G). *The algorithm* Output_G *has* $O(j(|N|) \cdot |N|^q)$ *time complexity and* $O(|N|^q)$ *space complexity.*

Creating a structural tree query from a graph query is unfavorable for this worst case complexity, since it is exponential in the number of variables and the corresponding structural tree query with value joins for a graph query has up to twice the number of variables as the graph query. For realistic cases however, this is a technique to transform tree-relation join conditions that are not verifiable in constant time into identity joins. Alternatively, it is possible in the match algorithms to create (in the top-down approach reasonably small) on-the-fly indexes for the non-tree structural relations, assuring a fast verification of these relations in Output. The quadratic increase of the exponential factor can hence be avoided.

5.3 Incremental Matrix Consumption for Trees and Graphs

The previous two algorithms are tailored to provide an in-memory representation of all answers of a query and are thus both in time and space complexity bound by the output size. An in-memory representation of the answers is useful to perform further processing based on the answers, e.g., for structural grouping, aggregation, or ordering. However, in many cases an incremental output of the answers is preferable, in particular if further processing can also be realized in an incremental manner. Incremental answer generation can be realized using the algorithm Output_{NLJ}, a slightly modified incremental *nested loop join* over the memoization matrix. The algorithm uses the structure of the matrix instead of join attributes, but is otherwise – leaving aside partitioning issues – a standard nested loop join and therefore omitted here for space reasons.

Proposition 3 (Complexity of Output_{NLJ}). *The algorithm* Output_{NLJ} *has time complexity* $O(|N|^q)$ *and space complexity* $O(q \cdot |N|^2)$ *on tree queries, on graph queries time complexity* $O(j(|N|) \cdot |N|^q)$ *and space complexity* $O(q \cdot |N|^2)$.

The advantage of Output_{NLP} is the low space complexity that is essentially bounded by the size of the memoization matrix. However, this advantage is paid for by an exponential time complexity in almost all cases. Furthermore, this exponential time complexity is reached in many practical cases, making this algorithm suitable only for cases where space consumption is clearly more important than run time of the evaluation algorithm.

$$
\begin{aligned}
[\![\,\text{NEXT}\,]\!]_D &= \{(c,c') : \exists (p,i,c),(p,i',c') \in E : i+1 = i'\} \\
[\![\,\text{NEXT}^+\,]\!]_D &= \{(c,c') : \exists (p,i,c),(p,i',c') \in E : i < i'\} \\
[\![\,\text{NEXT}^*\,]\!]_D &= \{(c,c') : \exists (p,i,c),(p,i',c') \in E : i \leq i'\}
\end{aligned}
$$

Table 3: Semantics of Order Relations

6. ORDER RELATIONS ON GRAPH DATA

In the previous sections, graph-shaped data is considered equivalent to tree-shaped data w.r.t. query evaluation. Although the worst case complexity of the matrix population algorithms is the same for both cases, the order of two sibling nodes becomes context dependent in graphs, cf. Section 2.1.

For the support of ordered queries in graph data, a ternary relation NEXT and its closures NEXT^+, NEXT^* are introduced (cf. Table 3). In fact, once the matrix consuming algorithms support join conditions, the handling of the ternary order relations is simple: it can be handled as additional join condition in the join and projection specification of each node (cf. Figure 6).

Besides this very rudimentary exploit of order relations as join conditions in the output algorithm, it is possible to take advantage of them in the matrix population algorithms, if the edge position from the data model is accessible. Assuming that $Next^*(x, y, y')$ must hold and that I is the set of positions of all y valuations and I' of y' respectively, it must obviously hold that $\forall i \in I : i \leq max(I')$ and $\forall i' \in I' : min(I) \leq i'$. If the domain of y is populated before y' (as the match algorithm does in its recursive descent), these conditions can be used to reduce the number of candidate valuations for y', and prune valuations for y: When populating the domain of y', the minimum position of valuations of y is known, so that the condition can be imposed on all valuations of y'. After populating y', all valuations of y that have a position greater than the maximum position of y' valuations can be dropped.

