SUBTREE-ELIMINATION ALGORITHMS IN DEDUCTIVE DATABASES

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DOCTOR OF PHILOSOPHY

By
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January 1991
I certify that I have read this dissertation and that in my opinion it is fully adequate, in scope and in quality, as a dissertation for the degree of Doctor of Philosophy.

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Abstract

A deductive database consists of a set of stored facts, and a set of logical rules (typically, recursive Horn clauses) that are used to manipulate these facts. A number of optimizations in such databases involve the transformation of sets of logical rules (programs) to simpler, more efficiently evaluable programs. We consider a class of optimizations in which the transformation is a simple syntactic restriction on the form of the original program, and in which the correctness of the transformation indicates the existence of a normal form for the proof trees generated by the program. For example, the existence of basis-linearizability in a nonlinear program indicates that the program is inherently linear, and permits the use of special-purpose query evaluators for linear recursions. The canonical example of a basis-linearizable program is the program that computes the transitive closure of a binary relation; the corresponding normal form for the proof trees is that of right-linearity. Similarly, if a program is sequencable, then it is conducive to a pipelined evaluation. In addition, the existence of k-boundedness in a program permits the elimination of recursion overhead in evaluating the program. We investigate the complexity of detecting such optimization opportunities, and provide correct (but not always complete) algorithms for this purpose.

Each of the problems that are mentioned above may be described in terms of the subtree-elimination problem, which we define and analyze. We relate the detection of basis-linearizability, sequencability and 1-boundedness to the complexity classes \( \mathcal{NC} \), \( \mathcal{P} \) and \( \mathcal{NP} \), and show that the first two of these problems are, in general, undecidable. The techniques used in our analysis provide a complete description of the complexity of deciding the equivalence of conjunctive queries (single-rule, nonrecursive programs), and tight undecidability results for the detection of program equivalence.
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Chapter 1

Subtree eliminations

1.1 Introduction

A deductive database system represents the use of predicate logic as a programming language for database systems. One may think of this programming language as the extension of relational algebra ([11]) through the use of recursion. This extension provides a strict increase in the expressive power of the database query language ([2]), but makes query evaluation potentially more expensive; that is, a general-purpose query evaluator is likely to be inefficient when applied to a “simple” program. Many of the optimization strategies that have been incorporated into the experimental deductive database systems currently under construction ([23, 22, 21], for example) are based on the recognition of programs on which limited yet efficient query evaluators may be used. In this dissertation, we provide an alternative optimization strategy: the replacement of programs by semantically equivalent but syntactically simpler programs, such that efficient algorithms may be used with respect to the transformed programs. The optimizations that we investigate are based on the detection of “normal forms” for the proof trees generated by the program in question. The problems that we address are decision problems; that is, given a program and a normal form, we ask whether the normal form applies to the given program. In this thesis, we present a uniform framework for the description of normal forms, a mechanism for the construction of conditions that are sufficient (but not always necessary) for the detection of each such normal form, and complexity results for the detection of three common normal forms. Our results have implications to the complexity of deciding equivalence among recursive and nonrecursive programs.

1.2 Deductive databases

For our purposes, a deductive database system\(^1\) consists of a finite set of stored ground facts (the extensional database or EDB), and a finite set of rules (Horn clauses) that are used to manipulate the EDB. A set of rules is termed a program. The program comprises

\(^1\)See [35, 36] for a comprehensive treatment.
the intensional database or IDB. Relations are defined in terms of predicates; that is, for any predicate \( p \), the relation for \( p \) is the set of tuples \( \bar{a} \) such that \( p(\bar{a}) \) is true. In this report, we will use the terms “predicate” and “relation” interchangeably. A predicate that corresponds to an EDB relation is termed an extensional or EDB predicate, and a predicate that is defined by a rule is termed intensional or IDB. We assume without loss of generality that no predicate is both intensional and extensional.

1.2.1 Syntax

Programs will be written using Prolog syntax. A rule is of the form

\[ p(\bar{X}) \leftarrow b_1(\bar{Y}_1), \ldots, b_n(\bar{Y}_n). \]

The “\( \leftarrow \)”, represents the “if” operator, and a comma represents the “and” operator. The atomic formula (atom) \( p(\bar{X}) \) is termed the head of the rule, and the conjunction on the right of the “if” symbol is termed the body of the rule. Each atomic formula in the body is termed a subgoal. The rule defines the predicate \( p \), and \( p \) is hence intensional. The variables appearing in the head of the rule are termed distinguished, and all other variables are termed nondistinguished. Distinguished variables are universally quantified over the rule, and nondistinguished variables are implicitly existentially quantified in the body of the rule. That is, if \( W_1, \ldots, W_k \) are the distinguished variables in the rule and \( Z_1, \ldots, Z_m \) are the nondistinguished variables, then the rule represents the formula

\[ \forall W_1, \ldots, W_k(\exists Z_1, \ldots, Z_m b_1(\bar{Y}_1) \land \ldots \land b_n(\bar{Y}_n)) \supset p(\bar{X}) \]

Example 1.1 The following program \( P \) consists of the two rules \( r_1 \) and \( r_2 \), and defines the intensional predicate \( p \). We assume that \( b \) is an extensional predicate.

\[
\begin{align*}
r_1 & : p(X,Y) \leftarrow p(X,U), p(U,Y). \\
r_2 & : p(X,Y) \leftarrow b(X,Y).
\end{align*}
\]

\( p(X,Y) \) is the head of each rule. The conjunction \( p(X,U), p(U,Y) \) is the body of rule \( r_1 \), and \( b(X,Y) \) is the body of rule \( r_2 \). The meaning of rule \( r_1 \) is: for all \( X \) and \( Y \), \( p(X,Y) \) is true if for some \( U \), \( p(X,U) \) and \( p(U,Y) \) are both true; that is, \( r_1 \) represents the formula

\[ \forall X,Y ((\exists U p(X,U) \land p(U,Y)) \supset p(X,Y)) \]

\( \Box \)

If a predicate \( p \) appears in the head of a rule and \( q \) appears in the body of the rule, then \( p \) is said to depend on \( q \). A predicate \( p \) is termed recursive if \( p \) depends transitively upon itself, and a rule is termed recursive if a predicate \( q \) appearing in the body of the rule depends transitively upon the predicate \( p \) appearing in the head of the rule. All other predicates and rules are termed nonrecursive. A program is termed recursive if any rule is recursive, and nonrecursive otherwise. In the example above, the predicate \( p \) and rule \( r_1 \) are
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recursive (so the program is recursive), and the predicate \( b \) and the rule \( r_2 \) are nonrecursive. A nonrecursive rule is also termed a basis or initialisation rule. A rule is said to be linear if at most one subgoal in the rule is intensional, linear recursive if exactly one subgoal in the body is recursive with the head of the rule, and bilinear if exactly two subgoals are recursive with the head. Rule \( r_1 \) in Example 1.1 is bilinear, and rule \( r_2 \) is linear. Rule \( r_1 \) in Example 1.2 below is also linear. A program is termed linear if every rule in the program is linear, and linear recursive if every rule is linear recursive or nonrecursive.

1.2.2 Semantics

The accepted semantics for Horn-clause programs consists of the unique minimum Herbrand model or least fixed point ([38]). The idea is that we may think of the “application” of a rule as the bottom-up (forward-chaining) use of the Horn clause represented by the rule. Then, the relation for each intensional predicate is the smallest relation that satisfies each of the rules in the program; that is, the smallest relation that is closed under the application of the rules in the program as described above. Alternatively, we may generate the intensional relations by initialising each intensional predicate to be empty, adding all facts generated by basis rules and then applying the rules in a bottom-up (forward-chaining) manner until no new facts are generated. The first of these views, that of the relation for a predicate being the smallest relation satisfying the initialisation rules and closed under the recursive rules, is integral to the approach taken by this report. Since programs may be viewed as generalised closures, we have focussed our attention on optimizations that may be performed on programs that compute such common relations as the symmetric and transitive closures of a binary relation.

Example 1.2 The program

\[
\begin{align*}
\text{r}_1 & : p(X,Y) :- p(Y,X). \\
\text{r}_2 & : p(X,Y) :- b(X,Y).
\end{align*}
\]

computes the symmetric closure of the basis predicate \( b \). The recursive rule \( r_1 \) states that \( p \) is symmetric, the basis rule insists that \( b \subseteq p \) and minimality is imposed by the semantics of the program. Note that the program is linear (and linear recursive).

Example 1.3 We repeat here the program of Example 1.1.

\[
\begin{align*}
\text{r}_1 & : p(X,Y) :- p(X,U), p(U,Y). \\
\text{r}_2 & : p(X,Y) :- b(X,Y).
\end{align*}
\]

The first rule says that \( p \) is transitive and the second requires inclusion; thus, the program computes the transitive closure of \( b \). If we think of \( b \) as the “parent” relation, then this program computes the “ancestor” relation. This program is important in that there is no nonrecursive program computing the transitive closure of \( b \) ([2]), justifying our earlier claim that the addition of recursion to relational algebra increases the expressive power of the language.
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Figure 1.1: Proof tree.

Example 1.4 The program

\[ r_1 : p(X,Y) \leftarrow p(X,U), p(U,Y). \]
\[ r_2 : p(X,Y) \leftarrow p(Y,X). \]
\[ r_3 : p(X,Y) \leftarrow b(X,Y). \]

computes the symmetric, transitive closure of \( b \). □

A rule is said to be safe if for every rule, every distinguished variable appears in the rule body. A program is said to be Datalog if it is safe and function-free; the programs of Examples 1.1 – 1.4 are all Datalog programs. In this report, we will for the most part restrict our attention to Datalog programs. Such programs are commonly used because they are powerful enough for the description of many real-life problems, but always generate finite relations from a finite database (because the Herbrand universe is finite).

1.2.3 Proof trees

For the purposes of this report, it will be convenient to view the relation generated by a program in another way. We say that an atom is ground if no variable appears in it. A rule is termed instantiated if every atom in the rule is replaced with a ground atom with which it unifies, such that the implied unifications are consistent. A proof tree is a tree in which the vertices are ground atoms such that

1. The leaves of the tree are atoms appearing in the EDB; and

2. If an interior node \( a \) has the children \( b_1, \ldots, b_n \), then there is an instantiated rule in the program whose head is \( a \) and whose body is \( b_1, \ldots, b_n \).

If \( c \) is the root of a proof tree, then we say that the proof tree establishes the fact \( c \).

Example 1.5 Assume that the relation for \( b \) in Example 1.3 is \( \{ b(joe, bob), b(bob, ann) \} \). The proof tree of Figure 1.1 establishes \( p(joe, ann) \). □

Now, given any program and database, the relation produced by the program for some predicate \( p \) from this database is precisely the set of facts \( p(\bar{a}) \) that are established by proof trees.
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1.2.4 Optimizations

In typical database applications, the extensional database is much larger than the size of a program that manipulates it. Hence, the preferred optimization techniques are data-independent. Two programs are said to be equivalent if they generate the same relations for every predicate from every extensional database; the optimizations that we consider are based on program equivalence, and are hence independent of any particular database. A variety of efficient query evaluation techniques have been proposed (see [7],[36] for overviews) and these techniques vary in application domain and efficiency. In this report, we investigate opportunities for transforming programs into equivalent programs for which efficient query evaluation techniques become available. The following examples illustrate optimizations that may be performed on the closure programs of the preceding examples; these optimizations will serve as canonical examples for three optimization problems that we will consider throughout this dissertation.

Example 1.6 Consider the symmetric closure program (say, Δ) of Example 1.2. We may think of the basis relation b as the edge relation in a directed graph; that is, b(u, v) is true precisely when there is an edge u \rightarrow v in the graph. Then, the symmetric closure of the graph may be obtained by adding the edge v \rightarrow u to the graph, where u \rightarrow v is any edge in the original graph. That is, the program of Example 1.2 is equivalent to the following nonrecursive program Q.

r_1' : p(X, Y) :- b(Y, X).

r_2' : p(X, Y) :- b(X, Y).

The program Q is obtained from the program Δ by replacing the recursive subgoal p(Y, X) in the body of rule r_1 by the nonrecursive subgoal b(Y, X). The gains of such a replacement stem from the elimination of recursion overhead in evaluating the program with respect to a database; that is, we may use a query evaluator that is specific to nonrecursive programs.

Example 1.7 Consider the bilinear program Δ of Example 1.3, computing the transitive closure of the basis predicate b. It is a well-known fact that Δ is equivalent to the following linear recursive program Q.

r_1' : p(X, Y) :- b(X, U), p(U, Y).

r_2' : p(X, Y) :- b(X, Y).

The program Q is obtained from Δ by replacing the first recursive atom in the body of r_1, p(X, U), with the nonrecursive atom b(X, U). An intuitive understanding of the equivalence is as follows. Assume that b stands for the “parent” relation, and that p is the “ancestor” relation, as we have previously discussed. Then, the recursive rule in Δ says that “Y is X’s ancestor if X has some ancestor U whose ancestor is Y”, and the recursive rule in Q says that “Y is X’s ancestor if X has some parent U whose ancestor is Y.” The gains of replacing
\( \mathcal{P} \) by \( \mathcal{Q} \) is that fast query evaluators that are specific to linear recursions become available for application to the linear program \( \mathcal{Q} \). Specifically, assume that we wish to answer the query \( p(\text{joe}, Y) \); that is, "who are the ancestors of \( \text{joe} \". Then, the "magic sets" technique ([36]) applied to \( \mathcal{P} \) generates the entire \( p \) relation, and takes time that is quadratic in the size of \( b \) (in the worst case); however, "right-linear evaluation" ([36]) computes the answer in time that is linear in the size of \( b \).\(^2\) A proof of this claim is contained in [36]. □

Example 1.8 Finally, consider the program \( \mathcal{P} \) of Example 1.4, computing the symmetric, transitive closure of \( b \). Again, we may think of \( b \) as the edge relation in a directed graph: then, \( p(u, v) \) is true iff there is a path from \( u \) to \( v \) in the graph, obtained by following edges in a forward or backward manner (in a mixed fashion). A little thought should suffice to convince the reader that \( p \) may be computed by

1. First, computing the symmetric closure of the graph.
2. Then, computing the transitive closure of the result.

That is, the program \( \mathcal{P} \) is equivalent to the following program, where the new predicate \( q \) is the symmetric closure of \( b \).

\[
\begin{align*}
\text{r}_1 & : p(X, Y) := p(X, U), p(U, Y). \\
\text{s}_1 & : p(X, Y) := q(X, Y). \\
\text{r}_2 & : q(X, Y) := q(Y, X). \\
\text{r}_3 & : q(X, Y) := b(X, Y).
\end{align*}
\]

Now, since \( p \) is defined only by rules \( r_1 \) and \( s_1 \), and since \( q \) is defined by rules \( r_2 \) and \( r_3 \), we may apply the optimizations of the previous examples to create the equivalent program

\[
\begin{align*}
\text{r}_1 & : p(X, Y) := q(X, U), p(U, Y). \\
\text{s}_1 & : p(X, Y) := q(X, Y). \\
\text{r}_2 & : q(X, Y) := b(Y, X). \\
\text{r}_3 & : q(X, Y) := b(X, Y).
\end{align*}
\]

Finally, since \( q \) is now defined only by the nonrecursive rules \( r_2 \) and \( r_3 \), we may substitute these rules for the predicate \( q \) to obtain the linear recursive program

\[
\begin{align*}
\text{r}_2 & : p(X, Y) := b(X, U), p(U, Y). \\
\text{r}_3 & : p(X, Y) := b(U, X), p(U, Y). \\
\text{s}_1 & : p(X, Y) := b(Y, X). \\
\text{s}_2 & : p(X, Y) := b(X, Y).
\end{align*}
\]

The gains of such a replacement are again obtained from the use of a query evaluator that is specific to linear recursions. That is, magic sets takes quadratic time (in the size of \( b \)) to evaluate \( p(\text{joe}, Y) \) with respect to the original program, but right-linear evaluation takes linear time when applied to the linear recursive program above. □

---

\(^2\)Right-linear evaluation may be extended to the nonlinear transitive-closure program, but does not extend to arbitrary nonlinear programs.
1.3 Top-down expansions

Recall that the facts generated by a program from a database are precisely those facts that are established by proof trees. A top-down expansion is obtained by lifting the arguments of a piece of a proof tree to variables; that is, the top-down expansion specifies the relation between the leaves and the root of a proof-tree piece. Alternatively, one may think of a top-down expansion as a state in a top-down query evaluation.

Definition 1.1 Consider a (not necessarily function-free) program $\mathcal{P}$ with rules $r_1, \ldots, r_n$, and let $p$ be any intensional predicate defined by $\mathcal{P}$. Assume that $p$ has arity $k$. A top-down expansion of $p$ by $\mathcal{P}$ is defined inductively, as follows.

1. The tree with root $p(X_1, \ldots, X_k)$ and leaf $p(X_1, \ldots, X_k)$, where $X_1, \ldots, X_k$ are distinct variables, is a top-down expansion of $p$ by $\mathcal{P}$. By convention, this top-down expansion is said to have depth 0.

2. Let $r_1$ be a rule

$$ h := B. $$

in which the rule head $h$ has principal functor $p$. The tree $T$ with root $h$ and leaves $B$ (in which the order of subgoals in $B$ is preserved) is a top-down expansion of $p$ by $\mathcal{P}$. The depth of this top-down expansion is 1.

3. Consider any top-down expansion $T$ of $p$. Assume that $q(\bar{Z})$ is the $i$th leaf in $T$. Let $R$ be a top-down expansion of depth 1, in which all variables have been renamed to make them distinct from the variables in $T$, and let $\tau$ be the mgu of $q(\bar{Z})$ with the root of $R$. Let $S$ be the expansion $R$, in which each variable $Y$ appearing in the root of $R$ is replaced by $\tau(Y)$ throughout $R$. Replace every variable $Y$ in $T$ that appears in the root of $S$ by $\tau(Y)$, and replace the $i$th leaf in the result by the subtree $S$. The result is a top-down expansion of $p$ by $\mathcal{P}$; the depth of the expansion is the depth of the resulting tree.

Recall that a variable appearing in a rule is distinguished if it appears in the head of the rule, and nondistinguished otherwise. The reason that nondistinguished variables are renamed at each stage of the expansion is that these variables are implicitly existentially quantified in the body of the rule. Distinguished variables are renamed only to make them distinct from variables (perhaps nondistinguished) in the parent tree.

