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Conference Paper · January 2002
DOI: 10.1145/564691.564727

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Holistic Twig Joins: Optimal XML Pattern Matching

Nicolas Bruno  
Columbia University  
nicolas@cs.columbia.edu

Nick Koudas  
AT&T Labs–Research  
koudas@research.att.com

Divesh Srivastava  
AT&T Labs–Research  
divesh@research.att.com

ABSTRACT

XML employs a tree-structured data model, and, naturally, XML queries specify patterns of selection predicates on multiple elements related by a tree structure. Finding all occurrences of such a twig pattern in an XML database is a core operation for XML query processing. Prior work has typically decomposed the twig pattern into binary structural (parent-child and ancestor-descendant) relationships, and twig matching is achieved by: (i) using structural join algorithms to match the binary relationships against the XML database, and (ii) stitching together these basic matches. A limitation of this approach for matching twig patterns is that intermediate result sizes can get large, even when the input and output sizes are more manageable.

In this paper, we propose a novel holistic twig join algorithm, TwigStack, for matching an XML query twig pattern. Our technique uses a chain of linked stacks to compactly represent partial results to root-to-leaf query paths, which are then composed to obtain matches for the twig pattern. When the twig pattern uses only ancestor-descendant relationships between elements, TwigStack is I/O and CPU optimal among all sequential algorithms that read the entire input: it is linear in the sum of sizes of the input lists and the final result list, but independent of the sizes of intermediate results. We then show how to use (a modification of) B-trees, along with TwigStack, to match query twig patterns in sub-linear time. Finally, we complement our analysis with experimental results on a range of real and synthetic data, and query twig patterns.

1. INTRODUCTION

XML employs a tree-structured model for representing data. Queries in XML query languages (see, e.g., [8, 5, 2]) typically specify patterns of selection predicates on multiple elements that have some specified tree-structured relationships. For example, the XQuery expression:

book[title = 'XML']//author[fn = 'jane' AND ln = 'doe']

matches author elements that (i) have a child subelement fn with content jane, (ii) have a child subelement ln with content doe, and (iii) are descendants of book elements that have a child title subelement with content XML. This expression can be represented as a node-labeled twig (or small tree) pattern with elements and string values as node labels.

Finding all occurrences of a twig pattern in a database is a core operation in XML query processing, both in relational implementations of XML databases, and in native XML databases. Prior work (see, for example, [12, 24, 17, 19, 18, 27, 1]) has typically decomposed the twig pattern into a set of binary (parent-child and ancestor-descendant) relationships between pairs of nodes, e.g., the parent-child relationships (book, title) and (author, fn), and the ancestor-descendant relationship (book, author). The query twig pattern can then be matched by (i) matching each of the binary structural relationships against the XML database, and (ii) "stitching" together these basic matches.

For solving the first sub-problem of matching binary structural relationships, Zhang et al. [27] proposed a variation of the traditional merge join algorithm, the multi-predicate merge join (MPMGJN) algorithm, based on the (DocId, LeftPos : RightPos, LevelNum) representation of positions of XML elements and string values (see Section 2.3 for details about this representation). Their results showed that the MPMGJN algorithm could outperform standard RDBMS join algorithms by more than an order of magnitude. More recently, Al-Khalifa et al. [1] took advantage of the same representation of positions of XML elements to devise I/O and CPU optimal join algorithms for matching binary structural relationships against an XML database.

The second sub-problem of stitching together the basic matches obtained using binary "structural" joins requires identifying a good join ordering in a cost-based manner, taking selectivities and intermediate result size estimates into account. In this paper, we show that a basic limitation of this (traditional) approach for matching query twig patterns is that intermediate result sizes can get very large, even when the input and final result sizes are much more manageable. As a result, we seek a better solution to the problem of matching query twig patterns efficiently.

In this paper, we propose a novel holistic twig join approach for matching XML query twig patterns, wherein no large intermediate results are created. Our technique uses the (DocId, LeftPos : RightPos, LevelNum) representation of positions of XML elements and string values (that succinctly captures structural relationships between nodes in the XML database). It also uses a chain of linked stacks to
1.1 Outline and Contributions

We begin by presenting background material (data model, query twig patterns, and positional representations of XML elements) in Section 2. Our main contributions are:

- **We develop two families of holistic path join algorithms** in Section 3 to match XML query root-to-leaf paths efficiently. The first, PathStack, generalizes the Stack-Tree-Desc binary structural join algorithm of [1], while the second, PathMPM, generalizes the MPMGJN binary join algorithm of [27]. We analyze PathStack and show that it is I/O and CPU optimal among all sequential algorithms that read the entire input, and has worst-case complexities linear in the sum of input and output sizes but independent of the sizes of intermediate results.

- **We then develop TwigStack in Section 4**, a holistic twig join algorithm that (i) refines PathStack to ensure that results computed for one root-to-leaf path of a twig pattern are likely to have matching results in other paths of the twig pattern, and (ii) merges results for the different root-to-leaf paths in the query twig pattern, to compute the desired output. When the query twig uses only ancestor-descendant relationships between elements, we analytically demonstrate that TwigStack is I/O and CPU optimal among all sequential algorithms that read the entire input.

- **Finally, in Section 5 we present experimental results on a range of real and synthetic data, and query twig patterns, to complement our analytical results**:
  - We show the substantial performance benefits of using holistic twig joins over binary structural joins (for arbitrary join orders).
  - We show that among holistic path join algorithms, PathStack is significantly faster than PathMPM. This validates the analytical results demonstrating the I/O and CPU optimality of PathStack.
  - For the case of twig patterns, we show that the use of TwigStack is better (both in time and space) than the independent use of PathStack on each root-to-leaf path, even when the twig pattern contains parent-child structural relationships.
  - We show how to use a modification of B-trees, denoted XB-trees, along with TwigStack, to perform matching of query twig patterns in sub-linear time.

We describe related work in Section 6, and conclude by discussing ongoing and future work in Section 7.

2. BACKGROUND

2.1 Data Model and Query Twig Patterns

An XML database is a forest of rooted, ordered, labeled trees, each node corresponding to an element or a value, and the edges representing (direct) element-subelement or element-value relationships. Node labels consist of a set of (attribute, value) pairs, which suffices to model tags, IDs, IDREFs, etc. The ordering of sibling nodes implicitly defines a total order on the nodes in a tree, obtained by a preorder traversal of the tree nodes. Figure 1 shows the tree representation of a sample XML document. (The utility of the numbers associated with the tree nodes will be explained in Section 2.3.)