7. EXPERIMENTAL EVALUATION

The experimental evaluation is based on both synthetic and real data. The set of structural relations is extended by the additional relation ATTRIBUTE in order to support attribute queries. The tests have been executed on an AMD Athlon 2400XP machine with 1GB main memory. The algorithms are implemented in Java executed on JVM version 1.5.0_06-b05. All tests show the processing time without data parsing. Each measurement is averaged over 500 runs. The algorithms have been implemented straightforwardly close to the form presented without additional optimizations.

Synthetic data is used to demonstrate and confirm the complexity of the presented algorithms. The real data scenarios stem from the University of Washington XMLData repository[1], and demonstrate the competitiveness of the algorithms in their basic form.

The first experiment confirms on synthetic data that the memoization of intermediary results is essential, not only for the complexity but also for the experimental query evaluation time. The $\text{Match}_\downarrow$ algorithm without memoization of variable domains (i.e., the helper structure ρ and all access

[1] `http://www.cs.washington.edu/research/xmldatasets/`

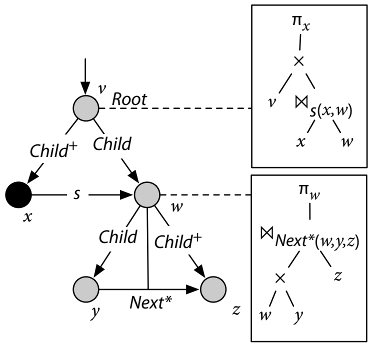

Figure 6: Join and Projection Specification with Order Relation

to it is removed from the algorithm) exhibits an exponential growth of time consumption in the size of the query (cf. Figure 7), because several common sub-matrices are built repeatedly. Though the exponential growth of the output size can be a factor, the query used in these experiments is unary and produces a linear output. In contrast, Figure 8 depicts the effect of increasing arity in a worst-case scenario, where the query is entirely unrestrictive and a binding for one answer variable is related to all bindings of all other variables.

Figures 9 and 10 show a *comparison between the two approaches* for matrix population discussed in this article. A path query consisting of four variables and CHILD^* (descendant) relations only, but without label restrictions, is used. This query exhibits worst case complexity for the top-down algorithm $\text{Match}_\downarrow$, as the match context is never restricted by a previous context. As expected, the plot shows a quadratic runtime growth in the data size for the top-down algorithm. The bottom-up approach exhibits, as expected, a cubic runtime when lacking index structures for the CHILD^* relation, whereas the runtime of the bottom-up algorithm with CHILD^* index and top-down is almost entirely identical (to the extent that the two plots are nearly indistinguishable in Figure 10).

The above experiments clearly reinforce the theoretical complexity results derived in this work. Moreover, at least the top-down algorithm performs quite well even in its basic form discussed here in real query scenarios. Figure 11 shows how the runtime of the top-down algorithm scales with the data size for path-, tree-, and graph-shaped queries. These queries are executed against the MONDIAL database of geographical information, cf. `http://www.dbis.informatik.uni-goettingen.de/Mondial/`. The plot shows additionally that already for path queries the bottom-up algorithm exhibits polynomial runtime; the naive bottom-up approach has an average runtime that is very close to its worst-case. On the other hand, the $\text{Match}_\downarrow$ exhibits a linear runtime in all queries, even in the graph query case. This shows manifestly the power of the context-aware processing of a top-down approach.

The final test on increasing fragments of a large XML document (the Nasa dataset from the above mentioned repository) shows that the runtime of $\text{Match}_\downarrow$ scales nicely with the data size and is very competitive even in the basic form implemented for these experiments.