Note that the definition of a top-down expansion requires that subgoals in a rule are written in a way that preserves the order of the subgoals in every rule. Throughout this report, we will assume that both proof trees and top-down expansions are written in a way that preserves the left-to-right order of the subgoals in every rule\textsuperscript{3}.

\textsuperscript{3}This assumption refers to the writing down of proof trees, and has no bearing on the order in which subgoals are evaluated by a query evaluator.
CHAPTER 1. SUBTREE ELIMINATIONS

Figure 1.2: Top-down expansion.

Note also that the construction of a top-down expansion is polynomial in the size of the expansion (since unification is polynomial [36]). For Datalog programs, this procedure may easily be performed in LOGSPACE.

Example 1.9 Consider the program of Example 1.3. Recall that this program computes $p$ as the transitive closure of the basis predicate $b$: that is, we may think of $b$ as the parent relation and $p$ as the ancestor relation. The trees of Figure 1.2 are top-down expansions of $p(X,Y)$ using the rules in this program.

Note that the variable $U$ is renamed at depth 2 in the tree of Figure 1.2 (b). Intuitively, the top-down expansion states that $Y$ is an ancestor of $X$ if $X$ has some parent $U'$, $U'$ has some parent $U$ and $U$ has the parent $Y$. That is, $Y$ is $X$'s great-grandparent in this case.

We will also speak of a top-down expansion of an atom $p(\bar{X})$; that is, we will specify an atom to be unified with the root of the tree. Let $T$ be a top-down expansion and $p(\bar{X})$ an atom. Assume that this atom unifies with the root of $T$ under the most general unifier $\tau$. Then, the expression $\tau(T)$ represents the expansion obtained by replacing every variable $Y$ in $T$ that appears in the root by $\tau(Y)$. We say that $\tau(T)$ is a top-down expansion of $p(\bar{X})$ by $\mathcal{P}$.

Example 1.10 Consider the program

$$r_1: p(f(X)) :- q(X, U).$$
$$r_2: q(X, X) :- b(X).$$

Figure 1.3 (a) shows a top-down expansion of $p$ with depth 2, and Figure 1.3 (b) exhibits a top-down expansion of $p(f(f(A)))$.

In Figure 1.3 (a), the variable $X$ in rule $r_2$ has been renamed to the variable $Y$. □
1.3. TOP-DOWN EXPANSIONS

\[
\begin{align*}
p(f(Y)) & \quad p(f(f(A))) \\
\downarrow & \quad \downarrow \\
q(Y,Y) & \quad q(f(A), f(A)) \\
\downarrow & \\
b(Y) & \quad b(f(A)) \\
(a) & \\
(b)
\end{align*}
\]

Figure 1.3: Top-down expansion with specified root.

1.3.1 Conjunctive queries

A single-rule, nonrecursive program is called a *conjunctive query* ([10]). That is, a conjunctive query is of the form

\[
p(\overline{X}) : - B.
\]

where \( B \) is a conjunction of atomic formulae all of whose principal functors are EDB predicate names. Each top-down expansion with EDB predicates at the leaves defines a conjunctive query in a natural way; that is, if \( T \) is such a top-down expansion, then the corresponding conjunctive query is

\[
h : - B.
\]

where \( h \) is the root of \( T \), and where \( B \) is the conjunction of the fringe of \( T \).

**Example 1.11** The top-down expansion of Figure 1.2 (b) represents the conjunctive query

\[
p(X,Y) : - b(X, U'), b(U', U), b(U, Y).
\]

\[
\square
\]

We will also speak of top-down expansions with IDB predicates at the leaves as conjunctive queries. The intention, in this case, is that the conjunctive query is applied nonrecursively.

**Example 1.12** The top-down expansion of Figure 1.2 (a) represents the conjunctive query

\[
p(X,Y) : - p(X, U), p(U, Y).
\]

The idea is that this conjunctive query represents all ways in which two \( p \)-facts (presumably generated by the program) may be combined to produce a new \( p \)-fact using the top-down expansion. \( \square \)

\[\text{\footnotesize{This conjunctive query is often written \( \{XY ', b(X, U'), b(U', U), b(U, Y)\}\); however, we will use the notation illustrated above for the purposes of uniformity.}}\]
We may now view a program as the (possibly infinite) union of the conjunctive queries that it generates, such that the bodies of the conjunctive queries are occupied by only extensional predicates. In fact, we will also speak of an arbitrary union of conjunctive queries as a "program".

1.3.2 Containment and equivalence

Let $\mathcal{P}$ and $\mathcal{Q}$ be programs defining the predicate $p$ (perhaps among other IDB predicates). We say that $\mathcal{P}$ is contained in $\mathcal{Q}$ with respect to $p$ (written $\mathcal{P} \subseteq_p \mathcal{Q}$, or just $\mathcal{P} \subseteq \mathcal{Q}$ if $p$ is understood) iff for every database, the relation for $p$ that is produced by $\mathcal{P}$ is a subset of that produced by $\mathcal{Q}$. The programs $\mathcal{P}$ and $\mathcal{Q}$ are said to be equivalent with respect to $p$ (written $\mathcal{P} \equiv_p \mathcal{Q}$) iff $\mathcal{P} \subseteq \mathcal{Q}$ and $\mathcal{Q} \subseteq \mathcal{P}$; as before, we omit all references to the predicate $p$ if this predicate is understood from the context.

Since a conjunctive query is a single-rule, nonrecursive program, these definitions apply equally to such queries. However, for the purpose of deciding containment among conjunctive queries, we need make no reference to the predicates being defined by the queries because each conjunctive query defines a unique predicate. That is, if the heads of two conjunctive queries are labelled by two different predicates, then there is no containment; otherwise, the containment is defined with respect to the common predicate defined by the queries.

Chandra and Merlin ([10]) have proposed a syntactic test for the containment of one conjunctive query in another. Consider the conjunctive queries

\[ C_1 : p(\bar{X}) : - B_1, \]
\[ C_2 : q(\bar{Y}) : - B_2. \]

where $B_1$ and $B_2$ are conjunctions. Let $f$ be a function on the variables in $C_2$. We extend $f$ to all symbols in $C_2$ by requiring $f$ to be the identity on constants. Finally, we may extend $f$ to terms (and atomic formulae) in the obvious way; that is, we define $f(q(d_1, \ldots, d_k))$ to be $f(q)(f(d_1), \ldots, f(d_k))$. We say that $f$ is a containment mapping from $C_2$ into $C_1$ (written $f : C_2 \rightarrow C_1$) iff the following are true.

1. $f(q(\bar{Y})) = p(\bar{X})$.
2. For each atom $t$ in $B_1$, the atom $f(t)$ appears in $B_1$.

For any atom in $C_2$, $f(t)$ is termed the destination of $t$ under $f$.

The value of containment mappings is illustrated in the following theorem of Chandra and Merlin ([10]).

**Theorem 1.1** Containment mapping theorem (Chandra and Merlin).
For any conjunctive queries $C_1$ and $C_2$, $C_1 \subseteq C_2$ iff there is a containment mapping $f : C_2 \rightarrow C_1$. □

In Chapter 2 of this dissertation, we will present a dual to the containment mapping, the conjunct mapping, which is also a necessary and sufficient condition for the detection...
of conjunctive query containment. The value of the concept of conjunct mappings is that the concept permits of a complete description of the complexity of deciding containment among conjunctive queries; the description is also contained in Chapter 2.

Example 1.13 Consider the conjunctive queries $C_1$ and $C_2$, as defined below.

\[
C_1 : p(X) := a(X, B), b(A, B), b(C, B), c(B, B), c(A, D).
\]

\[
C_2 : p(X) := a(X, V), b(U, V), c(U, W).
\]

The function $f$ defined by $f(X) = X$, $f(V) = B$, $f(U) = A$, $f(W) = D$ is a containment mapping from $C_2$ into $C_1$. The destination (under $f$) of $p(X)$ is $p(X)$, of $a(X, V)$ is $a(X, B)$, of $b(U, V)$ is $b(A, B)$ and of $c(U, W)$ is $c(A, D)$.

However, there is no containment mapping $g : C_1 \rightarrow C_2$. Assume such a $g$ exists. Then, the destination of $c(B, B)$ under $g$ would have to be $c(U, W)$ (the only $c$-atom in $C_2$). However, $g(c(B, B)) = c(U, W)$ requires that $g(B)$ be both $U$ and $W$, contradicting the functionality of $g$. □

Now, we may define the containment of top-down expansions (with IDB predicates permitted at the leaves) as the containment of the corresponding conjunctive queries. Given the relations between rules, top-down expansions and conjunctive queries, we will sometimes also speak of the containment of a top-down expansion in a rule. Finally, recall that we may think of a program as a (possibly infinite) union of conjunctive queries, where the bodies of these queries are atomic formulae whose principal functors are EDB predicates. Sagiv and Yannakakis ([29]) use this idea to reduce program containment to the containment of conjunctive queries. The theorem of Sagiv and Yannakakis says that, for a program $P$ to be contained in a program $Q$, each conjunctive query generated by $P$ must be contained in some conjunctive query generated by $Q$; that is, there can be no “mixing and matching”.

**Theorem 1.2 (Sagiv and Yannakakis).**

Consider programs $P$ and $Q$, defining the IDB predicate $p$. Then, $P \subset_p Q$ iff for every conjunctive query $C_P$ generated by $P$ with EDB predicates at the leaves and $p$ at the root, there is a conjunctive query $C_Q$ generated by $Q$ with EDB predicates at the leaves such that $C_P \subset C_Q$. □

### 1.3.3 Tree shapes

As we will show in the next section, the optimizations of the previous section can be described in terms of normal-form proof trees. That is, each optimization is made possible because all facts generated by the relevant program are generated by proof trees of a certain “shape”.

Recall that proof trees (and top-down expansions) are written in a way that preserves the left-to-right order of the subgoals in any rule. The idea of a proof-tree shape is the intuitively obvious one, given this assumption. Following Helm ([13]), we may formalise the concept by defining a shape as a list over the rule names.
Definition 1.2 Let \( P \) be a program with rules \( r_1, \ldots, r_n \). A *tree shape* (or just *shape*) is a list that is defined as follows.

1. The empty list \([\ ]\) is a shape. This list represents all top-down expansions of depth 0.

2. Let \( r_i \) be a rule defining the predicate \( p \), with intensional subgoals (in order) \( t_1, \ldots, t_k \) (that is, the principal functor of each \( t_i \) is an intensional predicate name). Then, the list

\[
[ r_i [ r_j [ \ldots [ ] \ldots ] ] ]
\]

is a shape. This shape represents the top-down expansion of \( p \) with depth 1, in which \( r_i \) is used to construct the expansion. The \((j + 1)\)th component of this list is said to *represent the leaf* \( t_j \).

3. Let \( S \) be a nonempty shape, representing some top-down expansion \( T \) of some predicate \( p \). Assume that the \( i \)th occurrence of the empty list in \( S \) represents the \( i \)th leaf \( q(\bar{Z}) \) in \( T \). Assume further that the head of rule \( r_j \) unifies with this leaf under the mgu \( \tau \), and that \( r_j \) has the intensional subgoals (in order) \( q_1(\bar{Z}_1), \ldots, q_k(\bar{Z}_k) \). Construct the top-down expansion \( T' \) by expanding the \( i \)th leaf \( q(\bar{Z}) \) in \( T \) through rule \( r_j \). Let \( S' \) be the shape \( S \), where the empty list representing the \( i \)th leaf \( q(\bar{Z}) \) in \( T \) is replaced by the list

\[
[ r_j [ r_i [ r_j [ \ldots [ ] \ldots ] ] ] ]
\]

Then \( S' \) is a shape, representing the top-down expansion \( T' \). Further, the \( l \)th occurrence of the empty list in the above list is said to represent the \( l \)th leaf \( q_l(\tau(\bar{Z}_l)) \) in the newly-added subtree.

It is clear that every top-down expansion has a well-defined shape. We will also speak of the shape of a top-down expansion of a specified atom, and of the shape of a proof tree.

Example 1.14 Figure 1.2 contains top-down expansions generated by the program of Example 1.3. The expansion of Figure 1.2 (a) has the shape \([r_1[\ ]]\), and expansion (b) in that figure has the shape \([r_1[r_2][r_2][r_2]]\). Similarly, Figure 1.3 exhibits top-down expansions generated by the program of Example 1.10. Figure 1.3 (a) contains a top-down expansion with the shape \([r_1[r_2]]\), and part (b) of that figure contains a top-down expansion with the same shape, but with the specified root \( pl(f(f(A))) \). □

The structure of a shape can be simplified if the program in question is linear (recall that a program is linear if at most one atom in the body of any rule is intensional). In the linear case, each top-down expansion may be represented as a *string* over the rule names, and sets of top-down expansions may be represented by regular expressions over the rule names ([25]).
1.3. **TOP-DOWN EXPANSIONS**

Example 1.15 Consider the linear logic program of Example 1.10. The top-down expansions of Figure 1.3 have the shape $r_1 r_2$; note that the order in which the rule names appear in the shape corresponds to the order in which rules are applied in a top-down fashion, starting with the root. The set of all top-down expansions generated by the program, with EDB predicates at the leaves, may be denoted by the regular expression $r_1^* r_2$. □

**Extending functions**

We formalise our earlier notions of the extensions of functions on the variables in an expansion, as follows. Let $f$ be any function defined on some of the variables in a top-down expansion $T$. We extend $f$ to all variables, and to constants, by requiring $f$ to be the identity on all variables on which it is not defined, and on all constants. Similarly, for any term, we define $f(q(d_1, \ldots, d_k))$ to be $f(q)(f(d_1), \ldots, f(d_k))$. Finally, we define $f(T)$ to be the result of replacing every atom $a$ in $T$ by $f(a)$. The idea, as before, is that we merely replace every occurrence of every variable on which $f$ is defined by its image under $f$. In the remainder of this chapter, we will assume that all functions have been extended as described above.

**Labels**

Consider any sequence $T_1, \ldots, T_n$ of top-down expansions, not necessarily of different shapes. We will assume that each node in each expansion is labelled to be distinct from all other nodes in the expansion, and from all nodes in every other expansion. Given a label $l$, the node to which $l$ refers will be written $node(l)$. We assume that labels are preserved through the application of functions to a top-down expansion, as described above. Now, given any containment mapping $f : T_2 \rightarrow T_1$ where $T_1$ and $T_2$ are labelled top-down expansions, we assume the selection of a labelled destination for each labelled node in $T_2$ under $f$; that is, for each node $node(k)$ that is a leaf or the root in $T_2$, we select a unique label $l$ such that $f(node(k)) = node(l)$.

**Uniqueness of shapes**

It is easily seen that every shape uniquely defines a top-down expansion, up to the renaming of variables. The idea is that the top-down application of rules “commute”, and we may therefore construct a top-down expansion of a given shape using any order of rule applications. More formally, let $T_1$, $T_2$ and $T_3$ be top-down expansions in which all variables in each expansion are renamed to be distinct, and where $T_2$ and $T_3$ have depth 1 (i.e. each represents the application of a single rule). Let $node(l)$ and $node(k)$ be distinct leaves in $T_1$. Assume that we expand the leaf $node(l)$ in $T_1$ through $T_2$ under any unifier $\tau_1$, and expand $node(k)$ in the result through $T_3$ under any unifier $\tau_2$ to create some expansion $S$ (see Figure 1.4).

Then, we may create $S$ in the following way:

1. Expand $node(k)$ in $T_1$ through $T_3$ using the unifier $\sigma_2 = \tau_2(\tau_1)$ (recall that all functions are extended to be the identity on variables on which they are not defined).
Figure 1.4: Changing the order of expansion.
2. Define the unification $\sigma_1$ to be the identity on variables in $T_1$ and $T_3$, and to be $\tau_2(\tau_1)$ on the variables in $T_2$. Expand $\text{node}(l)$ in the result of 1 above through $T_2$ using the unification $\sigma_2$.

That is, the unifications $\sigma_1$ and $\sigma_2$ permit us to construct the same expansion $S$ by applying the expansions $T_2$ and $T_3$ to $\text{node}(l)$ and $\text{node}(k)$ in reverse order. Hence, if we use the mgu at each stage, then both orders of applications must yield equally general top-down expansions. An induction on $n$ allows us to reach the same conclusion if the leaves $\text{node}(k_1), \ldots, \text{node}(k_n)$ are expanded through the depth-1 expansions $S_1, \ldots, S_n$ respectively. A straightforward induction on the size of a shape permits us to claim that every shape uniquely defines a top-down expansion, up to renaming of variables. Hence, we may abuse notation by speaking of the containment of a shape (or top-down expansion) in a shape.

Note that the uniqueness of shapes allows us to construct a top-down expansion from top-down expansions $T_1$, $T_2$ and $T_3$ of arbitrary depth, by renaming the variables of the expansions apart, expanding some leaf in $T_1$ through $T_2$ using the mgu of the leaf in $T_1$ with the root of $T_2$, and similarly expanding any leaf in the result through $T_3$.

### 1.3.4 Changing shapes

We present some results that will be of use in the following sections. The idea is that containment mappings between top-down expansions remain essentially unchanged under certain operations that are performed on the expansions in question, and expansions can therefore be robustly manipulated to change their shapes.

#### Replicating expansions

Let $T_1, \ldots, T_n$ be a sequence of expansions, not necessarily of different shapes. Assume that the label of each node in $T_i$ is a list of the form $[i, l]$, where $l$ is an integer unique to the relevant node in $T_i$. We will speak of replicating some tree $T_i$ in the above sequence. To create $k$ copies $T_{i1}, \ldots, T_{ik}$ of $T_i$, we construct $k$ rename functions $\text{ren}_1, \ldots, \text{ren}_k$ that rename each variable in $T_i$ to be distinct from any variables in $T_1, \ldots, T_n$ (or their copies, if any), such that the ranges of these rename functions are distinct. Then, for each $j$, $T_{ij}$ is $\text{ren}_j(T_i)$. Further, the labels of each copy of $T_i$ are propagated by setting the label of $\text{node}(m)$ in $T_{ij}$ to $[j|m]$.