![Figure 1: A sample XML Tree representation](image)

Queries in XML query languages like XQuery [2], Quilt [5] and XML-QL [8] make use of (node labeled) twig patterns for matching relevant portions of data in the XML database. The twig pattern node labels include element tags, attribute-value comparisons, and string values, and the query twig pattern edges are either parent-child edges (depicted using a single line) or ancestor-descendant edges (depicted using a double line). For example, the XQuery expression:

```
book[title = 'XML' AND year = '2000']
```

which matches book elements that (i) have a child title subelement with content XML, and (ii) have a child year subelement with content 2000, can be represented as the twig pattern in Figure 2(a). Only parent-child edges are used in this case. Similarly, the XQuery expression in the introduction can be represented as the twig pattern in Figure 2(b). Note that an ancestor-descendant edge is used between the book element and the author element.

In general, at each node in the query twig pattern, there is a node predicate on the attributes (e.g., tag, content) of the node in question. For the purposes of this paper, exactly
what is permitted in this predicate is not material. Similarly, the physical representation of the nodes in the XML database is not relevant to the results in this paper. It suffices for our purposes that there be efficient access mechanisms (such as index structures) to identify the nodes in the XML database that satisfy any given node predicate \( q \), and return a stream of matches \( T_q \).

2.2 Twig Pattern Matching

Given a query twig pattern \( Q \) and an XML database \( D \), a match of \( Q \) in \( D \) is identified by a mapping from nodes in \( Q \) to nodes in \( D \), such that: (i) query node predicates are satisfied by the corresponding database nodes (the images under the mapping), and (ii) the structural (parent-child and ancestor-descendant) relationships between query nodes are satisfied by the corresponding database nodes. The answer to query \( Q \) with \( n \) nodes can be represented as an \( n \)-ary relation where each tuple \((d_1, \ldots, d_n)\) consists of the database nodes that identify a distinct match of \( Q \) in \( D \).

Finding all matches of a query twig pattern in an XML database is a core operation in XML query processing, both in relational implementations of XML databases, and in native XML databases. In this paper, we consider the twig pattern matching problem:

Given a query twig pattern \( Q \), and an XML database \( D \) that has index structures to identify database nodes that satisfy each of \( Q \)'s node predicates, compute the answer to \( Q \) on \( D \).

Consider, for example, the query twig pattern in Figure 2(a), and the database tree in Figure 1. This query twig pattern has one match in the data tree that maps the nodes in the query to the root of the data and its first and third subtrees.

2.3 Representing Positions of Elements and String Values in an XML Database

The key to an efficient, uniform mechanism for set-at-a-time (join-based) matching of query twig patterns is a positional representation of occurrences of XML elements and string values in the XML database (see, e.g., [6, 7, 27]), which extends the classic inverted index data structure in information retrieval [22].

We can represent the position of a string occurrence in the XML database as a 3-tuple \((\text{DocId}, \text{LeftPos}, \text{LevelNum})\), and analogously, the position of an element occurrence as a 3-tuple \((\text{DocId}, \text{LeftPos} : \text{RightPos}, \text{LevelNum})\), where (i) \text{DocId} is the identifier of the document; (ii) \text{LeftPos} and \text{RightPos} can be generated by counting word numbers from the beginning of the document \text{DocId} until the start and the end of the element, respectively; and (iii) \text{LevelNum} is the nesting depth of the element (or string value) in the document. Figure 1 shows 3-tuples associated with some tree nodes, based on this representation (the DocId for all nodes is chosen to be one).

Structural relationships between tree nodes whose positions are recorded in this fashion can be determined easily: (i) ancestor-descendant: a tree node \( n_2 \) whose position in the XML database is encoded as \((D_2, L_2 : R_2, N_2)\) is a descendent of a tree node \( n_1 \) whose position is encoded as \((D_1, L_1 : R_1, N_1)\) iff \( D_1 = D_2, L_1 < L_2, \text{ and } R_2 < R_1^1; (ii) parent-child: a tree node \( n_2 \) whose position in the XML database is encoded as \((D_2, L_2 : R_2, N_2)\) is a child of a tree node \( n_1 \) whose position is encoded as \((D_1, L_1 : R_1, N_1)\) iff \( D_1 = D_2, L_1 < L_2, R_2 < R_1, \text{ and } N_1 + 1 = N_2. \) For example, in Figure 1, the author node with position \((1,6:20,3)\) is a descendant of the book node with position \((1,1:150,1)\), and the string “jane” with position \((1,8,5)\) is a child of the author node with position \((1,7:9,4)\). A key point worth noting about this representation of node positions in the XML data tree is that checking an ancestor-descendant relationship is as simple as checking a parent-child relationship (we can check for an ancestor-descendant structural relationship without knowledge of the intermediate nodes on the path). Also, this representation of positions of nodes allows for checking order (e.g., node \( n_2 \) follows node \( n_1 \) and structural proximity (e.g., node \( n_2 \) is a descendent within \( 3 \) levels of \( n_1 \) ) relationships.

3. HOLISTIC PATH JOIN ALGORITHMS

3.1 Notation

Let \( q \) (with or without subscripts) denote twig patterns, as well as (interchangeably) the root node of the twig pattern. In our algorithms, we make use of the following twig node operations: \text{isLeaf}: Node \rightarrow Bool, \text{isRoot}: Node \rightarrow Bool, \text{parent}: Node \rightarrow Node, \text{children}: Node \rightarrow \{\text{Node}\}, \text{and subTreeNodes}: Node \rightarrow \{\text{Node}\}. Path queries have only one child per node, otherwise children\( q \) returns the set of children nodes of \( q \). The result of subTreeNodes\( q \) is the node \( q \) and all its descendants.

Associated with each node \( q \) in a query twig pattern there is a stream \( T_q \). The stream contains the positional representations of the database nodes that match the node predicate at the twig pattern node \( q \) (possibly obtained using an efficient access mechanism, such as an index structure). The nodes in the stream are sorted by their (DocId, LeftPos) values. The operations over streams are: \text{eof}, \text{advance}, \text{next}, \text{nextL}, and \text{nextR}. The last two operations return the LeftPos and RightPos coordinates in the positional representation of the next element in the stream, respectively.