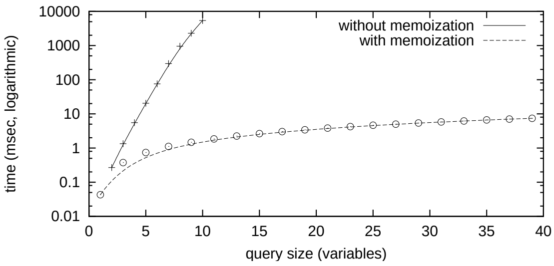

Figure 7: Effect of Memoization over Query Size

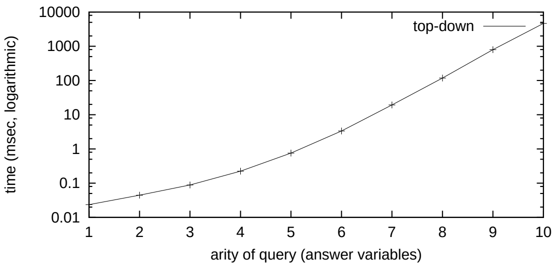

Figure 8: Worst-Case Effect of Query Arity

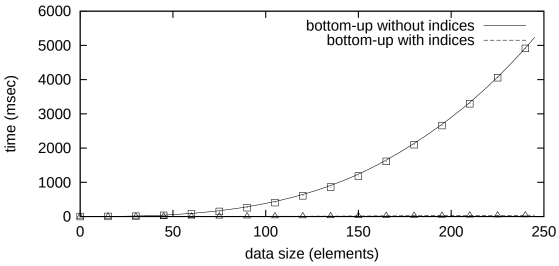

Figure 9: Comparison of Bottom-Up with and without Relation Indices

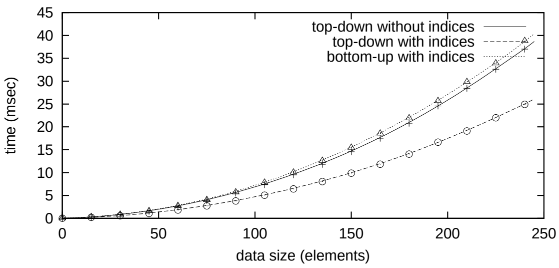

Figure 10: Comparison of Top-Down and Bottom-Up Approach

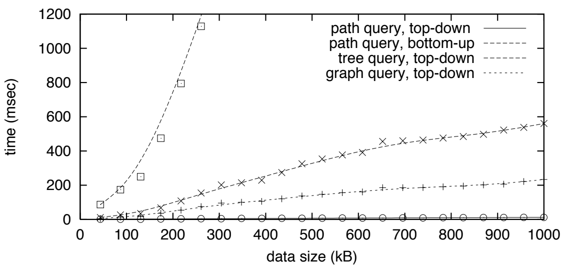

Figure 11: Path, Tree, and Graph Queries over Real-life Data

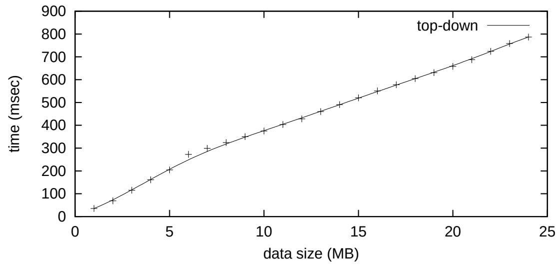

Figure 12: Top-Down Algorithm over Large, Real-life Data

8. EXTENSIONS AND OUTLOOK

Though the experimental evaluation shows that even the basic form of the proposed top-down algorithm performs nicely, there are quite a number of extensions and further optimizations likely to give interesting results: First of all, there are extensions of the top-down matching algorithm to a *complete unification algorithm*, needed for pattern matching as in Xcerpt [24]. This algorithm must handle negated and optional query parts as in general tree patterns [9].