**Theorem 1.3 Expansion Theorem**

Let $T_1$ and $T_3$ be top-down expansions with distinct variables, and let $T_2$ and $T_4$ be expansions with distinct variables. Assume that $f : T_2 \rightarrow T_1$ and $g : T_4 \rightarrow T_3$ are containment mappings. Assume that $R$ is obtained by expanding the leaf $\text{node}(l)$ in $T_1$ through $T_3$. Let $\text{node}(k_1), \ldots, \text{node}(k_n)$ be leaves in $T_2$ such that $f(\text{node}(k_i)) = \text{node}(l)$, and let $S$ be the result of expanding each leaf $\text{node}(k_i)$ in $T_2$ through the $i$th replica $T_{4i}$ of $T_4$. Then, there is a containment mapping $h : S \rightarrow R$ that preserves the destinations of $f$ and $g$; that is, if $f(\text{node}(c)) = \text{node}(d)$ and $\text{node}(c)$ is a leaf in $S$, then $h(\text{node}(c)) = \text{node}(d)$; and, if $g(\text{node}(c)) = \text{node}(d)$, then $h(\text{node}([i|c]) = \text{node}(d_i)$ for all $i$. Figure 1.5 depicts this claim.
Proof. Let the roots of $T_1, T_2, T_3$ and $T_4$ be $r_1, r_2, r_3$ and $r_4$ respectively. Similarly, let the root of $T_{4j}$ be $r_{4j}$ for all $j$. Let $\tau$ be the most general unifier of $\text{node}(i)$ with the root $r_3$ of $T_3$, and $\sigma$ the most general unifier of the sequence $r_{41}, \ldots, r_{4n}$ with the sequence of leaves $\text{node}(k_1), \ldots, \text{node}(k_n)$ in $T_2$. Since $g$ is a containment mapping from $T_4$ into $T_3$, the domain-disjoint functions $g_j = g(\text{ren}_j^{-1})$ are containment mappings from $T_{4j}$ into $T_3$ that preserve the destinations of $g$. Define the function $\rho$ as follows.

$$\rho(V) = \begin{cases} \tau(f(V)) & \text{for } V \text{ in } T_2 \\ \tau(g_j(V)) & \text{for } V \text{ in } T_{4j} \end{cases}$$

Now, $\rho$ is a unification under which the leaves $\text{node}(k_1), \ldots, \text{node}(k_n)$ may be expanded through the subtrees $T_{41}, \ldots, T_{4n}$ respectively (to create some expansion $S'$, say). Consider any leaf $\text{node}(m)$ in $T_2$; assume that the destination of $\text{node}(m)$ under $f$ is $\text{node}(i)$ in $T_1$. Then, $\text{node}(m)$ in $S'$ is syntactically identical to $\text{node}(i)$ in $R$. Similarly, consider any leaf $\text{node}(m)$ in $T_4$; assume that the destination of $\text{node}(m)$ under $g$ is $\text{node}(i)$ in $T_3$. Then for each $j$, $\text{node}([j|m])$ in $S'$ is syntactically identical to $\text{node}(i)$ in $R$. That is, the identity I is a containment mapping from $S'$ into $R$ that preserves the destinations of $f$ and $g$. If $\sigma$ is the most general unifier of $\text{node}(k_1), \ldots, \text{node}(k_n)$ with the roots $r_{41}, \ldots, r_{4n}$ of $T_{41}, \ldots, T_{4n}$, then by the properties of the most general unifier there is some function $h$ such that $\rho = h(\sigma)$; hence, $h$ is a containment mapping from $S$ into $S'$ such that $h(\text{node}(i)) = \text{node}(i)$ for all nodes in $S$, and our result follows by composing $h$ and $I$. \(\square\)
1.4. SUBTREE ELIMINATIONS

Figure 1.6: Assumption for the Splicing Theorem.

Theorem 1.4 Splicing Theorem
Let $T_1$, $T_2$, $T_3$ and $T_4$ be top-down expansions with distinct variables. Assume that $node(l)$ is a leaf in $T_1$ and $node(m)$ is a leaf in $T_2$, and that there is a containment mapping $f : T_4 \rightarrow T_2$. Let $node(k_1), \ldots, node(k_n)$ be the leaves in $T_4$ whose destination under $f$ is $node(m)$ (see Figure 1.6). Construct the expansion $R$ by expanding $node(l)$ in $T_1$ through $T_2$, and expanding $node(m)$ in the result through $T_3$. Construct $S$ by expanding $node(l)$ in $T_1$ through $T_4$, and expanding each leaf $node(k_j)$ in the result through the $j$th replica $T_{3j}$ of $T_3$. Then, there is a containment mapping $h$ from $S$ into $R$ such that the destination of each leaf $node(i)$ in $S$ is as follows.

1. If $node(i)$ is a node in $T_1$, then $h(node(i)) = node(i)$.
2. If $node(i)$ is a node in $T_4$, then $h(node(i)) = f(node(i))$.
3. If $i$ is of the form $[p|3]$, then $h(node(i)) = node(p)$.

Figure 1.7 depicts the idea.

Proof. The identity is a containment mapping from $T_1$ into $T_1$, and the function $g_j = ren_j^{-1}$ is a containment mapping from the $j$th replica of $T_3$ into $T_3$; our result follows by two applications of the Expansion Theorem. □

1.4 Subtree eliminations

1.4.1 Normal-form optimizations

In this section, we will present a variety of optimizations that are defined in terms of normal-form conjunctive queries. The domain on which we will define these optimizations is that of single-IDB programs; that is, programs in which there is only one intensional predicate, $p$. We do not assume that the programs are either safe or function-free. The following
Figure 1.7: Illustrating the Splicing Theorem.
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Figure 1.8: A one-bounded expansion.

The program $P$ will serve as the canonical example of a single-IDB program; the IDB predicate defined by the program is the predicate $p$.

Let $P$ consist of the $n$ recursive rules

\[ r_i : p(\bar{X}_{i0}) :- p(\bar{X}_{11}), \ldots, p(\bar{X}_{ik_i}), C_i. \]

\[ \vdots \]

\[ r_n : p(\bar{X}_{n0}) :- p(\bar{X}_{n1}), \ldots, p(\bar{X}_{nk_n}), C_n. \]

and the $m$ nonrecursive rules

\[ b_i : p(\bar{Y}_{i0}) :- D_i. \]

\[ \vdots \]

\[ b_j : p(\bar{Y}_{j0}) :- D_j. \]

\[ \vdots \]

\[ b_m : p(\bar{Y}_{m0}) :- D_m. \]

where the $C_i$ and $D_j$ are arbitrary conjunctions of EDB predicates. Examples 1.1 - 1.4 exhibit such programs.

Let us define a top-down expansion to be closed if all its leaves are EDB predicates.

1.4.2 One-boundedness: definition and results

Define a top-down expansion to be one-bounded if at most the root is expanded through a recursive rule; that is, if the top-down expansion has depth at most 2 (see Figure 1.8). The program $P$ is said to be one-bounded iff one-boundedness is a normal form for the proof trees generated by the program; that is, iff every closed conjunctive query generated by $P$ is contained in some closed one-bounded conjunctive query.

If $P$ is one-bounded, then $P$ can be converted into an equivalent nonrecursive program $Q$ by expanding each recursive atom in each rule through each nonrecursive rule. That is, the equivalent nonrecursive program $Q$ is constructed as follows.
Let \( q \) be a new predicate symbol. Construct the program \( Q \), with \( n + m + 1 \) rules \( \{ r'_i \mid 1 \leq i \leq n \} \cup \{ b'_i \mid 1 \leq i \leq m \} \cup \{ c \} \), as follows. If \( r_i \) is a recursive rule, then replace \( r_i \) by the rule
\[
r'_i : p(X_{i0}) :\text{q}(X_{i1}, \ldots, q(X_{ik}), C_i).
\]
That is, we replace all recursive occurrences of \( p \) in \( r_i \) with a corresponding occurrence of \( q \).

Next, we introduce the rule \( c \), which merely initialises \( p \) to \( q \):
\[
c : p(V_1, \ldots, V_k) :\text{q}(V_1, \ldots, V_k).
\]
The \( V \)'s are distinct variables. Finally, each nonrecursive rule \( b_i \) is replaced by the rule
\[
b'_i : q(Y_{i0}) :D_i.
\]
which initialises \( q \) using the nonrecursive rules for \( p \). Assume \( P \) is one-bounded; then, the closed top-down expansions of \( P \) are isomorphic to the closed top-down expansions of \( Q \); that is, each such top-down expansion generated by either program can also be generated by the other program. The equivalence of \( P \) and \( Q \) then follows by the theorem of Sagiv and Yannakakis (Theorem 1.2).

**Example 1.16** Consider the program \( P \) of Example 1.2. The program \( Q \) is the program
\[
r'_1 : p(X, Y) :\text{q}(Y, X).
c : p(X, Y) :\text{q}(X, Y).
b'_1 : q(X, Y) : b(X, Y).
\]
The intermediate predicate \( q \) can, in this case, be eliminated to obtain the linear program \( Q' \) of Example 1.6, repeated below.
\[
r'_1 : p(X, Y) : b(Y, X)
\]
\[
r_2 : p(X, Y) : b(X, Y).
\]
The closed one-bounded expansions of \( P \) are easily seen to be isomorphic to the closed expansions of \( Q' \), as indicated by Figure 1.9. \( \square \)

The gains of converting \( P \) into \( Q \) in this way are obtained from the elimination of recursion overhead in query processing.
Expansions of $\mathcal{P}$

Expansions of $\mathcal{Q}'$

Figure 1.9: Illustrating Example 1.16.
CHAPTER 1. SUBTREE ELIMINATIONS

Results

One-boundedness is easily seen to be decidable; we sketch a proof in Section 1.5. The complexity of one-boundedness has been investigated by Kanellakis ([20]) for a restricted class of programs. A sirup is a single-IDB, Datalog program with a single recursive rule, and a basis rule of the form

\[ p(X_1, \ldots, X_k) :\neg b(X_1, \ldots, X_k). \]

where the \( X \)s are distinct variables, and where the EDB predicate \( b \) appears nowhere else in the program. Kanellakis ([20]) has shown that one-boundedness in \( \mathcal{NP} \)-hard for linear sirups; that is, for programs that in addition to the basis rule above contain the recursive rule

\[ p(\overline{Y}) :\neg p(\overline{Z}), e_1(\overline{W}_1), \ldots, e_n(\overline{W}_n). \]

Kanellakis' result, however, assumes an unbounded number of repetitions of EDB predicates in the body of the recursive rule. In Chapter 2, we will show that one-boundedness is \( \mathcal{NP} \)-hard even if there are no more than 4 repetitions of any EDB predicate in the body of the recursive rule. In the same chapter, we will show that one-boundedness is decidable in polynomial time for linear sirups in which no EDB predicate is repeated in the body of the recursive rule. Finally, in Section 1.5, we will present a polynomial-time algorithm that is sufficient (but not necessary) to detect one-boundedness in arbitrary single-IDB programs; the idea is a reduction to the decision procedure for linear sirups.

1.4.3 Base-case linearizability: definition and results

Recall our running assumption that top-down expansions are written in a way that preserves the left-to-right order of the subgoals in every rule. Define a top-down expansion generated by \( \mathcal{P} \) to be right-linear if only the rightmost occurrence of \( p \) is ever recursively expanded in the expansion (see Figure 1.10). The program \( \mathcal{P} \) is said to be linearizable by basis iff right-linearity is a normal form for the proof trees generated by the program; that is, iff every closed conjunctive query generated by \( \mathcal{P} \) is contained in some closed right-linear conjunctive query.

If \( \mathcal{P} \) is basis-linearizable, then \( \mathcal{P} \) can be converted into an equivalent linear recursive program, as follows.

Let \( g \) be a new predicate symbol. Construct the program \( \mathcal{Q} \), with \( n + m + 1 \) rules \( \{ r'_i \mid 1 \leq i \leq n \} \cup \{ b'_i \mid 1 \leq i \leq m \} \cup \{ c \} \), as follows. If \( r_i \) is a nonlinear rule \( (k_i > 1) \), then replace \( r_i \) by the linear rule

\[ r'_i : p(X_{i0}) :\neg q(X_{i1}), \ldots, q(X_{ik-1}), p(X_{ik}), c_i. \]

That is, we replace all but the last recursive occurrence of \( p \) in \( r_i \) with a corresponding occurrence of \( q \). If \( r_i \) is linear \( (k_i = 1) \), then \( r'_i \) is the same as \( r_i \):

\[ r'_i : p(X_{i0}) :\neg p(X_{i1}), c_i. \]
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Next, we introduce the rule $c$, which merely initialises $p$ to $q$:

$$c : p(V_1, \ldots, V_k) :\dashv q(V_1, \ldots, V_k).$$

The $V$s are distinct variables. Finally, each nonrecursive rule $b_i$ is replaced by the rule

$$b_i' : q(V_{i0}) :\dashv D_i,$$

which initialises $q$ using the nonrecursive rules for $p$.

If $\mathcal{P}$ is basis-linearizable, then the closed right-linear top-down expansions of $\mathcal{P}$ are isomorphic to the closed top-down expansions of $\mathcal{Q}$; that is, each such top-down expansion generated by either program can also be generated by the other program. The equivalence of $\mathcal{P}$ and $\mathcal{Q}$ then follows by the theorem of Sagiv and Yannakakis (Theorem 1.2).

Example 1.17 Consider the program $\mathcal{P}$ of Example 1.3. The program $\mathcal{Q}$ is the program

$$r'_1 : p(X, Y) :\dashv q(X, U), p(U, Y).$$
$$c : p(X, Y) :\dashv q(X, Y).$$
$$b'_1 : q(X, Y) :\dashv b(X, Y).$$

The intermediate predicate $q$ can, in this case, be eliminated to obtain the linear program $\mathcal{Q}'$ of Example 1.7, repeated below.

$$r'_1 : p(X, Y) :\dashv b(X, U), p(U, Y).$$
$$r_2 : p(X, Y) :\dashv b(X, Y).$$

The closed right-linear expansions of $\mathcal{P}$ are easily seen to be isomorphic to the expansions of $\mathcal{Q}'$, as indicated by Figure 1.11. $\square$
CHAPTER 1. SUBTREE ELIMINATIONS

The gains of replacing \( \mathcal{P} \) by \( \mathcal{Q} \) are obtained through the use of special-purpose query evaluators for linear recursive programs. In fact, Ullman and van Gelder ([37]) have shown that the evaluation of programs with the polynomial fringe property (a superset of linear recursive programs) may be performed in \( \mathcal{NC} \).

Results

Basis-linearizability was proposed by Zhang et al. ([40]\textsuperscript{5}), who studied this property in terms of a bilinear sirup with rectified rule heads (i.e., no variable is repeated in the head of any rule), such that there is at most one EDB subgoal in the body of the recursive rule. That is, they consider programs of the following form.

\[
p(X_1, \ldots, X_k) := p(Y), p(Z), e(W).
p(X_1, \ldots, X_k) := b(X_1, \ldots, X_k).
\]

They claim a polynomial-time decision procedure for the detection of basis-linearizability for such programs, although their proof has a flaw in a key lemma; we will discuss the error in Chapter 3. In Chapter 3, we will show that basis-linearizability is decidable for bilinear sirups with an unbounded number of EDB subgoals in the recursive rule, as long as the EDB predicates are distinct; that is, we consider programs of the following form, in which the \( e_s \) are distinct.

\[
p(X_1, \ldots, X_k) := p(Y), p(Z), e_1(W_1), \ldots, e_n(W_n).
p(X_1, \ldots, X_k) := b(X_1, \ldots, X_k).
\]

The techniques of Chapter 2 can be used to show that our decision procedure is polynomial. We will show in Chapter 3 that the proof of [40] does not directly extend to such programs.

\textsuperscript{5}This paper has recently been published in the ACM Transactions on Database Systems, but the proof has been omitted.
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and in fact we also cover (as they do not) the case in which the program can be linearized in a different way; however, our proof has been motivated in large part by their treatment.

Ramakrishnan et al. ([25]) have shown that the decision procedure of Chapter 3 does not extend to the case in which EDB repetitions are permitted in the body of the recursive rule, and show that detecting basis-linearizability is \(\mathcal{NP}\)-hard in this case; however, their reduction involves an unbounded number of repetitions of EDB predicates in the recursive rule. In Chapter 2, we show that the detection of basis-linearizability is \(\mathcal{NP}\)-hard for bilinear sirups, even if no EDB predicate appears more than 4 times in the body of the recursive rule.

In Chapter 4, we show that the detection of basis-linearizability in head-rectified, single-IDB Datalog programs is undecidable even if the program has one bilinear rule, an unbounded number of linear rules and only 5 basis rules. Our treatment also shows that program containment is undecidable for a restricted class of linear Datalog programs.

Finally, in Section 1.5, we provide polynomial-space and polynomial-time algorithms that are sufficient (but not necessary) for the detection of basis-linearizability in arbitrary single-IDB Datalog programs.

1.4.4 Sequencability: definition and results

Define a top-down expansion generated by \(\mathcal{P}\) to be sequenced if a recursive atom generated by the (top-down) application of a recursive rule \(r_i\) is never expanded through the rule \(r_j\), if \(i > j\) (see Figure 1.12). The program \(\mathcal{P}\) is said to be sequencable iff sequencing is a normal form for the proof trees generated by the program; that is, iff every closed conjunctive query generated by \(\mathcal{P}\) is contained in some closed, sequenced conjunctive query. If \(\mathcal{P}\) is sequencable, then it may be replaced by the following program \(\mathcal{Q}\).