In our stack-based algorithms, PathStack and TwigStack, we also associate with each query node \( q \) a stack \( S_q \). Each data node in the stack consists of a pair: (positional representation of a node from \( S_q \), pointer to a node in \text{SLeaf}(q)\). The operations over stacks are: \text{empty}, \text{pop}, \text{push}, \text{topL}, and \text{topR}. The last two operations return the LeftPos and RightPos coordinates in the positional representation of the top element in the stack, respectively. At every point during the computation, (i) the nodes in stack \( S_q \) (from bottom to top) are guaranteed to lie on a root-to-leaf path in the XML database, and (ii) the set of stacks contain a compact encoding of partial and total answers to the query twig pattern, which can represent in linear space a potentially exponential (in the number of query nodes) number of answers to the query twig pattern, as illustrated below.

Example 3.1. Figure 3 illustrates the stack encoding of answers to a path query for a sample data set. The answer \([A_2, B_3, C_1]\) is encoded since \( C_1 \) points to \( B_3 \), and \( B_3 \) points to \( A_2 \). Since \( A_1 \) is below \( A_2 \) on the stack \( S_A \), \([A_1, B_3, C_1]\) is also an answer. Finally, since \( B_1 \) is below \( B_3 \) on the stack \( S_B \), and \( B_1 \) points to \( A_1 \), \([A_1, B_1, C_1]\) is also an answer. Note that \([A_2, B_3, C_1]\) is not an answer, since \( A_2 \) is above the node \( A_1 \) on stack \( S_A \) to which \( B_1 \) points.
3.2 PathStack

Algorithm PathStack, which computes answers to a query path pattern, is presented in Figure 4, for the case when the streams contain nodes from a single XML document. When the streams contain nodes from multiple XML documents, the algorithm is easily extended to test equality of Bcdid before manipulating the nodes in the streams and stacks.

Algorithm PathStack(q)
01 while ¬end(q)
02 qmin = getMinSource(q) // clean stacks
03 for qj in subtreeNodes(q) // clean stacks
04 while ¬empty(Sj) ∧ top(Sj) < next1(Tqmin))
05 pop(Sj)
06 moveStreamToStack(Tqmin, Sj, next1(Tqmin), pointer to top(Sparent(qmin)))
07 if (isLeaf(qmin))
08 showSolutions(Sqmin, 1)
09 pop(Sqmin)

Function end(q)
return ∀qj ∈ subtreeNodes(q): isLeaf(qj) ⇒ eof(Tq)

Function getMinSource(q)
return qmin ∈ subtreeNodes(q) such that next1(Tqmin) is minimal

Procedure moveStreamToStack(Tq, Sj, p)
01 push(Sj, next(Tq, p))
02 advance(Tq)

Figure 4: Algorithm PathStack

The key idea of Algorithm PathStack is to repeatedly construct (compact) stack encodings of partial and total answers to the query path pattern, by iterating through the stream nodes in sorted order of their LftPos values; thus, the query path pattern nodes will be matched from the query root down to the query leaf. Line 2 in Algorithm PathStack identifies the stream containing the next node to be processed. Lines 3-5 remove partial answers from the stacks that cannot be extended to total answers, given knowledge of the next stream node to be processed. Line 6 augments the partial answers encoded in the stacks with the new stream node. Whenever a node is pushed on the stack Sqmin, where qmin is the leaf node of the query path, the stacks contain an encoding of total answers to the query path, and Algorithm showSolutions is invoked by Algorithm PathStack (lines 7-9) to “output” these answers.

A natural way for Algorithm showSolutions to output query path answers encoded in the stacks is as n-tuples that are in sorted leaf-to-root order of the query path. This will ensure that, over the sequence of invocations of Algorithm showSolutions by Algorithm PathStack, the answers to the query path are also computed in leaf-to-root order. Figure 5 shows such a procedure for the case when only ancestor-descendant edges are present in the query path.

Procedure showSolutions(SN, SP)
// Assume, for simplicity, that the stacks of the query
// nodes from the root to the current leaf node we
// are interested in can be accessed as S[1],...,S[n].
// Also assume we have a global index[i]...n
// of pointers to the stack elements.
// index[i] represents the position in the i-th stack that
// we are interested in for the current solution, where
// the bottom of each stack has position 1.
// Mark we are interested in position SP of stack SN.
01 index[SN] = SP
02 if (SN == 1) // we are in the root
03 // output solutions from the stacks
04 output (S[1],index[1],...,S[1],index[1])
05 else // recursive call
06 for i = 1 to │SN│ index[SN].pointer_to_parent
07 showSolutions(SN−1,0)

Figure 5: Procedure showSolutions

When parent-child edges are present in the query path, we also need to take the LevelNum information into account. PathStack does not need to change, but we need to ensure that each time showSolutions is invoked, it does not output incorrect tuples, in addition to avoiding unnecessary work. This can be achieved by modifying the recursive call (lines 6-7) to check for parent-child edges, in which case only a single recursive call (showSolutions(SN−1, S[SN].index[SN].pointer_to_parent)) needs to be invoked, after verifying that the LevelNum of the two nodes differ by one. Looping through all nodes in the stack S[SN−1] would still be correct, but it would do more work than is strictly necessary.

If we desire the final answers to the query path be presented in sorted root-to-leaf order (as opposed to sorted leaf-to-root order), it is easy to see that it does not suffice that each invocation of showSolutions output answers encoded in the stack in the root-to-leaf order. To produce answers in the sorted root-to-leaf order, we would need to “block” answers, and delay their output until we are sure that no answer prior to them in the sort order can be computed. The details of how to achieve this naturally are presented in [3] and are omitted here for reasons of space.

Example 3.2. Consider the leftmost path, book-title-XML, in each of the query twins of Figure 2. If we used the binary structural join algorithms of [27, 1], we would first need to compute matches to one of the parent-child structural relationships: book-title, or title-XML. Since every book has a title, this binary join would produce a lot of matches against an XML books database, even when there are only a few books whose title is XML. If, instead, we first computed matches to title-XML, we would also match pairs under chapter elements, as in the XML data tree of Figure 1, which do not extend to total answers to the query path pattern. Using Algorithm PathStack, partial answers are compactly represented in the stacks, and not output. Using the XML data tree of Figure 1, only one total answer, identified by the mapping [ book → (1,1 : 150,1), title → (1,2 : 4,2), XML → (1,3,3) ], is encoded in the stacks.
3.3 Analysis of PathStack

The following proposition is a key to establishing the correctness of Algorithm PathStack.