Arc consistency, as used in constraint solving algorithms, can be used to reduce the size of the matrix structure. First experiments have shown, however, that verification of arc consistency does not always improve evaluation time: in cases where the runtime of $\mathsf{Match}_{\downarrow}$ is linear in the data size, applying arc consistency renders the runtime quadratic. This effect arises when the number of actually performed joins is reduced drastically through the query context.

Above this, *partial unnesting of matrices* can be used to remove existentially quantified variables eagerly at matrix population time: a link to and from an existentially quantified variable valuation is replaced by a direct link. In this way, the space complexity of path queries can be reduced from $O(|\,Vars(Q)| \cdot |N|^2)$ to $O(n \cdot |N|^2)$, n being the arity of the query. One step in this direction is the support of more expressive structural relations, e.g., conditional axes [19] that allow collapsing entire paths both for population and consumption of the matrix. Indeed, [20] uses a similar approach for the computation of complete answer aggregates over tree data.

Relational *query planning* and *execution* techniques could be incorporated to improve duplicate elimination [3] and to optimize the partitioning of relations between spanning tree and join specifications as well as the choice of an efficient join specification.

Finally, we plan to investigate a *combination* of bottom-up and top-down matching techniques, in order to combine the benefits of both a sophisticated bottom-up approach, i.e., early pruning in the case of selective query leaves, and the contextual narrowing of a top-down approach.

9. RELATED WORK

As previously mentioned, the complexity of conjunctive queries and monadic queries *over trees* is studied thoroughly in [15, 12]. A restriction of the bottom-up algorithm discussed in this article to conjunctive *tree queries* is roughly similar to the complete answer aggregates algorithm of [20] and has the same complexity.

Matching conjunctive queries against trees and graphs can be seen as a constraint solving problem. It is well established that tree-shaped constraint problems (i.e., tree queries) can be solved in $O(q \cdot v^2)$ [11] where q is the number of variables and v the variable domain size. This result assumes, however, $O(1)$ verification time for all relations. Furthermore, the implication from arc to global constraint consistency used in this result, does not hold for graph-shaped constraint problems.

In [15] it is shown that there are special cases where arc consistency is at least sufficient to retrieve one single consistent solution: if all binary constraints have the $\underline{\text{X}}$-property (read: X-underbar) over an order $<$, arc-consistency is sufficient to guarantee that the minimal solution (in terms of the same ordering $<$) is consistent. It follows that the evaluation of n-ary graph queries with $\underline{\text{X}}$-relations is only exponential in the number of free variables. It can further be derived that the general problem is NP-complete and thus an algorithm as proposed here with worst case exponential runtime is the best achievable to present knowledge.

Another field of important related work are structural indexing techniques [5, 8, 18]. Indexes are an orthogonal aspect to the matrix method that can be used to improve the runtime of the presented algorithms. Considering entire paths or trees at once through physical operators such as twig joins [5] is a promising and widely researched technique for tree data. Their application to the discussed algorithms is straightforward. However, most structural indexing techniques do not exhibit obvious extensions to graph data.

10. CONCLUSION

With the rise of XML and RDF, processing both graph- and tree-shaped n-ary queries against semi-structured data becomes ever more important. The memoization matrix is a compact recursive non-redundant data structure that holds the solution sets to such queries. In case of tree queries, it contains the exact solutions to the queries, whereas in case of graph queries intermediary results: the solutions to the query represented by a spanning tree chosen for the population of the matrix. By separating the evaluation of n-ary queries in two phases, viz. the population and the consumption of the memoization matrix, we demonstrate several insights in tree- and graph-shaped query evaluation: **(1)** We show that the shape of the data, whether tree or graph, does for the most part not affect the query complexity for n-ary conjunctive queries. **(2)** We show that a unified algorithm for both tree- and graph-shaped semi-structured queries is feasible and both in worst-case complexity and in experimental performance competitive for reasonable queries and data. **(3)** By this, we extend previously known results for the evaluation of tree and graph queries against tree data to graph data and show where complexity and experimental performance is affected by the change.

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