Let \(q_1 \ldots q_n\) be new and distinct predicate symbols, and construct the program \(\mathcal{Q}\) from program \(\mathcal{P}\), as follows. First, replace the rule \(r_1\) by the two rules \(r'_1\) and \(s_1\), where \(r'_1\) is the same as \(r_1\):

\[
\begin{align*}
r'_1 & : p(\bar{X}_{10}) := p(\bar{X}_{11}), \ldots, p(\bar{X}_{1k_1}), C_1. \\
s_1 & : p(V_1, \ldots, V_k) := q_1(V_1, \ldots, V_k).
\end{align*}
\]

The \(V\)s are distinct variables. Next, replace each recursive rule \(r_i\) \((i > 1)\) by the two rules:

\[
\begin{align*}
r'_i & : q_{i-1}(\bar{X}_{(i-1)0}) := q_{i-1}(\bar{X}_{i1}), \ldots, q_{i-1}(\bar{X}_{ik_i}), C_i. \\
s_i & : q_{i-1}(V_1, \ldots, V_k) := q_i(V_1, \ldots, V_k).
\end{align*}
\]

As before, the \(V\)s are distinct variables. Finally, replace each nonrecursive rule \(b_i\) by the rule

\[
b'_i : q_n(\bar{Y}_{10}) := D_i.
\]

\(\mathcal{Q}\) computes those facts which would be produced by a bottom-up evaluation of \(\mathcal{P}\), in which we initialise \(p\) using the \(b_i\), and then, in sequence, close under \(r_n, r_{n-1}, \ldots, r_1\). It is easily
Figure 1.12: A sequenced expansion.
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\[ p(X,Y) \]
\[ p(X,U) \quad p(U,Y) \]
\[ \begin{array}{c}
  p(U,X) \\
  b(U,X)
\end{array} \]

\[ p(X,Y) \]
\[ p(X,U) \quad p(U,Y) \]
\[ \begin{array}{c}
  q(X,U) \\
  q(U,X) \\
  b(U,X)
\end{array} \]

\[ \mathcal{P} \quad \mathcal{Q} \]

Figure 1.13: Illustrating Example 1.18.

seen that the normal-form closed conjunctive queries of $\mathcal{P}$ are isomorphic to the closed conjunctive queries of $\mathcal{Q}$. Therefore, if $\mathcal{P}$ is sequencable, then $\mathcal{P}$ and $\mathcal{Q}$ are equivalent.

Example 1.18 For the program of Example 1.4, the program $\mathcal{Q}$ is the program

\[ r'_1 : p(X,Y) :- p(X,U), p(U,Y). \]
\[ s_1 : p(X,Y) :- q(X,Y). \]
\[ r'_2 : q(X,Y) :- q(Y,X). \]
\[ s_2 : q(X,Y) :- b(X,Y). \]
\[ b'_1 : q_2(X,Y) :- c(X,Y). \]

Figure 1.13 sketches the idea behind the isomorphism between the closed sequenced expansions of $\mathcal{P}$ and the closed expansions of $\mathcal{Q}$. □

The gains of replacing $\mathcal{P}$ by $\mathcal{Q}$ are obtained in several ways. For example, the evaluation of the transformed program $\mathcal{Q}$ can be pipelined. Most importantly, however, the detection of sequencability can often set up further optimizations, as in Example 1.8. Sequencability is also essential to the detection of separability ([24]) in linear programs.

Results

Sequencability is not known to be decidable for any interesting classes of programs. In Chapter 4, we will show that the detection of sequencability is undecidable for head-rectified, single-IDB Datalog programs with only two recursive rules and 9 basis rules. Our treatment provides a tight undecidability result for program equivalence.
Sequencability has only been studied for linear Datalog programs with two recursive rules and a single basis rule, and the decidability of sequencability is open even on this restricted domain. A variety of sufficient conditions have been proposed ([25], [17]) in this case. In Chapter 2, we show that sequencability is \( \mathcal{NP} \)-hard for such programs if EDB predicates are allowed to appear up to 3 times in the body of each recursive rule, and in fact that all the proposed sufficient conditions are also \( \mathcal{NP} \)-hard in this case. We also show that a popular sufficient condition is polynomial if no EDB predicates are allowed to repeat in any recursive rule.

Finally, we provide in Section 1.5 a polynomial-space algorithm that is sufficient (but not necessary) for the detection of sequencability in arbitrary Datalog programs.

1.4.5 Subtree eliminations as a descriptive mechanism

The normal forms implied by these problems are susceptible to a uniform description, as the elimination of subtrees of a certain shape from the proof trees generated by a program. As a dual to the concept of a closed top-down expansion, let us define a top-down expansion to be open iff the only rules used to construct the expansion are recursive rules.

Definition 1.3 Let \( \mathcal{P} \) be the canonical single-IDB program of the preceding subsection. A subtree elimination instance is the program \( \mathcal{P} \) and a finite set \( S \) of finite shapes over the recursive rules \( r_1 \ldots r_n \) (that is, the shapes define open expansions). Let \( \mathcal{Q} \) be the set of closed top-down expansions generated by \( \mathcal{P} \), such that no subtree of the expansion is described by a shape in \( S \). Then the answer to the instance is "yes" iff \( \mathcal{P} \equiv \mathcal{Q} \) (recall that we speak of any union of closed top-down expansions as a program). \( \Box \)

The set of such instances is called the subtree-elimination problem (SEP). Since \( \mathcal{Q} \) is a subset of the conjunctive queries generated by \( \mathcal{P} \), and by the theorem of Sagiv and Yannakakis (Theorem 1.2), we may conclude that the answer to an SEP instance is "yes" iff each conjunctive query generated by \( \mathcal{P} \) is contained in some conjunctive query generated by \( \mathcal{Q} \).

The transformations of the previous sections may all be described within the framework of SEP. The idea is that the violations of the required normal form are represented as subtree shapes.

One-boundedness

Let \( \mathcal{P} \) be the canonical single-IDB program of this section. Let a minimum-depth violation of one-boundedness (or just a violation) be an open top-down expansion of depth 2, and let \( S = \{s_1, \ldots, s_n\} \) be the set of shapes of the minimum-depth violations. It is easily seen that the set of one-bounded top-down expansions generated by \( \mathcal{P} \) is precisely the set of expansions in which no subtree has the shape \( s_i \) for any \( i \). Thus, \( \mathcal{P} \) is one-bounded iff the answer to the SEP instance \( \langle \mathcal{P}, S \rangle \) is "yes".

Example 1.19 For the program of Example 1.2, the set \( S \) is the singleton \( \{[r_1 | r_1][]\} \), representing the single minimum-depth violation of Figure 1.14. \( \Box \)
1.4. SUBTREE ELIMINATIONS

\[
p(X, Y) \\
\downarrow \\
p(Y, X) \\
\downarrow \\
p(X, Y)
\]

Figure 1.14: Minimum-depth violation of one-boundedness.

\[
p(X, Y) \\
\downarrow \\
p(X, U) \quad p(U, Y) \\
\downarrow \\
p(X, V) \quad p(V, U)
\]

Figure 1.15: Minimum-depth violation of basis-linearizability.

Linearizability by basis

Let a minimum-depth violation of right-linearity (or just a violation) be an open top-down expansion of depth 2, in which the rightmost recursive subgoal that is a child of the root is not expanded, and in which at least one other child of the root is expanded. Let \( S = \{s_1, \ldots, s_n\} \) be the set of shapes of the minimum-depth violations. It is easily seen that the set of right-linear top-down expansions generated by \( \mathcal{P} \) is precisely the set of expansions in which no subtree has the shape \( s_i \) for any \( i \). Thus, \( \mathcal{P} \) is linearizable by basis iff the answer to the SEP instance \( < \mathcal{P}, S > \) is “yes”.

Example 1.20 For the program of Example 1.3, the set \( S \) is the singleton \( \{[r_1[r_1]]\} \), representing the single minimum-depth violation of Figure 1.15. □

Sequencability

Let a minimum-depth violation of sequencability (or just a violation) be an open top-down expansion of depth 2, in which if \( r_i \) is used to expand the root, then at least one child of the root is expanded through some rule \( r_j \) such that \( j < i \). Let \( S = \{s_1, \ldots, s_n\} \) be the set of shapes of the minimum-depth violations. It is easily seen that the set of sequenced top-down expansions generated by \( \mathcal{P} \) is precisely the set of expansions in which no subtree has the shape \( s_i \) for any \( i \). Thus, \( \mathcal{P} \) is sequencable iff the answer to the SEP instance \( < \mathcal{P}, S > \) is “yes”.
Example 1.21 For the program of Example 1.4, the set $S$ is the singleton $\{[r_2[r_1[][]]]\}$. The corresponding minimum-depth violation is depicted in Figure 1.16. □

1.5 Subtree-elimination algorithms

We now present a uniform framework for the generation of sufficient conditions for the solution of an SEP instance. In each case, the program that we consider is the generic single-IDB program $P$ of Section 1.4.1.

1.5.1 Basis-independence

Recall that an expansion is termed open if only recursive rules are used in the construction of the expansion, and closed if all the leaves are EDB predicates. Our sufficient conditions will focus on the rectification of open top-down expansions; that is, we will show that every open expansion generated by $P$ is contained in a normal-form open expansion. This procedure is sufficient to prove that every closed top-down expansion is contained in a closed, normal-form expansion, as we show below; the only wrinkle is introduced if the containing expansion has depth 0. Recall that the top-down expansion of depth 0 (the expansion with shape []) is the top-down expansion generating the conjunctive query

$$p(X_1, \ldots, X_k) : - p(X_1, \ldots, X_k),$$

where the $X$s are distinct variables. Now, assume that an expansion $T_1$ is contained in [], and that $f$ is the containment mapping proving the containment. By the properties of the containment mapping, $T_1$ must have some leaf that is syntactically identical to its root.

Theorem 1.5 Assume that $T_1$ is an open top-down expansion that is contained in the expansion of depth 0. Then every closed top-down expansion obtained by applying basis rules to the leaves of $T_1$ is contained in an initialisation rule.

Proof. Since $T_1$ is contained in the depth-0 expansion, there must be some leaf (labelled $l$, say) that is syntactically identical to the root. Hence, if the basis rule $b_i$ is used to expand $node(l)$ in $T_1$, then the result is contained in $b_i$ by the Expansion Theorem. □
1.5. SUBTREE-ELIMINATION ALGORITHMS

By our assumption that all violations in our SEP instance are open, we conclude that each basis rule (considered as a top-down expansion) is in the indicated normal form; that is, no such expansions are prohibited. Now, every closed top-down expansion is either a basis rule, or is obtained by expanding every $p$-leaf in an open expansion through some basis rule. Hence, by the Expansion Theorem and Theorem 1.5, the rectification of all open expansions is sufficient to prove that the answer to a given SEP instance is "yes"; that is, that every closed top-down expansion is contained in a closed, normal-form expansion. Note that this result holds independently of the set of initialisation rules in $P$; that is, the transformations that we will consider are basis-independent.

The following theorem shows that if an expansion $T$ is contained in the empty expansion, then the result of expanding any leaf of $T$ through the expansion $U$ is contained in either the empty expansion or in $U$.

**Theorem 1.6** Assume that $T_1$ is an open top-down expansion that is contained in the expansion of depth 0 (the expansion with shape []). Let $T_3$ be the expansion obtained by expanding $node(l)$ in $T_1$ through the expansion $T_2$. Then, either $T_3 \subseteq []$, or there is a containment mapping from $T_{21}$ (a replica of $T_2$) into $T_3$ such that for any leaf $node([1,j])$ in $T_{21}$, the destination of $node([1,j])$ is $node(j)$ in $T_3$.

**Proof.** Let $f$ be a containment mapping from $[]$ into $T_1$. As before, there is some leaf (say, $node(k)$) in $T_1$ that is syntactically identical to the root of $T_1$. There are two cases. If $k \neq l$, then $f$ is a containment mapping from $[]$ into $T_3$. If $k = l$, then the subtree rooted at $node(l)$ in $T_1$ is $\tau(T_2)$, where $\tau$ is the mgu of the root of $T_2$ with $node(l)$ in $T_1$; hence, $\tau(\text{ren}_1^{-1})$ is a containment mapping from $T_{21}$ into $T_3$, where $\text{ren}_1$ is the rename function that creates $T_{21}$ from $T_2$. \qed

1.5.2 Generating sufficient conditions

Ramakrishnan, Sagiv, Ullman and Vardi ([25]) have proposed a framework for the construction of conditions that are sufficient (but not necessary) to prove that the proof trees of a program satisfy a normal form. Let $< P, S >$ be an SEP instance, where $S = \{v_1, \ldots, v_k\}$ is a complete set of violations to the desired normal form. The process of [25] consists of two steps:

1. For each $v_i$, show that there is a containment mapping of a restricted form from some normal-form top-down expansion $q_i$ into $v_i$.

2. Show that the results of (1) may be used to inductively rectify all top-down expansions of $P$.

Such a technique is called a proof-tree transformation technique.

**One-boundedness**

By Theorem 1.5 and the Expansion Theorem, the containment of every open expansion of depth at least two in an open expansion of depth at most one suffices to prove one-boundedness in $P$. 
Theorem 1.7 Assume that every minimum-depth violation of one-boundedness is contained in an open expansion of depth at most 1. Then \( P \) is one-bounded.

Proof. By induction on the number \( i \) of rule applications in the top-down expansion, we will show that every expansion of depth at least 2 is contained in an expansion of depth at most 1. The basis, \( i = 2 \), follows by assumption. For the induction, assume the truth of the hypothesis for \( 2 \leq l < i \).

Consider a top-down expansion \( T_1 \) obtained through \( i \) rule applications. \( T_1 \) is obtained by expanding some leaf node(\( n \)) in some expansion \( T_2 \) (constructed using \( i - 1 \) rule applications) through some rule \( r_j \) (see Figure 1.17). By our inductive hypothesis, \( T_2 \) is contained in a tree \( T_3 \) of depth at most one; assume that \( f \) is a containment mapping proving the containment. If \( T_3 \) has depth 0, then by Theorem 1.6, \( T_3 \subset \) [] or \( T_3 \subset r_j \), and our result follows.

Assume that \( T_3 \) has depth 1. By the Expansion Theorem, we may expand each node in \( T_3 \) whose destination under \( f \) is node(\( n \)) through \( r_j \), to produce an expansion \( T_4 \) of depth 2 such that \( T_1 \subset T_4 \) (see Figure 1.17). However, by assumption, \( T_4 \) is contained in a top-down expansion of depth at most 1, and our result follows because the composition of containment mappings is a containment mapping. \( \square \)

Example 1.22 Consider the program of Example 1.2. The minimum-depth violation of one-boundedness is contained in the top-down expansion of depth 1, under the identity mapping \( f(X) = X, f(Y) = Y \) (see Figure 1.18). Hence, the program is one-bounded. \( \square \)

A similar procedure on closed top-down expansions may be used to show that one-boundedness is decidable. That is, \( P \) is one-bounded iff every closed expansion of depth 3 is contained in a closed expansion of depth at most 2. Our treatment has, however, been motivated by the interests of exposition, and by the setting up of an efficient algorithm for the detection of one-boundedness; the latter is contained in the next section.
Linearizability by basis

By definition, the open expansion of depth 0 is right-linear. By Theorem 1.5 and the Expansion Theorem, if we show that every non-right-linear open expansion is contained in a right-linear open expansion, then we may conclude that \( P \) is basis-linearizable. The following treatment is an extension of a result of [25]; they consider a Datalog program with a single recursive rule, which is bilinear.

Let \( T_1 \) and \( T_2 \) be open expansions, let node\( (l) \) be the rightmost \( p \)-leaf in \( T_1 \) and let node\( (k) \) be the rightmost \( p \)-leaf in \( T_2 \). We say that a containment mapping \( f : T_2 \rightarrow T_1 \) is acceptable for right-linearity (or just acceptable) iff node\( (l) \) is the destination (under \( f \)) of no leaf, or is the destination of node\( (k) \) only.

Example 1.23 Consider the program of Example 1.3. Figure 1.19 shows that the minimum-depth violation of right-linearity is contained in a right-linear expansion under the acceptable mapping \( f(X) = X, f(Y) = Y, f(A) = V, f(B) = U \). □

Theorem 1.8 Assume that every minimum-depth violation of right-linearity is contained in a right-linear expansion, and that the containment is provable by an acceptable containment mapping. Then \( P \) is basis-linearizable.

Proof. By induction on the number \( i \) of rule applications in the top-down expansion, we show that every non-right-linear expansion is contained in a right-linear expansion. The basis, \( i = 0 \) (representing the top-down expansion of depth 0), is trivial. For the induction, assume the truth of the hypothesis for \( 0 \leq l < i \), where \( i > 0 \).
Consider a top-down expansion $T_1$ obtained through $i$ rule applications. If $T_1$ is right-linear, then the result follows; if $T_1$ is a minimum-depth violation, then the result follows by assumption. Otherwise, $T_1$ is obtained by expanding some leaf $\text{node}(n)$ in some expansion $T_2$ (constructed using $i - 1$ rule applications) through some rule $r_j$ (see Figure 1.20).

By our inductive hypothesis, $T_2$ is contained in a right-linear tree $T_3$. If $T_3$ has depth 0, then our result follows by Theorem 1.6.

Assume that $T_3$ has depth at least 1. By the Expansion Theorem, we may expand each node in $T_3$ whose destination under $f$ is $\text{node}(n)$ through $r_j$, to produce an expansion $T_4$ such that $T_1 \subset T_4$. If $T_4$ is right-linear, the result follows. Otherwise, $T_4$ is a tree that is obtained from some right-linear tree by expanding some non-rightmost $p$-leaves in the right-linear tree through the rule $r_j$. We call such an expansion almost right-linear.

We may rectify $T_4$ in a bottom-up manner, using the Splicing Theorem and the fact that the composition of containment mappings is a containment mapping, as follows. At any stage in the process, we have a situation as shown in Figure 1.21; that is, we have an almost-right-linear tree $T_5$ whose rightmost $p$-node is expanded through a violation $V$, such that the rightmost $p$-node of $V$ is a leaf or is expanded through some right-linear tree $T_6$.

By assumption, there is an acceptable mapping from some right-linear expansion $R$ into $V$. Hence, by the Splicing Theorem, we may splice $R$ in for $V$: the $p$-leaves of $R$ remain
Figure 1.21: The rectification procedure of Theorem 1.8.
leaves, except for the rightmost $p$-leaf in $R$ which may be expanded through the right-linear tree $T_5$. An inductive repetition suffices to complete the rectification.  

By the observations of Example 1.23, we may now claim that the transitive-closure program of Example 1.3 is basis-linearizable.

**Complexity** If $\mathcal{P}$ is a Datalog program, then the minimum-depth violations may be constructed in polynomial time, and the containments under acceptable mappings may be tested in polynomial space by the chase algorithm of [25]. In the non-Datalog case, the chase may not terminate; however, we may generate sufficient conditions by placing a bound on the depth of the containing right-linear expansion. A suitable heuristic may be one based on size preservation; that is, we may insist that the containing query be no bigger than the contained expansion.