**Proposition 3.1.** If we fix node Y, the sequence of cases between node Y and nodes X on increasing order of LeftPos (L) is: {1[2]}^3*.4*. Cases 1 and Cases 2 are interleaved, then all nodes in Case 3 before any node in Case 4, and finally all nodes in Case 4 (see Figure 6).

<table>
<thead>
<tr>
<th>Property</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>X.R-Y.L</td>
<td>X.L-Y.L</td>
<td>X.L-Y.R</td>
<td>X.R-Y.R</td>
<td>X.L-Y.R</td>
</tr>
</tbody>
</table>

**Figure 6: Cases for PathStack and TwigStack**

**Lemma 3.1.** Suppose that for an arbitrary node q in the path pattern query, we have that getMinSource(q) = q_n. Also, suppose that t_{q_{min}} is the next element in q_n's stream. Then, after t_{q_{min}} is pushed onto stack S_{q_{min}}, the chain of stacks from S_{q_{min}} to S_q verifies that their labels are included in the chain of nodes in the XML data tree from t_{q_{min}} to the root.

For each node t_{q_{min}} pushed onto stack S_{q_{min}}, it is easy to see that the above lemma, along with the iterative nature of Algorithm showSolutions, ensures that all answers in which t_{q_{min}} is a match for query node q_{min} will be output. This leads to the following correctness result:

**Theorem 3.1.** Given a query path pattern q and an XML database D, Algorithm PathStack correctly returns all answers for q on D.

We next show optimality. Given an XML query path of length n, PathStack takes n input lists of tree nodes sorted by (DocId, LeftPos), and computes an output sorted list of n-tuples that match the query path. It is straightforward to see that, excluding the invocations to showSolutions, the I/O and CPU costs of PathStack are linear in the sum of sizes of the n input lists. Since the cost of showSolutions is proportional to the size of the output list, we have the following optimality result:

**Theorem 3.2.** Given a query path pattern q with n nodes, and an XML database D, Algorithm PathStack has worst-case I/O and CPU time complexities linear in the sum of sizes of the n input lists and the output list. Further, the worst-case space complexity of Algorithm PathStack is the minimum of (i) the sum of sizes of the n input lists, and (ii) the maximum length of a root-to-leaf path in D.

It is particularly important to note that the worst-case time complexity of Algorithm PathStack is independent of the sizes of any intermediate results.

3.4 PathMPMJ

A straightforward generalization of the MPMGJN algorithm [27] for path queries proceeds one stream at a time to get all solutions. Consider the path query q_1/q_2/q_3. The basic idea is as follows: Get the first (next) element from the stream T_{q_1}, and generate all solutions that use that particular element from T_{q_1}. Then, advance T_{q_2} and backtrack T_{q_1} and T_{q_3} accordingly (i.e., to the earliest position that might lead to a solution). This procedure is repeated until T_{q_1} is empty. The generate all solutions step recursively starts with the first marked element in T_{q_1}, gets all solutions that use that element (and the calling element in T_{q_2}), then advances the stream T_{q_2} until there are no more solutions with the current element in T_{q_2}, and so on. We refer to this algorithm as PathMPMJNaive in our experiments.

It turns out that maintaining only one mark per stream (for backtracking purposes) is too inefficient, since all marks need to point to the earliest segment that can match the current element in T_{q_1} (the stream of the root node). A better strategy is to use a stack of marks, as described in Algorithm PathMPMJ in Figure 7. In this optimized generalization of MPMGJN, each query node will not have a single mark in the stream, but “k” marks where k is the number of its ancestors in the query. Each mark points to an earlier position in the stream, and for query node q, the i’th mark is the first mark in q_t such that the element in q_t starts after the current element in the stream of q’s i’th ancestor.

**Algorithm PathMPMJ(q)**

01 while (root(T_{q})) (isRoot(q)) /
    nextI(q) < nextI(parent(q)))
02 for (q ∈ subtrees(q)) // advance descendants
03 while (nextI(q) < nextI(parent(q)))
04 advance(T_{q_3})
05 PushMark(T_{q_1})
06 if (isLeaf(q)) // solution in the streams' heads
    outputSolution()
07 else PathMPMJ(child(q))
08 advance(T_{q_2})
09 for (q ∈ subtrees(q)) // backtrack descendants
10 PopMark(T_{q_1})

**Figure 7: Algorithm PathMPMJ**

**Theorem 3.3.** Given a query path pattern q and an XML database D, Algorithm PathMPMJ correctly returns all answers for q on D.

While the two extensions of MPMGJN appear similar, the difference between their performance is noticeable, as we shall see in the experimental section. Further, as was the case with MPMGJN, Algorithm PathMPMJ is not asymptotically optimal either.

4. TWIG JOIN ALGORITHMS

4.1 Limitations of Using PathStack

A straightforward way of computing answers to a query twig pattern is to decompose the twig into multiple root-to-leaf path patterns, use PathStack to identify solutions to each individual path, and then merge-join these solutions to compute the answers to the query. This approach, which we
experimentally evaluate in Section 5, faces the same fundamental problem as the techniques based on binary structural joins, towards a holistic solution: many intermediate results may not be part of any final answer, as illustrated below.

**Example 4.1.** Consider the query sub-twig rooted at the author node of the twig pattern in Figure 2(b). Against the XML database in Figure 1, the two paths of this query: author-fn-jane, and author-ln-doe, have two solutions each, but the query twig pattern has only one solution.

In general, if the query (root-to-leaf) paths have many solutions that do not contribute to the final answers, using PathStack (as a sub-routine) is suboptimal, in that the overall computation cost for a twig pattern is proportional not just to the sizes of the input and the final output, but also to the sizes of intermediate results. In this section, we seek to overcome this suboptimality using Algorithm TwigStack.