**Sequencability**

By convention, the open expansion of depth 0 is sequenced. By Theorem 1.5 and the Expansion Theorem, if we show that every non-sequenced open expansion is contained in a sequenced open expansion, then we may conclude that $\mathcal{P}$ is sequencable. The following result is an extension of an algorithm proposed independently by [25] and [17]; they consider Datalog programs with only two recursive rules, both of which are linear.

For any $i < j$, define an $r_i$-$r_j$ violation of sequencability (or just an $r_i$-$r_j$ violation) to be an open expansion of depth 2, such that $r_j$ is used to expand the root, one or more of the children are expanded through $r_i$, and all other children of the root are leaves.

Let us further define an $r_i$-$r_j$-sequenced expansion to be a sequenced expansion using only the rules $r_i$ and $r_j$ such that $r_i$ is used at most once (that is, $r_i$ can only be used to expand the root).

**Example 1.24** Consider the program of Example 1.4. The minimum-depth violation of sequencability in this program is the expansion $[r_2[r_1([[]]])]$ (see Figure 1.22); this expansion is an $r_1$-$r_2$ violation. The minimum-depth violation is contained in the $r_1$-$r_2$-sequenced expansion $[r_1[r_2([[]])[r_2]])$, as shown in the figure; the containment follows because both expansions have the same root and leaves.  

Let us define a node violation of $r_i$ to be the root of an $r_i$-$r_j$ violation for any $j$.

**Theorem 1.9** Assume that for all $i$ and $j$, each $r_i$-$r_j$ violation is contained in some $r_i$-$r_j$-sequenced expansion. Then $\mathcal{P}$ is sequencable.

**Proof.** By induction on the number $m$ of rule applications in a top-down expansion $T$ generated by $\mathcal{P}$, we prove that $T$ is contained in a sequenced expansion. The proof is similar to that of Theorem 1.8; we merely sketch the inductive step. Assume that the $m$th rule applied is $r_i$. By the inductive hypothesis and the Expansion Theorem, $T$ is contained in some top-down expansion $T'$, which is obtained by expanding some leaves in a sequenced expansion through $r_i$. We inductively rectify $T'$ using the Splicing Theorem, by "shuffling
up" the node violations of $r_i$ as follows. Consider any node violation at maximum depth; assume it is the root of the $r_i$-$r_j$ violation $V$, in which some leaves may be expanded through sequenced expansions in which every rule used is of the form $r_k$ for $k \geq j$ (where $j > i$). By assumption, $V$ is contained in an $r_i$-$r_j$-sequenced expansion $S$. By the Splicing Theorem, we may splice $S$ in for $V$; this process either reduces the number of node violations of $r_i$ by 1 or replaces the node violation by a node violation at a smaller depth. Further, the splicing-in of $S$ for $V$ does not create any $r_k$-$r_l$-violations for $k \neq i$. Hence, we may proceed in stages, in each stage removing all node violations of $r_i$ at maximum depth, until the tree $T'$ is sequenced. The situation is depicted in Figure 1.23. In the figure, $R_1 \ldots R_k$ are sequenced subtrees in which the rules $r_1, \ldots, r_i$ are not used. \[ \square \]

By the observations of Example 1.24, we may conclude that the program of Example 1.4 (computing the symmetric, transitive closure) is sequencable.

**Complexity** As before, the tests of Theorem 1.9 may be performed in polynomial space for Datalog programs through the chase algorithm of [25]. In the non-Datalog case, we may construct sufficient conditions by placing a bound on the depth of each containing $r_i$-$r_j$-sequenced expansion, perhaps by using the size-maintaining heuristic that was presented in the previous subsection.

### 1.5.3 Fast algorithms

Finally, we present restricted algorithms for the detection of one-boundedness and basi-linearizability. In Chapter 2, we will show that for Datalog programs, these algorithms are polynomial in the size of $P$: they perform polynomial-time reductions to restricted programs for which the detection of the appropriate normal form is known to be decidable in polynomial time. The idea behind the algorithms is to further restrict the destinations of an atom under a mapping that proves the containment of a violation in a normal-form
expansion. That is, we essentially rename different occurrences of the recursive atoms in each rule.

Let us assume that for any $i$ and $j$, the $j$th subgoal in the rule $i$ is given the superscript $ij$, and that this superscript is carried through all top-down expansions. That is, if $r_i$ is used to expand a $p$-atom and the $j$th subgoal has principal functor $q_i$, then the $j$th child of the expanded atom is referred to as a $q^{ij}$-atom (or just $q^{ij}$). The root of the expansion, and the body of the top-down expansion of depth 0, are merely $p$-atoms. Figure 1.24 illustrates this notation on the non-right-linear top-down expansion of Figure 1.19, representing the minimum-depth violation of basis-linearizability in the program of Example 1.3.

**One-boundedness**

For all $i$, define a violation of degree $i$ to be a minimum-depth violation of one-boundedness in which exactly $i$ children of the root are expanded. Now, for any open top-down expansions $T_1$ and $T_2$, we say that a containment mapping $f : T_1 \rightarrow T_2$ is restricted if the destination of any $q^{ij}$-atom in $T_1$ under $f$ is a $q^{ij}$-atom in $T_2$. Note that the number and size of the violations of degree 1 are polynomial in the size of $\mathcal{P}$, and that each violation can be constructed in polynomial time.

---

*Note that this concept is distinct from the idea of labels in a top-down expansion*
Theorem 1.10 Assume that every violation of degree 1 is contained in a top-down expansion of depth no more than 1, and that the containments are proved by restricted mappings. Then, \( \mathcal{P} \) is one-bounded.

Proof. We prove by induction on \( i \) that every violation of degree \( i \) is contained in a tree of depth at most one, and that the containment is proved by a restricted mapping; our result then follows by Theorem 1.7. The basis, \( i = 1 \), follows by assumption.

Now, assume the truth of the inductive hypothesis for \( 1 \leq l < i \). Consider any violation \( T \) of degree \( i \). This violation must be obtained by expanding some \( p^{th} \)-leaf at depth 1 in some violation \( V \) of degree \( i - 1 \) through some rule \( r_j \). By our inductive hypothesis, \( V \) is contained in some expansion \( W \) of depth at most 1 under a restricted containment mapping.

If the depth of \( W \) is 0, then by Lemma 1.6 and the Expansion Lemma, \( T \) is contained in \( \square \) or \( r_j \) under a restricted mapping.

If the depth of \( W \) is 1, then let \( W' \) be the result of expanding the \( p^{th} \)-leaf in \( W \) through the rule \( r_j \) (see Figure 1.25). By the Expansion Lemma, \( T \) is contained in \( W' \) under a restricted mapping. However, \( W' \) is a violation of degree 1, and is (by assumption) contained in a tree of depth at most 1 under a restricted mapping; our result follows because...
the composition of restricted mappings is a restricted mapping. □

This theorem leads to the following algorithm that is sufficient (but not necessary) to prove one-boundedness.

**Algorithm 1.1**

**INPUT:** A single-IDB program $\mathcal{P}$.

**OUTPUT:** "yes" only if $\mathcal{P}$ is one-bounded.

1. Construct all violations of degree 1, and all expansions of depth at most 1.

2. If each violation of degree 1 is contained in an expansion of depth at most 1 under a restricted mapping, then answer "yes"; otherwise, answer "no".

□

There are a polynomial number of degree-1 violations, so Step (1) may be accomplished in polynomial time. Step (2) involves a polynomial number of containment tests, each involving the existence of a restricted mapping from an expansion of depth 0 or 1 into a violation. Testing for the existence of a mapping from a depth-0 expansion into any expansion is clearly polynomial. Consider tests of the second kind; that is, tests for the existence of a restricted mapping from a depth-1 expansion $T$ into a violation $V$. Each atom in $T$ has at most 2 possible destinations in $V$ under a restricted mapping, and we will show in Chapter 2 that such tests may be accomplished in polynomial time. Hence, Algorithm 1.1 is in $\mathcal{P}$.

**Basis-linearizability**

A similar process may be applied to create sufficient conditions for the detection of basis-linearizability.

As before, we define a violation of degree $i$ to be a minimum-depth violation of right-linearity in which exactly $i$ children of the root are expanded. Now, for any violation $T_1$ and right-linear expansion $T_2$, we say that a containment mapping $f : T_1 \rightarrow T_2$ is restricted if for any $g^{ij}$-leaf in $T_1$ that is not the rightmost $p$-leaf in $T_1$, the destination of this $g^{ij}$-atom in $T_1$ under $f$ is a $g^{ij}$-atom in $T_2$. Note that a restricted containment mapping is acceptable for right-linearity. Again, we observe that the number and size of the violations of degree 1 are polynomial in the size of $\mathcal{P}$, and that each violation can be constructed in polynomial time.

**Theorem 1.11** Assume that every violation of degree 1 is contained in a right-linear top-down expansion, and that the containments are proved by restricted mappings. Then, $\mathcal{P}$ is basis-linearizable.

**Proof.** We prove by induction on $i$ that every violation of degree $i$ is contained in a right-linear expansion, and that the containment is proved by a restricted mapping; our result then follows by Theorem 1.8. The basis, $i = 1$, follows by assumption.
Now, assume the truth of the inductive hypothesis for \(1 \leq l < i\). Consider any violation \(T\) of degree \(i\). This violation must be obtained by expanding some \(p^{ab}\)-leaf at depth \(l\) in some violation \(V\) of degree \(i - 1\), such that this leaf is not the rightmost child of the root, through some rule \(r_j\) (see Figure 1.26). By our inductive hypothesis, \(V\) is contained in some right-linear expansion \(W\) under a restricted containment mapping.

If the depth of \(W\) is 0, then by Theorem 1.6, \(T\) is contained in \(r_j\) or \([],\) under a restricted mapping.

If the depth of \(W\) is 1 or larger, then let \(W'\) be the result of expanding every \(p^{ab}\)-leaf in \(W\) whose destination is the newly-expanded leaf in \(V\) through the rule \(r_j\). By the Expansion Theorem, \(T\) is contained in \(W'\) under a restricted mapping. Note that \(W'\) is obtained by expanding some \(p^{ab}\)-leaves in a right-linear expansion through \(r_j\); that is, at any stage of the tree, at most two sibling \(p\)-atoms are expanded. By assumption, each violation of degree 1 is contained in a right-linear expansion under a restricted mapping, and a bottom-up rectification as in the proof of Theorem 1.8 serves to complete the proof. \(\square\)

This theorem yields the following sufficient (but not necessary) condition for the detection of basis-linearizability. We will show in Chapter 2 that the algorithm is polynomial:
the key is to test whether every degree-1 violation is contained in a right-linear tree of depth at most 2 under a restricted mapping\(^7\).

**Algorithm 1.2**

INPUT: A single-IDB program \(\mathcal{P}\).

OUTPUT: "yes" only if \(\mathcal{P}\) is basis-linearizable.

(1) Construct all violations of degree 1, and all right-linear expansions of depth at most 2.

(2) If each violation of degree 1 is contained in a right-linear expansion of depth at most 2 under a restricted mapping, then answer "yes"; otherwise, answer "no".

\[\square\]

There are a polynomial number of degree-1 violations and a polynomial number of right-linear trees of depth at most 2, so Step (1) may be accomplished in polynomial time. Step (2) involves a polynomial number of containment tests, each involving the existence of a restricted mapping from a right-linear expansion of depth 0, 1 or 2 into a violation. As we mentioned in our treatment of one-boundedness in the previous subsection, testing for the existence of a mapping from a depth-0 expansion into any expansion is polynomial. Consider tests for the existence of a restricted mapping from a depth-1 or depth-2 right-linear expansion \(T\) into a violation \(V\). Let \(N\) be the size of \(V\); remember that \(N\) is polynomial in the size of the program \(\mathcal{P}\). By the definition of a restricted mapping, one atom (say, \(a\)) in \(T\) has up to \(N\) possible destinations in \(V\), and each other atom has at most 2 possible destinations. Hence, by a case analysis on the destinations of \(a\), we may reduce the test to \(N\) tests for the existence of a mapping from \(T\) into \(V\) such that each atom in \(T\) has at most 2 allowed destinations in \(V\). We will show in Chapter 2 that such tests may be accomplished in polynomial time. Hence, Algorithm 1.2 is in \(\mathcal{P}\).

Sequencability

A similar algorithm may be devised for the detection of sequencability, but we omit the treatment in the interest of brevity.

### 1.6 Overview of Chapters 2, 3 and 4

In the remainder of this report, we will investigate the complexity of the subtree elimination problem, focussing on the detection of one-boundedness, basis-linearizability and sequencability.

In Chapter 2, we investigate the complexity of detecting containments among conjunctive queries. We extend the conjunctive query containment problem to the \(k\)-containment problem, and show that \(k\)-containment and \(kSAT\) are essentially the same problem. This investigation results in a complete description of the complexity of conjunctive query containment. These results are then extended to show that one-boundedness, basis-linearizability

\(^7\)The algorithm is polynomial for any given choice of depth for the right-linear trees.
and sequencability are \( \mathcal{NP} \)-hard for restricted classes of programs. In this chapter, we also prove that the sufficient conditions of Section 1.5.3 (Algorithms 1.1 and 1.2) are in \( \mathcal{P} \).

In Chapter 3, we provide a decision procedure for the detection of basis-linearizability in a class of recursive programs. The decision procedure can be seen to be polynomial using the techniques of Chapter 2.

Finally, in Chapter 4, we show that sequencability and basis-linearizability are undecidable for multi-rule, nonlinear programs. The techniques of this chapter also provide tight undecidability results for the detection of program equivalence.

### 1.6.1 Complexity results

The results of our investigation are presented in Table 1.1. The programs considered are all Datalog. The expression \( \leq i \text{ reps} \) means that each recursive rule in the program has at most \( i \) occurrences of an EDB predicate in the body of each recursive rule.
Chapter 2

The complexity of conjunctive query containment

2.1 Introduction

In this chapter, we will characterize the complexity of testing containments among pairs of conjunctive queries. Recall that a conjunctive query is a single-rule, nonrecursive program, and that the theorem of Sagiv and Yannakakis (Theorem 1.2) relates containments among recursive programs to containments among the conjunctive queries generated by these programs.

In Section 2.2, we characterize the complexity of the conjunctive query containment problem. Our results are obtained by defining and analysing a closely related problem, which we term the \( k \)-containment problem. We also show that a restricted version of the 2-containment problem is in \( \mathcal{NC} \), and is hence efficiently computable in parallel.

In Section 2.3, we extend the results of Section 2.2 to provide \( \mathcal{NP} \)-hardness results for the one-boundedness, sequencability and basis-linearizability problems. We also justify the title of Section 1.5.3 by showing that the algorithms of that section are in \( \mathcal{P} \), as we claimed.

2.2 The \( k \)-containment problem

Let us consider the complexity of the conjunctive query containment problem. In this section, we will define the \( k \)-containment problem as a parametrized version of the conjunctive query containment problem, and show that while the 2-containment problem is in \( \mathcal{P} \), the 3-containment is \( \mathcal{NP} \)-complete. We also show that for Datalog (that is, function-free) conjunctive queries, the 2-containment problem is in \( \text{NLOGSPACE} \) (and hence in \( \mathcal{NC} \)).
2.2. THE K-CONTAINMENT PROBLEM

2.2.1 Conjunctive query containment

Recall from Section 1.3.1 that a conjunctive query is a single-rule, nonrecursive program. That is, a conjunctive query is of the form

\[ p(X) \leftarrow \mathcal{B} \]

where \( \mathcal{B} \) is an arbitrary conjunction of atomic formulae. Strictly speaking, the predicate \( p \) must not occur within \( \mathcal{B} \); however, we will ignore this restriction when it is clear from the context that such an expression is to be applied nonrecursively.

Consider the (not necessarily function-free) conjunctive queries

\[
C_1 : a_0(U_0) \leftarrow a_1(U_1), \ldots, a_m(U_m).
\]
\[
C_2 : b_0(W_0) \leftarrow b_1(W_1), \ldots, b_l(W_l).
\]

We assume without loss of generality that there are no repetitions of any atomic formula in the body of \( C_1 \), or in the body of \( C_2 \) (although predicates may appear repeatedly). That is, for no \( i \) and \( j \), \( i \neq j \), are \( a_i(U_i) \) and \( a_j(U_j) \) syntactically identical (or \( b_i(W_i) \) and \( b_j(W_j) \) identical). Subgoal repetitions can clearly be identified and eliminated in polynomial time. The conjunctive queries \( C_1 \) and \( C_2 \) will serve as generic conjunctive queries in the remainder of this chapter.

The theorem of Chandra and Merlin

The following treatment is a synopsis of Section 1.3.2, which presents a syntactic test for the containment of a conjunctive query in another (see Theorem 1.1). The basic tool used is the containment mapping, as described below in terms of the generic conjunctive queries \( C_1 \) and \( C_2 \) presented at the beginning of this section.

Let \( f \) be a function on the symbols in \( C_2 \) that leaves constants unchanged. We may extend \( f \) to terms (and atoms) in the obvious way; that is, we define \( f(q(d_1, \ldots, d_k)) \) to be \( f(q)(f(d_1), \ldots, f(d_k)) \), where the \( d_i \) are arbitrary terms. Such a function is said to be a containment mapping from \( C_2 \) into \( C_1 \) if the following are both true.

1. \( f(b_0(W_0)) = a_0(U_0) \).
2. For \( 1 \leq j \leq l \) there is an \( i \), \( 1 \leq i \leq m \), such that \( f(b_j(W_j)) = a_i(U_i) \).

If there is a containment mapping \( f : C_2 \rightarrow C_1 \), then for every atom \( t \) in \( C_2 \), we say that \( f(t) \) is the destination of \( t \) under \( f \). Since \( f \) is a function and there are (by assumption) no subgoal repetitions in \( C_1 \), each atom in \( C_2 \) has a unique destination under \( f \).

The theorem of Chandra and Merlin (Theorem 1.1) states that for any conjunctive queries \( C_1 \) and \( C_2 \), \( C_1 \subseteq C_2 \) if and only if there is a containment mapping \( f : C_2 \rightarrow C_1 \).

Example 2.1 Consider the conjunctive queries \( C_3 \) and \( C_4 \), as defined below.

\[
C_3 : p(X) \leftarrow a(X, B), b(A, B), b(C, B), b(D, D), c(B, B), c(C, B), c(A, D).
\]
\[
C_4 : p(X) \leftarrow a(X, V), b(U, V), c(U, W).
\]
The function $f$ defined by $f(X) = X, f(V) = B, f(U) = A, f(W) = D$ is a containment mapping from $C_4$ into $C_3$. The destination (under $f$) of $p(X)$ is $p(X)$, of $a(X, V)$ is $a(X, B)$, of $b(U, V)$ is $b(A, B)$ and of $c(U, W)$ is $c(A, D)$.

However, there is no containment mapping $g : C_3 \rightarrow C_4$. If there were such a mapping $g$, then the destination of $c(B, B)$ under $g$ would have to be $c(U, W)$ (the only $c$-atom in $C_4$); however, the requirement $g(c(B, B)) = c(U, W)$ would imply $g(B) = U$ and $g(B) = W$, contradicting the assumed functionality of $g$. □

## 2.2.2 Conjecture mappings

The theorem of Chandra and Merlin is based on the existence of a mapping on symbols. An alternative viewpoint, and one which lends itself to a description of the complexity of deciding conjunctive query containment, is based on the existence of a mapping on atoms.

**Definition 2.1** Let $s$ and $t$ be two arbitrary atomic formulae. We say that there is a partial mapping from $s$ to $t$ (written $s \rightarrow t$) if there is a substitution for the variables in $s$ under which $s$ is made syntactically identical to $t$. □

Each partial mapping $s \rightarrow t$ (if it exists) implies a unique substitution for each variable in $s$; the set of such assignments is termed the assignment set induced by the partial mapping. Two assignment sets are said to be consistent if no variable is assigned a different value by the two assignment sets, and a pair of partial mappings is said to be consistent if the assignment sets induced by the mappings are consistent.

**Example 2.2** In Example 2.1, the partial mapping $b(U, V) \rightarrow b(A, B)$ induces the assignment set $\{ U := A, V := B \}$. Further, the partial mappings $a(X, V) \rightarrow a(X, B)$ and $b(U, V) \rightarrow b(A, D)$ are inconsistent, since the variable $V$ is assigned a different value by these mappings. Finally, as indicated in Example 2.1, there is no partial mapping $c(B, B) \rightarrow c(U, W)$. □

The existence of a partial mapping may be tested and the induced assignment set generated through term-matching (Ullman [36]), and may hence be accomplished in time that is polynomial in the total size of $s$ and $t$. Testing for consistency is clearly polynomial in the size of the assignment sets. The following lemma shows that for function-free atoms, both these procedures may be accomplished in LOGSPACE. The central idea is the fact that in the function-free case, the existence of a partial mapping and the consistency of a pair of partial mappings may each be tested by testing the equality or inequality of arguments in the relevant atoms.

**Example 2.3** Consider the queries of Example 2.1. There is a partial mapping $b(U, V) \rightarrow b(A, B)$, but no partial mapping $c(B, B) \rightarrow c(U, W)$. In the latter case, both arguments of $c(B, B)$ are equal, but the arguments of $c(U, W)$ are unequal. □

For any atom $p(\vec{X})$ and integer $i$, let $p(\vec{X})[i]$ denote the $i$th argument of $p(\vec{X})$.

**Theorem 2.1** Let $p(\vec{X})$ and $q(\vec{Y})$ be atoms. Then, there is a partial mapping $p(\vec{X}) \rightarrow q(\vec{Y})$ iff the following conditions are true.
1. \( p \) and \( q \) are the same predicate, and have the same arity (say, \( n \)).

2. For \( 1 \leq i \leq n \), if \( p(\vec{X})[i] \) is the constant \( c \), then \( q(\vec{Y})[i] \) is the same constant \( c \).

3. For \( 1 \leq i < j \leq n \), if \( p(\vec{X})[i] = p(\vec{X})[j] \), then \( q(\vec{Y})[i] = q(\vec{Y})[j] \).

**Proof.** If conditions 1, 2 and 3 are met, then the set

\[
\{ p(\vec{X})[i] := q(\vec{Y})[i] \mid 1 \leq i \leq n, \ p(\vec{X})[i] \text{ is a variable} \}
\]

is a substitution under which \( p(\vec{X}) \) is made syntactically identical to \( q(\vec{Y}) \). The converse follows by the definition of a partial mapping. \( \Box \)

**Theorem 2.2** Let \( p \) be a predicate of arity \( n \) and \( q \) a predicate of arity \( m \). Assume that the partial mappings \( p(\vec{X}) \rightarrow p(\vec{Y}) \) and \( q(\vec{W}) \rightarrow q(\vec{Z}) \) exist. These partial mappings are consistent iff for \( 1 \leq i \leq n, 1 \leq j \leq m \), if \( p(\vec{X})[i] = q(\vec{W})[j] \), then \( p(\vec{Y})[i] = q(\vec{Z})[j] \).

**Proof.** If the condition is met, then the set

\[
\{ p(\vec{X})[i] := p(\vec{Y})[i] \mid 1 \leq i \leq n, \ p(\vec{X})[i] \text{ is a variable} \}
\]

\[
\cup
\{ q(\vec{W})[j] := q(\vec{Z})[j] \mid 1 \leq j \leq m, \ q(\vec{W})[j] \text{ is a variable} \}
\]

is single-valued for each variable in \( \vec{X} \cup \vec{W} \), and is a substitution under which \( p(\vec{X}) \) is made syntactically identical to \( p(\vec{Y}) \) and \( q(\vec{W}) \) made syntactically identical to \( q(\vec{Z}) \). The converse follows by the definition of consistency. \( \Box \)

The importance of partial mappings lies in the duality that such mappings enjoy with containment mappings. More precisely, if there is a function \( f \) and atoms \( s \) and \( t \) such that \( f(s) = t \), then (by definition) there is a partial mapping \( s \rightarrow t \); in addition, the existence of a partial mapping \( s \rightarrow t \) uniquely defines a function \( f \) such that \( f(s) = t \). Further, the assignment set induced by the partial mapping is merely an extensional definition of the function \( f \).

**Example 2.4** Consider the queries \( C_3 \) and \( C_4 \) of Example 2.1. The function \( f \) defined by \( f(U) = A, f(V) = B \) maps \( b(U, V) \) to \( b(A, B) \) (that is, \( f(b(U, V)) = f(A, B) \)). The partial mapping \( b(U, V) \rightarrow b(A, B) \) exists, and the assignment set induced by the partial mapping is \( \{ U := A, V := B \} \). \( \Box \)

These observations lead us to the following characterization for conjunctive query containment.

**Definition 2.2** Let \( C_1 \) and \( C_2 \) be the generic conjunctive queries of the preceding subsection. We say that a conjunct mapping \( M \) from \( C_2 \) into \( C_1 \) (written \( M : C_2 \rightarrow C_1 \)) is a sequence \( < m_0, \ldots, m_l > \) of (not necessarily distinct) atoms in \( C_1 \) such that the following are all true.
1. \( m_0 \) is \( a_0(\bar{U}_0) \).

2. For \( 1 \leq j \leq l \), \( m_j \) is \( a_i(\bar{U}_i) \) for some \( i \in [1,m] \).

3. For each \( j \), \( 0 \leq j \leq l \), there is a partial mapping \( b_j(\bar{W}_j) \rightarrow m_j \).

4. Each pair of partial mappings is consistent.

For each \( j \), \( m_j \) is the \textit{destination} of \( b_j(\bar{W}_j) \) under the conjunct mapping. The partial mapping \( b_0(\bar{W}_0) \rightarrow a_0(\bar{U}_0) \) is termed the \textit{head mapping}.

The value of conjunct mappings is illustrated by the following theorem.

\textbf{Theorem 2.3 (Conjunct mapping theorem)} For any conjunctive queries \( C_1 \) and \( C_2 \), there is a containment mapping from \( C_2 \) into \( C_1 \) iff there is a conjunct mapping from \( C_2 \) into \( C_1 \).

\textit{Corollary} \( C_1 \subseteq C_2 \) iff there is a conjunct mapping \( M : C_2 \rightarrow C_1 \).

\textit{Proof.} Let \( C_1 \) and \( C_2 \) be as above. If there is a containment mapping \( f : C_2 \rightarrow C_1 \), then the sequence \( \langle f(b_0(\bar{W}_0)), \ldots f(b_l(\bar{W}_l)) \rangle \) defines a conjunct mapping from \( C_2 \) into \( C_1 \). Conversely, assume that \( M \) is a conjunct mapping from \( C_2 \) into \( C_1 \). The function defined by the union of the assignment sets induced by the partial mappings \( b_j(\bar{W}_j) \rightarrow m_j \), for \( 0 \leq j \leq l \), is a containment mapping from \( C_2 \) into \( C_1 \). The proof of the corollary follows by the containment mapping theorem.

\textbf{Example 2.5} Consider the conjunctive queries \( C_3 \) and \( C_4 \) of Example 2.1. There is a conjunct mapping \( M : C_4 \Rightarrow C_3 \) in which the destination of \( p(X) \) is \( p(X) \), of \( a(X, B) \), of \( b(U, V) \) is \( b(A, B) \) and of \( c(U, W) \) is \( c(A, D) \).

2.2.3 The \( k \)-containment problem

We extend the conjunctive query containment problem by permitting the placement of restrictions on the destinations that a conjunct mapping may include.

\textbf{Definition 2.3} Let \( C_1 \) and \( C_2 \) be the generic conjunctive queries of Section 2.2.1, and let \( \mathcal{D} \) be the sequence \( \langle D_0, D_1, \ldots D_l \rangle \), where

1. \( D_0 = \{ a_0(\bar{U}_0) \} \), and

2. For \( 1 \leq j \leq l \), \( D_j \subseteq \{ a_i(\bar{U}_i) \mid 1 \leq i \leq m \} \).

We say that \( C_1 \subseteq C_2 \) under \( \mathcal{D} \) (written \( C_1 \stackrel{\mathcal{D}}{\subseteq} C_2 \)) if there is a conjunct mapping \( M : C_2 \Rightarrow C_1 \) such that \( m_j \in D_j \), for all \( j \). Determining such a containment is an instance of the \textit{distinguished-destination problem}. The \( D_j \) are termed \textit{destination sets}, since they limit the possible destinations of each atom under a conjunct mapping. If any destination set \( D_j \) is empty, then \( C_1 \stackrel{\mathcal{D}}{\not\subseteq} C_2 \).
2.2. THE K-CONTAINMENT PROBLEM

\[ C_3 : p(X) \leftarrow a(X, B), b(A, B), b(C, B), b(D, D), c(B, B), c(C, B), c(A, D). \]

\[ C_4 : p(X) \leftarrow a(X, V), b(U, V), c(U, W). \]

Figure 2.1: Distinguished-destination instance.

Similarly, if we are given conjunctive queries \( C_1 \) and \( C_2 \), and destination sets \( D_1 \) and \( D_2 \), then we may define the equivalence of \( C_1 \) and \( C_2 \) under \( D_1 \) and \( D_2 \) (written \( C_1 \overset{D_1, D_2}{\equiv} C_2 \)) to be \( C_1 \subseteq C_2 \) and \( C_2 \subseteq C_1 \). \( \square \)

Example 2.6 Consider the conjunctive queries \( C_3 \) and \( C_4 \) of Example 2.1, and define \( D \) by the arrows in Figure 2.1. \( < C_1, C_2, D > \) is a distinguished-destination instance. Note that the atom \( b(D, D) \) is not an allowed destination for \( b(U, V) \), but is an allowed destination for \( c(U, W) \). \( \square \)

We further parametrize the problem by the maximum cardinality of the destination sets \( D_j \).

Definition 2.4 An instance of the \( k \)-containment problem is an instance of the distinguished-destination problem, in which \( |D_j| \leq k \) for all \( j \); that is, no destination set has more than \( k \) elements. \( \square \)

Example 2.7 The problem of Example 2.6 is an instance of the 4-containment problem. \( \square \)

2.2.4 Pruning

Given conjunctive queries \( C_1 \) and \( C_2 \) (the generic conjunctive queries of Section 2.2.1) and a set \( D \) of destination sets, we may prune the destination sets in \( D \) as follows. For each \( j \), let \( D_j \) be the set \( \{d_{jq} | 1 \leq q \leq n_j \} \), where \( n_j \) is the cardinality of \( D_j \).

Definition 2.5 We say that the distinguished-destination problem \( < C_1, C_2, D > \) is pruned iff

1. For all \( p, s \), if \( d_{ps} \in D_p \) then \( b_p(W_p) \rightarrow d_{ps} \); that is, there is a partial mapping from every atom in \( C_2 \) to each of its allowed destinations; and
\[ C_3 : p(X) := a(X, B), b(A, B), b(C, B), b(D, D), c(B, B), c(C, B), c(A, D). \]

\[ C_4 : p(X) := a(X, V), b(U, V), c(U, W). \]

Figure 2.2: Pruning.

2. For all \( p, s \), if \( d_{ps} \in D_p \), then for all \( q \) there is a \( t \) such that \( d_{qt} \in D_t \) and the partial mapping \( b_p(I_{p\in p}) \rightarrow d_{ps} \) is consistent with the mapping \( b_q(W_q) \rightarrow d_{qt} \); that is, every allowed destination for some atom is consistent with at least one allowed destination for every other atom.

\[ \square \]

Define any \( d_{ps} \in D_p \) to be a violation of Class 1 if it violates condition (1), and a violation of Class 2 if it violates condition (2). If \( d_{ps} \) is a violation of Class 1 or 2, then by the definition of a conjunct mapping, the destination of \( b_p(W_p) \) cannot be \( d_{ps} \) under any conjunct mapping. Hence, the removal of a Class 1 or Class 2 violation \( d_{ps} \) from the destination set \( D_p \) does not affect the existence of a containment. We prune the destination sets \( D_j \) by iteratively removing all violations to produce a set \( D' \) such that \( C_1 \subseteq C_2 \) iff \( C_1 \subseteq C_2 \).

Example 2.8 Consider the distinguished-destination instance of Example 2.6. There is no partial mapping \( c(U, W) \rightarrow b(D, D) \) (since \( b \) and \( c \) are different predicates), and the partial mapping \( c(U, W) \rightarrow c(B, B) \) is inconsistent with every choice of destination for \( b(U, V) \). The pruned distinguished-destination instance is shown in Figure 2.2. Note that the instance is now a 2-containment problem.

\[ \square \]

Algorithm 2.1

INPUT: \( C_1, C_2, D \) as above.

OUTPUT: \( D' \), containing no violations, such that \( C_1 \subseteq C_2 \) iff \( C_1 \subseteq C_2 \).

1. \( \text{change} \rightarrow \text{true} \)
2. \( \text{while} \ \text{change} \)
3. \( \quad \text{change} \rightarrow \text{false} \)
4. \( \quad \text{for} \ 0 \leq j \leq l \)
5. \( \quad \text{for} \ s \in D_j \)
2.2. THE $K$-CONTAINMENT PROBLEM

$\%$ If $s$ is a Class 1 violation, remove it.
\begin{align*}
&\text{if } b_j(\bar{W}_j) \neq s \\
&D_j \leftarrow D_j \setminus \{s\} \\
&\text{else}
\end{align*}

$\%$ If $s$ is a Class 2 violation, remove it.
\begin{align*}
&\text{violation } \leftarrow \text{false} \\
&\text{for } 0 \leq i \leq l \\
&\text{temp } \leftarrow \text{true} \\
&\text{for } t \in D_i \\
&\text{if } b_j(\bar{W}_j) \rightarrow s \text{ is consistent with } b_i(\bar{W}_i) \rightarrow t \\
&\text{temp } \leftarrow \text{false} \\
&\text{violation } \leftarrow \text{violation } \lor \text{temp}
\end{align*}

\begin{align*}
&\text{if } \text{violation} \\
&D_i \leftarrow D_i \setminus \{s\} \\
&\text{change } \leftarrow \text{true}
\end{align*}

$D'$ is the set of the resulting $D_j$. $\square$

The correctness of the algorithm follows from the fact that the removal of a violation cannot affect the existence of a containment. Termination is guaranteed since each assignment of true to change (at line 1) accompanies the deletion of a destination from a destination set. The algorithm is easily seen to run in polynomial time, and in LOGSPACE for Datalog queries by Theorems 2.1 and 2.2.

In the remainder of this chapter, we assume that all distinguished-destination instances have been pruned.

2.2.5 Equivalence of the containment and distinguished-destination problems

It turns out that the conjunctive query containment and distinguished-destination problems are essentially the same problem, in the sense that these problems are polynomially equivalent.

Given conjunctive queries $C_1$ and $C_2$ and an integer $k$ such that no predicate appears more than $k$ times in the body of $C_1$, we may construct a $k$-containment instance by setting $D_0$ to be a singleton set containing the head of $C_1$, and setting each other $D_j$ to be the set of the atoms in the body of $C_1$ that have the same principal functor as $b_j$. That is, each atom in the body of $C_2$ is allowed to map to every occurrence of the same predicate in the body of $C_1$.

The following algorithm performs the reduction in the opposite direction.

**Algorithm 2.2**

**INPUT:** a $k$-containment instance $C_1, C_2$ and $D$.

**OUTPUT:** conjunctive queries $C'_1$ and $C'_2$ such that no predicate appears more than $k$ times in the body of $C'_1$, and such that $C'_1 \subseteq C'_2$ iff $\forall D \in C_1 \subseteq C_2$. 

(1) The heads of $C_1'$ and $C_2'$ are those of $C_1$ and $C_2$, respectively.\footnote{To preserve the safety of the queries, we may create a new predicate $f$, and place the atom $f(\bar{u}_0)$ in the body of $C_1'$ and the atom $f(\bar{w}_0)$ in the body of $C_2'$.}

(2) Let the $j$th atom in the body of $C_2$ be $e(\bar{w}_j)$. Since $\mathcal{D}$ is pruned, each member of the destination set $D_j$ must also have principal functor $e$. Let $D_j = \{ e(\bar{u}_{jq}) | 1 \leq q \leq n_j \}$, where (by assumption) $n_j \leq k$. Create a new predicate symbol $g_j$. Then, add the atom $g_j(\bar{w}_j)$ to the body of $C_2'$, and an atom $g_j(\bar{u}_{jq})$ to the body of $C_1'$ for $1 \leq q \leq n_j$.

\[ \square \]

**Example 2.9** Consider the pruned distinguished-destination instance of Example 2.8. The algorithm produces the following queries.

\[ C_1' : p(X) := d(X, B), e(A, B), e(C, B), g(C, B), g(A, D). \]
\[ C_2' : p(X) := d(X, V), e(U, V), g(U, W). \]

\[ \square \]

The algorithm is clearly polynomial. In step 2, each predicate $g_j$ is made to appear at most $n_j \leq k$ times in the body of $C_1'$, and thus no predicate appears more than $k$ times in the body of $C_1$. Finally, to prove that $C_1 \subseteq C_2$ iff $C_1' \subseteq C_2'$, we observe the following.