### 4.2 TwigStack

Algorithm TwigStack, which computes answers to a query twig pattern, is presented in Figure 8, for the case when the streams contain nodes from a single XML document. As with Algorithm PathStack, when the streams contain nodes from multiple XML documents, the algorithm is easily extended to test equality of Doc3D before manipulating the nodes in the streams and on the stacks.

```plaintext
Algorithm TwigStack(q)
// Phase 1
01 while ¬end(q)
02 qact = getNext(q)
03 if ¬isRoot(qact)
04 cleanStackKParent(qact, nextL(qact))
05 if ¬isEmpty(Sparent(qact))
06 cleanStackKParent(qact, next(qact))
07 moveStreamToStack(Tqact, Squeue, pointer to top(Sparent(qact)))
08 if ¬isLeaf(qact)
09 showSolutionsWithBlocking(Sqact, 1)
10 push(Sqact)
11 else advance(Tqact)
// Phase 2
12 mergeAllPathSolutions()

Function getNext(q)
01 if ¬isLeaf(q) return q
02 for qi ∈ children(q)
03 ni = getNext(qi)
04 if (ni ≠ qi) return ni
05 nmin = minargni nextL(Tni)
06 nmax = maxargni nextL(Tni)
07 while (nextL(Tni) < nextL(Tnmax))
08 advance(Tni)
09 if (nextL(Tni) < nextL(Tnmin)) return q
10 else return nmin

Procedure cleanStack(S, actL)
01 while ¬isEmpty(S) ∧ (top(S) < actL))
02 pop(S)

Figure 8: Algorithm TwigStack
```

Algorithm TwigStack operates in two phases. In the first phase (lines 1-11), some (but not all) solutions to individual query root-to-leaf paths are computed. In the second phase (line 12), these solutions are merge-joined to compute the answers to the query twig pattern.

The key difference between PathStack and the first phase of TwigStack is that before a node h_q from the stream T_q is pushed on its stack S_q, TwigStack (via its call to getNext) ensures that: (i) node h_q has a descendant h_qi in each of the streams T_qi, for qi ∈ children(q), and (ii) each of the nodes h_qi recursively satisfies the first property. Algorithm PathStack does not satisfy this property (and it does not need to do so to ensure (asymptotic) optimality for query path patterns). Thus, when the query twig pattern has only ancestor-descendant edges, each solution to each individual query root-to-leaf path is guaranteed to be merge-joinable with at least one solution to each of the other root-to-leaf paths. This ensures that no intermediate solution is larger than the final answer to the query twig pattern.

The second merge-join phase of Algorithm TwigStack is linear in the sum of its input (the solutions to individual root-to-leaf paths) and output (the answer to the query twig pattern) sizes, only when the inputs are in sorted order of the common prefixes of the different query root-to-leaf paths. This requires that the solutions to individual query paths be output in root-to-leaf order as well, which necessitates blocking; showSolutions (from Figure 5), which outputs solutions in sorted leaf-to-root order, cannot be used.

**Example 4.2.** Consider again the query of Example 4.1, which is the sub-twig rooted at the author node of the twig pattern in Figure 2(b), and the XML database tree in Figure 1. Before Algorithm TwigStack pushes an author node on the stack Sqauthor, it ensures that this author node has: (i) a descendant fn node in the stream Tm (which in turn has a descendant jane node in Tjane), and (ii) a descendant ln node in the stream Tm (which in turn has a descendant doe node in Tdoo). Thus, only one of the three author nodes (corresponding to the third author) from the XML data tree in Figure 1 is pushed on the stacks. Subsequent steps ensure that only one solution to each of the two paths of this query: author-fn-jane, and author-ln-doe, is computed. Finally, the merge-join phase computes the desired answer.

### 4.3 Analysis of TwigStack

In this section we discuss the correctness of algorithm TwigStack for processing twig queries, and then we analyze its complexity. Most of the proofs in this section are omitted for lack of space and can be found in [3].

**Definition 4.1.** Consider a twig query Q. For each node q ∈ subTreeNodes(Q) we define the head of q, denoted h_q, as the first element in T_q that participates in a solution for the sub-query rooted at q. We say that a node q has a minimal descendant extension if there is a solution for the sub-query rooted at q composed entirely of the head elements of subTreeNodes(q).

Proposition 3.1, based on Figure 6, is important for establishing the following lemma:

**Lemma 4.1.** Suppose that for an arbitrary node q in the twig query we have that getNext(q) = q_N. Then, the following properties hold:

1. q_N has a minimal descendant extension.
2. For each node q' ∈ subTreeNodes(q_N), the first element in T_{q'} is h_{q'}.
3. Either (a) \( q = q_N \) or (b) \( \text{parent}(q_N) \) does not have a minimal right extension because of \( q_N \) (and possibly other nodes). In other words, the solution rooted at \( p = \text{parent}(q_N) \) that uses \( h_p \) does not use \( h_q \) for node \( q \) but some other element whose \( L \) component is larger than that of \( h_q \).

Using the lemma above, we can prove [3] that when some node \( q_N \) is returned by \( \text{getNext} \), \( h_{q_N} \) is guaranteed to have a descendant extension in \( \text{subtreesNodes}(q_N) \). We can also prove [3] that any element in the ancestors of \( q_N \) that uses \( h_{q_N} \) in a descendant extension was returned by \( \text{getNext} \) before \( h_{q_N} \). Therefore we can maintain, for each node \( q \) in the query, the elements that are part of a solution involving other elements in the streams of \( \text{subtreesNodes}(q) \). Then, each time that \( q_N = \text{getNext}(q) \) is a leaf node, we output all solutions that use \( h_{q_N} \). It can be proved [3] that we can achieve that by maintaining one stack per node in the query.

**Theorem 4.1.** Given a query twig pattern \( q \) and an XML database \( D \), Algorithm \( \text{TwigStack} \) correctly returns all answers for \( q \) on \( D \).