1. Both instances involve the same head mapping, yielding the same induced assignment set.

2. If the $j$-th atom in the body of $C_2$ is $e(\bar{w}_j)$ with destination set $D_j = \{ e(\bar{u}_{jq}) | 1 \leq q \leq n_j \}$, then for any $q$, there is a partial mapping $e(\bar{w}_j) \rightarrow e(\bar{u}_{jq})$ inducing the assignment set $S$ iff there is a partial mapping $g_j(\bar{w}_j) \rightarrow g_j(\bar{u}_{jq})$ inducing the assignment set $S$.

### 2.2.6 Complexity of $k$-containment

The $k$-containment problem is clearly in $\mathcal{NP}$; merely guess a conjunct mapping and verify using the conjunct mapping theorem. It turns out that the $k$-containment problem and $k\text{SAT}$ are essentially the same problem. That is, for $k \geq 2$, the $k$-containment problem is no harder than $k\text{SAT}$; since 2SAT is known to be polynomial, we may conclude that the 2-containment problem is also polynomial. In fact, the reduction may be performed in logspace for Datalog queries, and the 2-containment problem is therefore in $\mathcal{NLOGSPACE}$ (and hence $\mathcal{NC}$ [9]). Further, for $k \geq 3$, $k\text{SAT}$ is no harder than the $k$-containment problem, and the 3-containment problem is therefore $\mathcal{NP}$-complete.
2.2. THE $K$-CONTAINMENT PROBLEM

$C_3: \quad p(X) :\leftarrow d(X, B) \quad e(A, B) \quad e(C, B) \quad g(C, B) \quad g(A, D)$.

\[
\begin{array}{ccccccc}
  t &=& 1 & \quad y &=& 1 & \quad z &=& 1 & \quad w &=& 1 & \quad r &=& 1 & \quad s &=& 1 \\
X &=& X & \quad X &=& X & \quad U &=& A & \quad U &=& C & \quad U &=& A \\
V &=& B & \quad V &=& B & \quad V &=& B & \quad W &=& B & \quad W &=& D \\
C_4: \quad p(X) :\leftarrow d(X, V) \quad e(U, V) \quad g(U, W)
\end{array}
\]

2SAT instance:
Class 1 clauses: \{t\} \{y\} \{z + w\} \{r + s\}
Class 2 clauses \{z + \bar{r}\} \{\bar{w} + s\}

Minimal satisfying truth assignments:
\[
\begin{align*}
t &=& y &=& z &=& s &=& 1 \\
t &=& y &=& w &=& r &=& 1
\end{align*}
\]

Figure 2.3: Testing the containment $C_3 \subseteq C_4$ in Example 2.9

Polynomial time

We will provide a polynomial-time reduction from any instance of the $k$-containment problem to an instance of $k$SAT, for $k \geq 2$. We assume that the conjunctive queries $C_1$ and $C_2$ are the generic queries described in Section 2.2.1.

The basic idea is that we carry a Boolean variable representing each choice of destination for each atom. The clauses produced are of two kinds.

1. Clauses that enforce the requirement that each atom in $C_2$ have a legal destination in $C_1$. We call such clauses Class 1 clauses.

2. Consistency constraints that disallow inconsistent pairs of partial mappings. Such clauses are termed Class 2 clauses.

Example 2.10 illustrates the construction.

Example 2.10 Consider the pruned 2-containment instance of Example 2.9. Let the following Boolean variables indicate the following choices of destinations (see Figure 2.3).
### Table: Boolean variable, atom, destination

<table>
<thead>
<tr>
<th>Boolean variable</th>
<th>atom</th>
<th>destination</th>
</tr>
</thead>
<tbody>
<tr>
<td>(t)</td>
<td>(p(X))</td>
<td>(p(X))</td>
</tr>
<tr>
<td>(y)</td>
<td>(d(X,V))</td>
<td>(d(X,B))</td>
</tr>
<tr>
<td>(z)</td>
<td>(e(U,V))</td>
<td>(e(A,B))</td>
</tr>
<tr>
<td>(w)</td>
<td>(e(U,V))</td>
<td>(e(C,B))</td>
</tr>
<tr>
<td>(r)</td>
<td>(g(U,W))</td>
<td>(g(C,B))</td>
</tr>
<tr>
<td>(s)</td>
<td>(g(U,W))</td>
<td>(g(A,D))</td>
</tr>
</tbody>
</table>

Recall that the Class 1 clauses represent the statement “Every atom in \(C_4\) has a legal destination”. Now, the only allowed destination for \(p(X)\) is \(p(X)\), yielding the Class 1 clause \(\{t\}\). Similarly, the allowed destinations for \(b(U,V)\) are \(b(A,B)\) and \(b(C,B)\); the corresponding Class 1 clause is \(\{z+w\}\). The set of Class 1 clauses is \(\{t\}\{y\}\{z+w\}\{r+s\}\).

The Class 2 clauses enforce consistency of the corresponding partial mappings. The mapping \(b(U,V) \rightarrow b(A,B)\) is inconsistent with \(c(U,W) \rightarrow c(C,B)\) (yielding the clause \(\{\bar{z}+\bar{r}\}\)), and the mapping \(b(U,V) \rightarrow b(C,B)\) is inconsistent with \(c(U,W) \rightarrow c(A,D)\) (yielding the clause \(\{\bar{w}+\bar{s}\}\)).

The 2SAT instance created is \(\{t\}\{y\}\{z+w\}\{r+s\}\{\bar{z}+\bar{r}\}\{\bar{w}+\bar{s}\}\), with the two satisfying truth-assignments \(t = y = z = s = 1\) and \(t = y = w = r = 1\). The first such assignment gives a conjunct mapping as indicated by the heavy arrows in Figure 2.3. Note that in the general case, the cardinality \(k\) of the Class 1 clauses is the parameter of the \(k\)-containment instance, and Class 2 clauses always have cardinality 2.

In general, more than one member of a Class 1 clause may be true in a satisfying truth assignment (signifying more than one possible destination for some atom). In this case, any one choice of destination suffices.

The following is a formal statement and proof of the algorithm.

**Algorithm 2.3**

**INPUT:** a pruned \(k\)-containment instance \(< C_1, C_2, D >\), with \(k \geq 2\).

**OUTPUT:** a \(k\)-SAT instance \(I\) that is satisfiable iff there is a \(k\)-containment.

1. If any destination set \(D_j\) is empty, output the unsatisfiable instance \(\{x\}\{\bar{x}\}\).

2. Create \((l+1)k\) Boolean variables \(\{x_{ji}|0 \leq j \leq l, 1 \leq i \leq k\}\) and \((l+1)k\) set variables \(\{A_{ji}|0 \leq j \leq l, 1 \leq i \leq k\}\); the former will be used to construct the \(k\)SAT instance, and the latter to hold induced assignment sets. Each destination set \(D_j\) is \(\{d_{ji}|1 \leq i \leq n_j\}\), where by assumption \(n_j \leq k\).

3. for \(0 \leq j \leq l\)
   4. add the clause \(\{x_{j1} + \ldots + x_{jn_j}\}\) to \(I\)
   5. for \(1 \leq q \leq n_j\)
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(6) \( A_{jq} \leftarrow \) the assignment set induced by the partial mapping \( b_j(W_j) - d_{jq} \)

(7) for \( 0 \leq j < i \leq l \)

(8) for \( 1 \leq q \leq n_j, 1 \leq p \leq n_i \)

(9) if \( A_{jq} \) is inconsistent with \( A[ip] \)

(10) add \( \{ \overline{x_{jq}} + \overline{x_{ip}} \} \) to \( I \)

\( \Box \)

The algorithm is clearly polynomial. As before, we term the clauses that are added to \( I \) at Step 4 Class 1 clauses, and those that are added at Step 10 Class 2 clauses. Since Class 1 clauses have cardinality at most \( n_j \leq k \) and Class 2 clauses are doubletons, \( I \) is a \( k\)SAT instance.

By the form of the Class 1 clauses, we may observe that in any satisfying truth-assignment for \( I \), some \( x_{jq} \) is true for each \( j \). Define a satisfying truth-assignment to be minimal iff exactly one \( x_{jq} \) is true for each \( j \).

**Lemma 2.1** \( I \) is satisfiable iff it has a minimal truth-satisfying assignment.

**Proof.** If \( I \) has a minimal satisfying truth-assignment, then it is clearly satisfiable. For the converse, assume that \( S \) is a satisfying truth-assignment for \( I \). By previous discussion, at least one member of each Class 1 clause is true under \( S \). Arbitrarily pick one such member of each Class 1 clause, and set every other member to be false. Such a procedure cannot make either a Class 1 clause or a Class 2 clause untrue if it was true under \( S \); hence, the result is a minimal satisfying truth-assignment for \( I \). \( \Box \)

**Lemma 2.2** If \( C_1 \subseteq C_2 \), then \( I \) is satisfiable.

**Proof.** If \( C_1 \subseteq C_2 \), no destination set \( D_j \) is empty, and the algorithm does not terminate at Step 1. Let \( < d_{0,q}, \ldots, d_{1,j} > \) be a conjunct mapping from \( C_2 \) into \( C_1 \), where \( d_{js} \in D_j \) for all \( j \). Construct a truth-assignment for \( I \) by setting \( x_{js} \) to be true, and all other variables to be false. Such an assignment satisfies all Class 1 clauses. Further, by the properties of a conjunct mapping, each Class 2 clause is satisfied as well. Hence, this truth-assignment satisfies \( I \). \( \Box \)

**Lemma 2.3** If \( I \) is satisfiable, then \( C_1 \subseteq C_2 \).

**Proof.** Assume \( I \) is satisfiable, and let \( S \) be a minimal satisfying truth-assignment for \( I \). Assume that the variables that are true under \( S \) are \( x_{0,s}, \ldots, x_{i,s} \). Then \( < d_{0,s}, \ldots, d_{i,s} > \) is a conjunct mapping from \( C_2 \) into \( C_1 \) that obeys \( D \), since the Class 1 clauses enforce the requirement that \( d_{js} \in D_j \), and the Class 2 clauses enforce the requirement that no two choices of destination are inconsistent. \( \Box \)
Note that a similar reduction may be performed from a $k$-equivalence problem $< C_1, C_2, D_1, D_2 >$ to a $k$SAT instance $I$. That is, we perform the reduction for $< C_1, C_2, D_1 >$ and $< C_2, C_1, D_2 >$ separately, to produce $k$SAT instances $I_1$ and $I_2$ respectively, where the variables in $I_1$ and $I_2$ are distinct; then, the conjunction of $I_1$ and $I_2$ yields a $k$SAT instance that is satisfiable iff $C_1 \equiv_{D_1} D_2$. 

**Theorem 2.4** Algorithm 2.3 is correct.

*Corollary 1.* The 2-containment (or 2-equivalence) problem is in $\mathcal{P}$. 

*Corollary 2.* The 2-containment (or 2-equivalence) problem is in $\mathcal{NLOGSPACE}$ (and hence $\mathcal{NC}$) for Datalog queries.

*Proof.* By Lemmas 2.3 and 2.4. Corollary 1 follows because 2SAT is in $\mathcal{P}$. Corollary 2 follows because 2SAT is complete for $\mathcal{NLOGSPACE}$, and $\mathcal{NLOGSPACE}$ is in $\mathcal{NC}$ ([9]). $\square$

**Related work** Sagiv and Yannakakis ([29]) propose an algorithm to decide containment among function-free conjunctive queries $C_1$ and $C_2$ in which each atom in $C_2$ has only two destinations consistent with the head mapping; the primary differences between their algorithm and Algorithm 2.3 are that their algorithm is based on function-free queries, and performs pruning only in terms of atoms whose destinations are inconsistent with the head mapping. Related work on polynomial-time algorithms includes the minimization algorithms of Aho et al. ([3, 4]) and Johnson and Klug ([19]). The most general result among these three papers is that of Johnson and Klug, who consider “fanout-free” conjunctive queries; they test for equivalence between two queries by minimizing each query, and then determining whether the minimal queries are isomorphic. The conjunctive query

$$C_1 : p(X) := a(X, C), b(B, C), b(C, C), c(B, D), c(C, D), c(C, C).$$

is not fanout-free. However, $C_1$ is equivalent to the conjunctive query

$$C_2 : p(X) := a(X, U), b(U, U), c(U, U).$$

as may be verified through two uses of Algorithm 2.4.

**$\mathcal{NP}$-completeness**

We now show that the $k$-containment problem is $\mathcal{NP}$-complete for $k \geq 3$, for a restricted class of conjunctive queries. We will begin by defining the concept of a valid labelling for a $k$SAT instance, and showing that a $k$SAT instance is satisfiable iff it has a valid labelling. We will then reduce the problem of finding a valid labelling for a given $k$SAT instance to that of solving a $k$-containment instance.
2.2. THE K-CONTAINMENT PROBLEM

3SAT instance: \[ c_1 = \{x_1 + x_2 + \bar{x}_3\} \quad c_2 = \{\bar{x}_1 + \bar{x}_4 + x_5\} \]

Satisfying truth assignment: \[ x_1 = \text{true}, x_4 = \text{false}, x_2, x_3, x_5 \text{ arbitrary} \]

Valid labelling: \[ << T_{11}, D_{12}, D_{13} > > \quad < D_{21}, T_{22}, D_{23} > > \]

Figure 2.4: Valid labelling.

Valid labelling  Let \( I \) be a \( k \)SAT instance consisting of the \( p \) clauses \( c_1, \ldots, c_p \) over the \( q \) variables \( x_1, \ldots, x_q \). Without loss of generality, we assume that \( I \) contains no tautological clauses (clauses that contain a pair of complementary literals); such clauses do not affect the satisfiability of \( I \), and may be removed in polynomial time. We also assume that no literal appears more than once in any clause; literal repetitions may similarly be removed in polynomial time. For all \( i \), let the \( i \)th clause have \( n_i \leq k \) literals. We will use the notation \( l_{ij} \) to denote the \( j \)th literal in clause \( c_i \).

Let \( \{T_{ij} \mid 1 \leq i \leq p, 1 \leq j \leq k\} \cup \{D_{ij} \mid 1 \leq i \leq p, 1 \leq j \leq n_i\} \) be a set of \( 2km \) distinct constants. A labelling \( A \) of \( I \) is an \( p \)-vector of tuples \( < A[i1], \ldots, A[in_i] > \), where \( A[ij] \) is either \( T_{ij} \) or \( D_{ij} \) for each \( i \) and \( j \). Intuitively, the assignment of \( T_{ij} \) to \( A[ij] \) represents a satisfying truth assignment under which the literal \( l_{ij} \) is “true”; similarly, \( D_{ij} \) denotes a “don’t care” for the value of \( l_{ij} \).

A labelling of \( I \) is valid if

1. For each \( i \), there is exactly one \( j \) such that \( A[ij] = T_{ij} \); that is, exactly one literal in each clause is “true”; and

2. For any \( A[ij] \) and \( A[ml] \), \( i \neq m \), if \( l_{ij} \) and \( l_{ml} \) are complementary literals, then either \( A[ij] = D_{ij} \) or \( A[ml] = D_{ml} \) (or both); that is, no pair of complementary literals in different clauses are both true.

Example 2.11

Consider the 3SAT instance \( I \) consisting of the two clauses \( c_1 = \{x_1 + x_2 + \bar{x}_3\} \) and \( c_2 = \{\bar{x}_1 + \bar{x}_4 + x_5\} \). The sequence \( << T_{11}, D_{12}, D_{13} > < D_{21}, T_{22}, D_{23} > > \) is a valid labelling for \( I \); that is, we set the first literal in clause \( c_1 \) and the second literal in clause \( c_2 \) to “true”, and set all other literals to “don’t care” (see Figure 2.4). □

\[ ^2\text{That is, } I \text{ is an instance of at-most-} k\text{-SAT} \]
It turns out that the existence of a valid labelling is necessary and sufficient for the existence of a satisfying truth-assignment.

**Theorem 2.5** A $k$SAT instance is satisfiable iff it has a valid labelling.

*Proof.* Consider a $k$SAT instance $\mathcal{I}$ as above. If $\mathcal{I}$ is satisfiable, then it has some satisfying truth-assignment $S$. Construct a labelling $V$ as follows: if any literal $l_{ij}$ is true under $S$, then $A[ij]$ is $T_{ij}$; otherwise, it is $D_{ij}$. Since $S$ satisfies each clause in $\mathcal{I}$, at least one $A[ij]$ is $T_{ij}$ for each $i$. Now, for each $i$, select any $A[ij]$ that is assigned $T_{ij}$, and assign $D_{im}$ to every other $A[im]$. This procedure cannot create violations of requirement 2 in the definition of a valid labelling, and the result is a valid labelling for $\mathcal{I}$.

For the converse, assume that $V$ is a valid labelling for $\mathcal{I}$. Construct a truth assignment for $\mathcal{I}$ as follows: for every literal $l_{ij}$ such that $A[ij]$ is $T_{ij}$, if $l_{ij}$ is the positive literal $x_p$, then set $x_p$ to true under $S$, and if it is the negative literal $\overline{x_p}$, then set $x_p$ to false; set all unassigned variables to false. This procedure assigns a unique value to each variable in $\mathcal{I}$, since a valid labelling never assigns $T$-values to complementary literals. Since at least one literal in each clause is true under $S$, $S$ is a satisfying truth-assignment for $\mathcal{I}$. □

The reduction The idea of a valid labelling permits a reduction from a $k$SAT instance $I$ to a $k$-containment instance as illustrated below.