**Proof.** [Sketch] In Algorithm \( \text{TwigStack} \), we repeatedly find \( \text{getNext}(q) \) for query \( q \) (line 2). Assume that \( \text{getNext}(q) = q_N \). Let \( A_{q_N} \) be the set of nodes in the query that are ancestors of \( q_N \). We know that \( \text{getNext} \) already returned all elements from the streams of nodes in \( A_{q_N} \) that are part of a solution that uses \( h_{q_N} \). If \( q \neq q_N \), in line 4 we pop from \( \text{parent}(q_N) \)'s stack all elements that are guaranteed not to participate in any new solution. After that, in line 5 we test whether \( h_{q_N} \) participates in a solution. We know that \( q_N \) has a descendant extension by Lemma 4.1, property 1. If \( q \neq q_N \) and \( \text{parent}(q_N) \)'s stack is empty, node \( q_N \) does not have an ancestor extension. Therefore it is guaranteed not to participate in any solution, so we advance \( q_N \) in line 11 and continue with the next iteration. Otherwise, node \( q_N \) has both ancestor and descendant extensions and therefore it participates in at least one solution. We then clean \( q_N \)'s stack (line 6) and push \( h_{q_N} \) to it (line 7). Finally, if \( q_N \) is a leaf node, we output the stored solutions from the stacks (lines 8-10).

While correctness holds for query twig patterns with both ancestor-descendant and parent-child edges, we can prove optimality only for the case where the query twig pattern has only ancestor-descendant edges. The intuition is simple: Since we push into the stacks only elements that have both a descendant and an ancestor extension, we are guaranteed that no element that does not participate in any solution is pushed into any stack. Therefore, the merge postprocessing step is optimal, and we have the following result.

**Theorem 4.2.** Consider a query twig pattern \( q \) with \( n \) nodes, and only ancestor-descendant edges, and an XML database \( D \). Algorithm \( \text{TwigStack} \) has worst-case I/O and CPU time complexities linear in the sum of sizes of the \( n \) input lists and the output list. Further, the worst-case space complexity of Algorithm \( \text{TwigStack} \) is the minimum of (i) the sum of sizes of the \( n \) input lists, and (ii) \( n \) times the maximum length of a root-to-leaf path in \( D \).

It is particularly important to note that, for the case of query twigs with ancestor-descendant edges, the worst-case time complexity of Algorithm \( \text{TwigStack} \) is independent of the sizes of solutions to any root-to-leaf path of the twig.

### 4.4 Suboptimality for Parent-Child Edges

Theorem 4.2 holds only for query twigs with ancestor-descendant edges. Unfortunately, in the case where the twig pattern contains a parent-child edge between two elements (e.g., see the query in Example 4.2), Algorithm \( \text{TwigStack} \) is no longer guaranteed to be I/O and CPU optimal. In particular, the algorithm might produce a solution for one root-to-leaf path that does not match with any solution in another root-to-leaf path.

Consider the query twig pattern with three nodes: \( A, B \) and \( C \), and parent-child edges between \( (A, B) \) and between \( (A, C) \). Let the XML data tree consist of node \( A_1 \), with children (in order) \( A_2, B_1, C_1 \), such that \( A_2 \) has children \( B_1, C_1 \). The three streams \( T_A, T_B \) and \( T_C \) have as their first elements \( A_1, B_1 \) and \( C_1 \) respectively. In this case, we cannot say if any of them participates in a solution without advancing other streams, and we cannot advance any stream before knowing if it participates in a solution. As a result, optimality can no longer be guaranteed.

### 4.5 Using XB-Trees

Algorithms PathStack and TwigStack need to process each node in the input lists to check whether or not it is part of an answer to the query (path or twig) pattern. When the input lists are very long, this may take a lot of time. In this section, we propose the use of a variant of B-trees, denoted XB-tree, on the input lists to speed up this processing.

#### 4.5.1 XB-Tree Description

As its name suggests, the XB-tree is a variant of the B-tree, designed for indexing the positional representation (DocId, LeftPos : RightPos, LevelNum) of elements in the XML tree. We describe the index structure when all nodes belong to the same XML document; the extension to multiple documents is straightforward.

The nodes in the leaf pages of the XB-tree are sorted by their LeftPos (\( L \) values); this is similar to the leaf pages of a B-tree on the L values. The difference between a B-tree and an XB-tree is in the data maintained at internal pages. Each node \( N \) in an internal page of the XB-tree consists of a bounding segment \([N_L, N_R]\) (where \( L \) denotes LeftPos and \( R \) denotes RightPos) and a pointer to its child page \( N, \text{page} \) (which contains nodes with bounding segments completely included in \([N_L, N_R]\)). The bounding segments of nodes in internal pages might partially overlap, but their \( L \) positions are in increasing order. Besides, each page \( P \) has a pointer to the parent page \( P, \text{parent} \) and the integer \( P, \text{parentIndex} \) which is the index of the node in \( P, \text{parent} \) that points back to \( P \). The construction and maintenance of an XB-tree is very similar to that of a B-tree, using the \( L \) value as the key; the difference is that the \( R \) values need to be propagated up the index structure.

#### 4.5.2 Using XB-Trees

We maintain a pointer \( act = (actPage, actIndex) \) to the actIndex-th node in page actPage of the XB-tree. There are two operations over the XB-tree that affect this pointer:

1. **advance**. If \( act = (actPage, actIndex) \) does not point to the last node in the current page, we simply advance \( actIndex \). Otherwise we replace \( act \) with the value \((actPage, parent, actPage, parentIndex)\) and recursively advance it.
2. drillDown. If act = (actPage, actIndex), actPage is not a leaf page, and N is the actIndex'th node in actPage, we replace act with (N.page, 0) so that it points to the first node in N.p.

Initially act = (rootPage, 0), pointing to the first node in the root page of the XB-tree. When act points to the last node in rootPage and we advance it, we finish the traversal.

We can modify the previous algorithms easily to use XB-trees. Algorithm TwigStackXB, in Figure 9, extends Algorithm TwigStack so that it uses XB-trees. The only changes are in the lines indicated by parentheses. The function isPlainValue returns true if the actual pointer in the XB-tree is pointing to a leaf node (actual value in the original stream). If we define isPlainValue(T) = true when T is not an XB-tree but a regular file, this algorithm reduces to the previous one.

![Algorithm TwigStackXB](image)

THEOREM 4.3. Given a query twig pattern q and an XML database D, Algorithm TwigStackXB correctly returns all answers for q on D. □

While we do not have any analytical results about the efficiency of Algorithm TwigStackXB, we show experimentally that it performs matching of query twig patterns in sub-linear time.

5. EXPERIMENTAL EVALUATION

In this section we present experimental results on the performance of the join algorithms introduced in Sections 3 and 4 using both real and synthetic data.

5.1 Experimental Setting

We implemented all XML join algorithms in C++ using the file system as the storage engine. All experiments were run on a 550MHz Pentium III processor with 768MB of main memory and a 2GB quota of disk space.

We used both synthetic and real-world data. The synthetic data sets are random trees generated using three parameters: depth, fan-out and number of different labels. For most of the experiments presented involving synthetic data sets, we generated full binary and ternary trees. Unless specified explicitly, the node labels in the trees were uniformly distributed. We tried other configurations (larger fanout and random depths in the tree) and also used the XMark [26] benchmarks. Those results are omitted for lack of space and can be found in [3].

The real data set is an “unfolded” fragment of the DBLP database. In the DBLP data set, each author is represented by a name, a homepage, and a list of papers. In turn, each paper contains a title, the conference where it was published, and a list of coauthors. We generated our unfolded fragment of DBLP as follows. We started with an arbitrary author and converted the corresponding information to XML format. For each paper, we replaced each coauthor name with the actual information for that author. We continued unfolding authors until we reached a previously traversed author, or a depth of 200 authors. The resulting XML data set has depth 805 and around 3 million nodes, representing 93,536 different papers from 36,900 unique authors.

5.2 Binary Structural Joins vs PathStack

In this experiment we compare our holistic PathStack algorithm against strategies that use a combination of binary structural joins [1]. For this purpose, we used a synthetic data set consisting of 1,000,000 nodes and six different labels: A1, A2, ..., A6. 2 We issued the path query \(A1/A2/.../A6\) and evaluated it using PathStack. Then, we evaluated all binary join strategies resulting from applying all possible join orders. Figure 10 shows the execution time of all join strategies, where each strategy is represented with a bar. We also show with a solid line the execution time of PathStack, and with a dotted line the time it takes to do a sequential scan over the input data (labeled SS).

For this query, PathStack took 2.53s, slightly more than the 1.87s taken by the sequential scan over the input data. In contrast, the strategies based on binary structural joins ranged from 16.1s to 53.07s. Our first conclusion is that optimization plays an important role for binary structural joins, since a bad join ordering can result in a plan that is more than three times worse than the best plan. Our second conclusion is that the holistic strategy is superior to the approach of using binary structural joins for arbitrary join orders; in this case, it results in more than a six-fold improvement in execution time over the best strategy that uses binary structural joins.

2Note that the actual XML data can contain many more labels, but that does not affect our techniques since we only access the indexes of labels present in the query.
5.3 Paths: PathStack vs PathMPMJ

In this section we study the efficiency of the different holistic path join algorithms of Section 3. We first compare the two versions of PathMPMJ. We used a 64K synthetic data set with labels $A_1, \ldots, A_{10}$, and issue path queries of different lengths. Figure 11 shows the execution times of both techniques, as well as the time taken for a sequential scan over the input data. PathMPMJNaive is much slower compared to the optimized PathMPMJ (generally over an order of magnitude). The reason is that PathMPMJNaive is too conservative when backtracking and reads several times unnecessary portions of the data (in our experiments, as much as 15 times more nodes than PathMPMJ). Since the performance of PathMPMJNaive degrades considerably with the size of the data set and the length of the input query, we do not consider this strategy for the remainder of this paper.

![Figure 11: PathMPMJ versus PathMPMJNaive](image)

We now compare PathStack against PathMPMJ. In Figure 12 we show the execution time and the number of nodes read from disk for path queries of different lengths and a synthetic data set of 1,000,000 nodes and 10 different labels. Clearly, PathStack results in considerably better performance than PathMPMJ, and this difference increases with longer path queries. This is explained by the fact that PathStack makes a single pass over the input data, while PathMPMJ needs to backtrack and read again large portions of data. For instance, for a path query of length 10, PathMPMJ reads the equivalent of five times the size of the original data, as seen in Figure 12(b). In Figure 12(a), for path queries of length two, the execution time of PathStack is considerably slower than that of the sequential scan, and closer to PathMPMJ. This behavior is due to the fact that for the path query of length two, the number of solutions is rather large (more than 100,000), so most of the execution time is used in processing these solutions and writing them back to disk. For longer path queries, the number of solutions is considerably smaller, and the execution of PathStack is closer to a sequential scan and much more efficient than PathMPMJ.

![Figure 10: Holistic and binary joins for path queries](image)

Figure 13 shows the execution time and number of values read for two simple path queries over the unfolded DBLP data set (note the logarithmic scale on the Y axis). Due to the specific nesting properties between nodes in this data set, the PathMPMJ algorithm spends much time backtracking and reads several times the same values. For instance, for the path query of length three in Figure 13, PathMPMJ reads two orders of magnitude more elements than PathStack.

5.4 Twigs: PathStack vs TwigStack

We now focus on twig queries, and compare TwigStack against the naive application of PathStack to each branch in the tree followed by a merge step. As shown in Section 4, TwigStack is optimal for ancestor/descendant relationships, but it is provably suboptimal for parent/child relationships. In this section, we analyze these two cases separately.

![Figure 14: Twig queries used in the experiments](image)

5.4.1 Ancestor-Descendant Relationships

We first used the query shown in Figure 14(a) over different synthetically generated data sets. Each data set was generated as a full ternary tree. The first subtree of the root node contained only nodes labeled $A_1, A_2, A_3$ and $A_4$. The second subtree contained nodes labeled $A_1, A_5, A_6$ and $A_7$. Finally, the third subtree contained all possible nodes. Clearly, there are many partial solutions in the first two subtrees but those do not produce any complete solution. Only the third subtree contains actual solutions. We varied the size of the third subtree relative to the sizes of the first two from 8% to 24% (beyond that point the number of solutions became too large). Figures 15(a-b) show the execution time of PathStack and TwigStack and the number of partial solutions each algorithm produces before the merging step. The consistent gap between TwigStack and PathStack results from the latter generating all partial solutions from the first two subtrees which are later discarded in the merge step ($A_1//A_2//A_3//A_4$) vs ($A_1//A_5//A_6//A_7$). As seen in Figure 15(b), the number of partial solutions produced by PathStack is several orders of magnitude larger than that of the TwigStack algorithm. The number of solutions to the query computed by both algorithms is, of course, the same.

We then used the twig query of Figure 14(b) and generated different synthetic data sets in the following way. As before, each data set is a full ternary tree. The first subtree does not contain any nodes labeled $A_2$ or $A_3$. The second subtree does not contain any $A_1$ or $A_7$ nodes. Finally, the third subtree does not contain any $A_5$ or $A_6$ nodes. Therefore, there is not even a single solution for the query twig, although each subtree contains a large number of partial solutions. The main difference with the previous experiment is that we need to materialize an intermediate join result before getting the final answer. Therefore, there is no ex-
execution strategy using PathStack that avoids materializing a big intermediate result. Figure 15(c) shows the execution time for PathStack and TwigStack for different data sizes (note the logarithmic scale). For the last data set (with 243K nodes), PathStack could not finish, since the intermediate result filled all the available space on disk (2GB).

5.4.2 Parent-Child Relationships
As explained in Section 4, TwigStack is not optimal for parent/child relationships. We now show that even in this case, TwigStack performs much better than PathStack. For that purpose, we modified the queries in Figures 14(a-b) adding the following constraint: all ancestor-descendant relationships are connected by a path of length between one and three (this can be checked by comparing the LevelNum values of the positional representations). Figure 16 shows the results for these experiments. Even in the presence of parent-child constraints, TwigStack is considerably more efficient than PathStack. In particular, Figure 16(b) shows that the number of partial solutions produced by TwigStack (though not minimal) is small. The non-minimality is evident from the observation that the number of partial solutions produced by TwigStack is sometimes larger than the number of total solutions to the query twig.

We also evaluated the query of Figure 14(c) over the unfolded DBLP data set. This query asks for authors with papers published in the year 2000, who have some coauthor with a paper published in 1990, who in turn has some coauthor with a paper in 1980. We vary the allowed depth in the relationship COAUTHOR // PAPER, i.e., the number of coauthors and papers we can traverse from a given author, from 0 (no solutions) to 37. The results are shown in Figure 17. We can see that for these queries, TwigStack is again more efficient than PathStack.

5.5 Sub-Linearity: Using XB-Trees
We now study the advantages of using XB-trees to process path and twig queries. In particular, we show that the number of nodes that need to be read from the XB-tree (counting both leaf and internal nodes) is significantly smaller than the size of the input, which causes sub-linear behavior in our algorithm. As we will see, XB-trees with small node capacities can effectively skip many leaf nodes, but the number of internal nodes traversed is large. On the other hand, for large node capacities there are fewer internal node accesses, but XB-trees cannot skip many leaf nodes because they could miss some solutions. We experimentally obtained the best results when using node capacities ranging from 4 to 64.

For the experiments in this section, we evaluated different queries using PathStack and TwigStack, with and without XB-trees. We varied the node capacity of the XB-trees between 2 and 1,024 values per index node. Figure 18(a) shows the number of values read in the XB-tree (separated into internal and leaf accesses) for the data set and path queries used in Section 5.3. Figure 18(b) shows the results when using the twig query of Figure 14(a), and the data sets of Section 5.4. Finally, Figure 18(c) shows the results for the twig query in Figure 14(c) over the unfolded DBLP data set.

In general, the total number of nodes visited in the XB-Tree is consistently smaller than the input data size for a wide range of node capacities. For the synthetic data set, we obtained better results for complex queries. In those situations, XB-trees can prune significant portions of the input data. In contrast, for simpler queries, we need to go deep in the XB-tree nodes, in many cases down to the leaves, since there are many solutions dispersed throughout the whole data set. For data sets with solutions concentrated around certain portions of the data, the impact of XB-trees is more significant, since many internal nodes can be skipped.
6. RELATED WORK

Join processing is central to database implementation [13]. For inequality join conditions, band join [9] algorithms are applicable when there exists a fixed arithmetic difference between the values of join attributes. Such algorithms are not applicable in our domain as there is no notion of fixed arithmetic difference. In the context of spatial and multimedia databases, the problem of computing joins between pairs of spatial entities has been considered, where commonly the predicate of interest is overlap between spatial entities [14, 20, 15] in multiple dimensions. The techniques developed in this paper are related to such join operations. However, the predicates considered as well as the techniques we develop are special to the nature of our structural join problem.

In the context of semi-structured and XML databases, query evaluation and optimization has attracted a lot of research attention. In particular, work done in the Lore DBMS [21, 16, 17], and the Niagara system [19], has considered various aspects of query processing on such data. XML data and various issues in their storage as well as query processing using relational database systems have recently been considered in [12, 24, 23, 4, 10, 11]. In [12, 24, 11], the mapping of XML data to a number of relations was considered along with translation of a subset of XML queries to relational queries. In subsequent work [23, 4, 10], the authors considered the problem of publishing XML documents from relational databases. Our holistic join strategy for query twig patterns can leverage these previous techniques.

The representation of positions of XML elements (DocId, StartPos : EndPos, LevelNum) is essentially that of Consens and Milo, who considered a fragment of the PAT text searching operators for indexing text databases [6, 7], and discussed optimization techniques for the algebra. This representation was used to compute containment relationships between “text regions” in the text databases. The focus of that work was on theoretical issues, without elaborating on efficient algorithms for computing these relationships.

Finally, the recent works of Zhang et al. [27] and Al-Khalifa et al. [1] are closely related to ours. They proposed binary structural join algorithms as primitives for matching query twig patterns. Our Algorithm PathMPM3 is a generalization of the MPMGJN algorithm of [27] to match query paths, and Algorithms PathStack and TwigStack are generalizations of the stack-based algorithms of [1] to match query paths and query twig patterns, respectively.

7. CONCLUSION

In this paper we developed holistic join algorithms for matching XML query twig patterns, a core operation central to much of XML query processing, both for native XML query processor implementations and for relational XML query processors. In particular, Algorithm TwigStack was shown to be I/O and CPU optimal for a large class of query twig patterns, and practically efficient.

There is more to efficient XML query processing than is within the scope of this paper. We have initiated efforts to address some of these issues. One such issue involves the use of axes like following-sibling in XPath expressions, in addition to the more commonly used child and descendant axes (used in this paper to specify twig patterns). How can we compute answers to XPath expressions with such axes? Another issue involves the piecing together of holistic twig joins with value-based joins (including links across documents) to build effective query plans.
8. REFERENCES