**Example 2.12** Consider the $k$SAT instance $I$ of Example 2.11, consisting of the two clauses $c_1 = \{x_1 + x_2 + \overline{x}_3\}$ and $c_2 = \{\overline{x}_1 + \overline{x}_4 + x_5\}$. We construct conjunctive queries $C_1$ and $C_2$ as follows.

Let us use the Datalog variable $L_{ij}$ to represent the $j$th literal in clause $c_i$. For example, $L_{11}$ represents the first literal in clause 1; that is, the occurrence of $x_1$ in $c_1$. Similarly, $L_{23}$ represents the literal $x_5$ in clause $c_2$. Further, the Datalog variables $T_{ij}$ and $D_{ij}$ respectively represent a choice of "true" or "don't care" for the $j$th literal in clause $c_i$.

The head of each of $C_1$ and $C_2$ will be the $O$-ary predicate $h$ (see Figure 2.5).

To represent the clause $c_1$, we construct the atom $c_1(L_{11}, L_{12}, L_{13})$ in the body of $C_2$, and the three possible destinations $c_1(T_{11}, D_{12}, D_{13}), c_1(D_{11}, T_{12}, D_{13}), c_1(T_{11}, D_{12}, D_{13})$. Note that any containment mapping from $C_2$ into $C_1$ enforces the fact that exactly one literal in clause $c_1$ is "true", as required by part (1) of the definition of a valid labelling (see Figure 2.5). We similarly construct an occurrence of a predicate $c_2$ in $C_2$ and three occurrences of this predicate in $C_1$ to represent the clause $c_2$.

Finally, we must impose requirement (2) in the definition of a valid labelling: that is, that no two complementary occurrences of any literal are both assigned "true". In our example, there is only one such violation: the first literal in $c_1$ and the first literal in $c_2$ are complementary. Hence, we construct a new "enforcer" predicate $e_{1121}$, and add the atom $e_{1121}(L_{11}, L_{21})$ to the body of $C_2$ and the three atoms $e_{1121}(T_{11}, D_{21}), e_{1121}(D_{11}, T_{21})$ and $e_{1121}(D_{11}, D_{21})$ to the body of $C_1$. The completed instance is shown in Figure 2.5.

Note that in general, the number of predicate repetitions added in the first stage is the maximum cardinality of any clause in the $k$SAT instance (i.e. $k$), and the number added in the second stage is always 3. □
3SAT instance: \[ c_1 = \{ x_1 + x_2 + \bar{x}_3 \} \quad c_2 = \{ x_1 + \bar{x}_4 + x_5 \} \]

Satisfying truth assignment: \( x_1 = \text{true}, x_4 = \text{false}, x_2, x_3, x_5 \) arbitrary.

Valid labelling: \(< < T_{11}, D_{12}, D_{13} > > \quad < D_{21}, T_{22}, D_{23} >> \)

\[
\begin{align*}
C_1 : h \leftarrow & c_1(T_{11}, D_{12}, D_{13}), \quad c_2(T_{21}, D_{22}, D_{23}), \quad \epsilon_{1121}(T_{11}, D_{21}), \\
& c_1(D_{11}, T_{12}, D_{13}), \quad c_2(D_{21}, T_{22}, D_{23}), \quad \epsilon_{1121}(D_{11}, T_{21}), \\
& c_1(D_{11}, D_{12}, T_{13}), \quad c_2(D_{21}, D_{22}, T_{23}), \quad \epsilon_{1121}(D_{11}, D_{21}).
\end{align*}
\]

\[
\begin{align*}
C_2 : h \leftarrow & c_1(L_{11}, L_{12}, L_{13}), \quad c_2(L_{21}, L_{22}, L_{23}), \quad \epsilon_{1121}(L_{11}, L_{21}).
\end{align*}
\]

Figure 2.5: Illustrating the construction.
We formalise the procedure as follows.

Let $I$ be a $k$SAT instance, for $k \geq 3$. We construct conjunctive queries $C_1$ and $C_2$ such that no predicate appears more than $k$ times in either query, such that no variable is repeated in any conjunct, and such that $C_1 \subseteq C_2$ iff $I$ has a valid labelling. Further, the construction will yield queries $C_1$ and $C_2$ such that $C_2 \subseteq C_1$; hence, $C_1 \equiv C_2$ iff $I$ is satisfiable. The time expended in the reduction is polynomial in the size of $C_1$ and $C_2$.

Algorithm 2.4
INPUT: A $k$SAT instance $I$
OUTPUT: Conjunctive queries $C_1$ and $C_2$ as above, such that $C_1 \subseteq C_2$ ($C_1 \equiv C_2$) iff $I$ is satisfiable

1. $C_1$ and $C_2$ each has the rule head $h$ (with no arguments). That is, the relation for $h$ is one of $true$ and $false$. 3

2. for $1 \leq i \leq p$
3. Consider the $i$th clause $c_i = \{l_{i1} + \ldots + l_{in_i}\}$
4. Create new nondistinguished variables $L_{i1}, \ldots, L_{in_i}$ and the predicate symbol $c_i$
5. Add to the body of $C_2$ the atom $c_i(L_{i1}, \ldots, L_{in_i})$
6. add $n_i \ c_i$-atoms to the body of $C_1$, where the $j$th argument of the $i$th such atom is $T_{ij}$ and the $r$th argument is $D_{ir}$ for all $r \neq j$
7. for $1 \leq i < j \leq p$
8. for $1 \leq l \leq n_i, 1 \leq m \leq n_j$
9. if $l_{il}$ and $l_{jm}$ are complementary literals
10. create a new predicate constant $e_{ijlm}$
11. add $e_{ijlm}(L_{il}, L_{jm})$ to the body of $C_2$
12. add $e_{ijlm}(T_{il}, D_{jm}), e_{ijlm}(D_{il}, T_{jm})$ and $e_{ijlm}(D_{il}, D_{jm})$ to $C_1$

The algorithm is clearly polynomial. Define conjuncts that are added to the bodies of $C_1$ and $C_2$ in Steps 5 and 6 to be $Class 1$ conjuncts, and those that are added at Steps 11 and 12 to be $Class 2$ conjuncts. $C_2$ contains no repetitions of any predicate. $C_1$ contains at most $k$ repetitions of $Class 1$ predicates, and three repetitions of $Class 2$ predicates. Note that all conjuncts are rectified (that is, have no repeated arguments), and have arity at most $k$.

3 For a reader who is offended by a 0-ary predicate, identical results may be obtained by making $h(X)$ the head of each rule, and adding the atom $a(X)$ to each rule body.
Lemma 2.4 There is a containment mapping \( f : C_2 \rightarrow C_1 \) iff \( \mathcal{I} \) has a valid labelling.

Proof. Assume \( f \) is a containment mapping from \( C_2 \) into \( C_1 \). Construct a labelling for \( \mathcal{I} \) by setting \( A[ij] \) to be \( f(L_{ij}) \) for all \( i \) and \( j \). The possible destinations for Class 1 atoms require that condition 1 in the definition of a valid labelling is satisfied; similarly, the possible destinations for Class 2 atoms enforce condition 2, and the labelling thus constructed is valid.

Assume \( V \) is a valid labelling for \( \mathcal{I} \). Construct a function \( f \) on the variables of \( C_2 \) by setting \( f(L_{ij}) \) to the value of \( A[ij] \) for all \( i \) and \( j \), and extend \( f \) to atoms (see Section 2.2.1). Since \( f(h) = h \), the head mapping exists. By condition 1 in the definition of a valid labelling, and by construction, each Class 1 atom in \( C_2 \) has exactly one possible destination in \( C_1 \) under \( f \). The possible destinations for Class 2 atoms, along with condition 2 in the definition of a valid labelling, ensure the functionality of \( f \). \( \square \)

Lemma 2.5 \( C_2 \subset C_1 \).

Proof. The function defined by \( f(D_{ij}) = f(T_{ij}) = L_{ij} \) is a containment mapping from \( C_1 \) into \( C_2 \). \( \square \)

Theorem 2.6 Algorithm 2.4 is correct.

Corollary. 3-containment (3-equivalence) is \( \mathcal{NP} \)-complete.

Proof. By Algorithm 2.3, Theorem 2.4 and Theorem 2.5, we conclude that 3-containment is polynomially equivalent to 3-containment, and is hence \( \mathcal{NP} \)-complete. \( \square \)

Related results Chandra and Merlin ([10]) have shown that testing conjunctive query containment is \( \mathcal{NP} \)-complete even for function-free queries, although their result assumes up to six repetitions of each predicate in the bodies of the queries. Sagiv and Yannakakis ([29]) have shown that the problem is \( \mathcal{NP} \)-complete even if no predicate appears more than three times in the body of either query; however, their reduction assumes the repetition of variables in the arguments of some conjuncts.

2.3 Applications

Let us turn to the complexity of the optimization problems that we discussed in Chapter 1. It turns out that the results of the previous section allow us to show that restricted versions of the one-boundedness, sequencability and basis-linearizability problems are \( \mathcal{NP} \)-hard, and that the algorithms of Section 1.5.3 are polynomial.

2.3.1 Approach and notation

The \( \mathcal{NP} \)-hardness results of this section are based on the following idea. Given any 3SAT instance, the techniques of the preceding section permit us to construct conjunctive queries

\[
C_1: \ h \ := \ B_1.
\]

\[
C_2: \ h \ := \ B_2.
\]
such that \( C_1 \subset C_2 \) iff the 3SAT instance is satisfiable. That is, \( B_1 \) and \( B_2 \) are the bodies of the conjunctive queries generated by Algorithm 2.5. Let us abuse notation by saying that \( B_1 \subset B_2 \) whenever there is a conjunct mapping \( M : B_2 \Rightarrow B_1 \); that is, a consistent choice of destinations (in \( B_1 \)) for the atoms in \( B_2 \). Now, the conjunctive query \( C_1 \) is contained in the conjunctive query \( C_2 \) iff there is a conjunct mapping from \( B_2 \) into \( B_1 \), since \( h \) (the head of \( C_1 \) and \( C_2 \)) is a 0-ary predicate. Hence, the original 3SAT instance is satisfiable iff \( B_1 \subset B_2 \). Note also that by construction, there is a conjunct mapping \( B_1 \Rightarrow B_2 \); that is, that \( B_2 \subset B_1 \).

**Example 2.13** Consider the conjunctive queries \( C_1 \) and \( C_2 \) of Example 2.12. The conjunctions \( B_1 \) and \( B_2 \) are as follows.

\[
B_1 : c_1(T_{11}, D_{12}, D_{13}), c_1(D_{11}, T_{12}, D_{13}), c_1(D_{11}, D_{12}, T_{13}),
\]
\[
c_2(T_{21}, D_{22}, D_{23}), c_2(D_{21}, T_{22}, D_{23}), c_2(D_{21}, D_{22}, T_{23}),
\]
\[
e_1121(T_{11}, D_{21}), e_1121(D_{11}, T_{21}), e_1121(D_{11}, D_{21}).
\]
\[
B_2 : c_1(L_{11}, L_{12}, L_{13}), c_2(L_{21}, L_{22}, L_{23}), e_1121(L_{11}, L_{21}). \; \Box
\]

Now, the \( \mathcal{NP} \)-hardness results of the following subsections are obtained by embedding the conjunctions \( B_1 \) and \( B_2 \) (perhaps with added arguments) into the bodies of recursive rules, such that the resulting rules have desired properties iff \( B_1 \subset B_2 \). Let us adopt the convention that for any variable \( X \), \( X|B_1 \) denotes the conjunction \( B_1 \) in which each conjunct is given the additional first argument \( X \).

**Example 2.14** Consider the conjunction \( B_2 \) of Example 2.13. The rule

\[
p(X) : - p(U), X|U|B_2.
\]

stands for the rule

\[
p(X) : - p(U), c_1(X, U, L_{11}, L_{12}, L_{13}), c_2(X, U, L_{21}, L_{22}, L_{23}), e_1121(X, U, L_{11}, L_{21}). \; \Box
\]

Finally, let us adopt the convention that in “unwinding” a recursion, every nondistinguished variable in a rule is renamed by “priming” at each stage of the expansion: that is, a nondistinguished variable \( U \) in the body of a rule is renamed

\[
\overbrace{U' \ldots U'}^i
\]

(written \( U^{(i)} \)) for some \( i \). For a linear recursion, the version of a nondistinguished variable \( U \) at depth \( i+1 \) is the variable \( U^{(i)} \).

**Example 2.15** Consider the linear rule of Example 2.14. Figure 2.6 exhibits our notation on expansions of \( p(X) \) using this rule. \( \Box \)

Let us return to the conjunctions \( B_1 \) and \( B_2 \) as described at the beginning of this section. Let \( B_j^{(i)} \) denote the conjunction \( B_j \) (that is, one of \( B_1 \) and \( B_2 \)) in which every variable is primed \( i \) times. It is clear that if \( B_1^{(i)} \subset B_2^{(k)} \) for any \( i \) and \( k \), then \( B_1 \subset B_2 \).
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Figure 2.6: Priming.

2.3.2 One-boundedness

Consider the safe, (not necessarily function-free) recursive rule

\[ r_1 : p(\vec{X}) := p(\vec{U}_1), \ldots, p(\vec{U}_n), a_1(\vec{W}_1), \ldots, a_k(\vec{W}_k). \]

where \( \vec{X} \) is a vector of distinct variables. Recall that the sirup \( r_1 \) is said to be \( 1 \)-bounded if every top-down expansion of \( p(\vec{X}) \) using \( r_1 \) is contained in a top-down expansion of depth at most 1. Recall also our convention that the top-down expansion representing the rule

\[ \epsilon : p(\vec{X}) := p(\vec{X}). \]

has depth 0. If \( r_1 \) is 1-bounded, then the program consisting of \( r_1 \) and any basis rule of the form

\[ r_2 : p(\vec{X}) := b(\vec{X}). \]

may be reduced to a nonrecursive program, in which \( r_1 \) is replaced by the rule

\[ r'_1 : p(\vec{X}) := b(\vec{U}_1), \ldots, b(\vec{U}_n), a_1(\vec{W}_1), \ldots, a_k(\vec{W}_k). \]

Kanellakis ([20]) has shown that deciding 1-boundedness is \( \mathcal{NP} \)-hard for linear sirups defining a predicate of arity four; however, the reduction involves an unbounded number of repetitions of EDB predicates in the body of the sirup. We present the following result.

**Theorem 2.7** Let \( r_1 \) be a linear, Datalog, head-rectified sirup defining a binary predicate, such that no EDB predicate appears more than four times in its body, or has arity greater than five. Testing 1-boundedness is \( \mathcal{NP} \)-hard for such rules.
Proof. Given a 3SAT instance \( \mathcal{I} \), construct the conjunctive queries \( C_1 : h \leftarrow B_1 \) and \( C_2 : h \leftarrow B_2 \), as in Algorithm 2.4. We construct a program \( \mathcal{P} \) that is 1-bounded iff there is a conjunct mapping \( M : B_2 \Rightarrow B_1 \). Recall that by construction, \( B_1 \Rightarrow B_2 \). \( \mathcal{P} \) is the sirup

\[
r : \text{p}(X, Y) : \text{p}(X, U), \text{e}(X, Y), \text{e}(V, Y), f(X, U), f(V, U), X|R|B_1, V|S|B_2
\]

where \( X, Y, U, V, R \) and \( S \) are distinct variables not appearing in \( B_1 \) or \( B_2 \), and where \( p, e \) and \( f \) are distinct predicate symbols not appearing in \( B_1 \) or \( B_2 \).

Consider the top-down expansions \( r^2 \), \( \epsilon \) and \( r \) (see Figure 2.5).

\( \mathcal{P} \) is 1-bounded iff \( r^2 \subset \epsilon \) or \( r^2 \subset r \). In either case, the head mapping induces the assignment set \( \{ X := X, Y := Y \} \). The nondistinguished variable \( U' \) appears in the \( p \)-atom generated by \( r^2 \), so that the only choice of destination for the body of \( \epsilon \) violates the head mapping, and thus \( r^2 \not\subset \epsilon \).
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Thus, if $\mathcal{P}$ is 1-bounded, then $r^2 \subseteq r$. The destination for the atom $p(X, U)$ in $r$ requires that $U := U'$. Then, the possible destinations for the atom $f(V, U)$ require that $V := X$ or $V := V'$, and the possible destinations for $e(V, Y)$ require that $V := X$ or $V := V'$. Thus, the conjunct mapping $M : r \Rightarrow r^2$ must assign $V := X$, and we may conclude that there is a conjunct mapping $V[S|B_2 \Rightarrow X|R|B_1$ or $V[S|B_2 \Rightarrow X|R'|B_1'$, as desired.

For the converse, assume $C_1 \subseteq C_2$; then $B_2 \Rightarrow B_1$. We may select the destination of $X|R|B_1$ to be $X|R|B_1$, and select the destination of every other atom in $r_1$ as in the previous paragraph, to obtain a conjunct mapping from $r$ into $r^2$. By Theorem 1.7, $\mathcal{P}$ is one-bounded. □

On the other hand, we may use Algorithm 2.3 to decide 1-boundedness in polynomial time, for linear sirups in which no predicate is repeated in the body of the recursive rule (i.e., $n = 1$ and the $a_i$ are distinct in $r_1$). The reason is that testing 1-boundedness reduces to two 2-containment tests.

Algorithm 2.5
INPUT: A sirup $r_1$ as described above, with $n = 1$ and with no predicate repetitions among the $a_i$.
OUTPUT: "yes" if the sirup is 1-bounded, "no" otherwise.

1. Construct the empty rule $\epsilon : p(\overline{x}) := p(\overline{x})$, and the top-down expansion $r_1 r_1$.

2. Use Algorithm 2.3 to determine whether $r_1 r_1 \subseteq \epsilon$ or $r_1 r_1 \subseteq r_1$. If either containment holds, return "yes"; otherwise, return "no".

□

Theorem 2.8 Algorithm 2.5 is correct.
Proof. Necessity follows by the definition of 1-boundedness, and sufficiency by Theorem 1.7. □

Theorem 2.9 Algorithm 2.5 runs in polynomial time for arbitrary sirups, and in NLOGSPACE (and hence in $\mathcal{NC}$) for Datalog queries.
Proof. Step (1) may be performed in polynomial time for arbitrary sirups, and in LOGSPACE for Datalog queries. The proof follows by Theorem 2.4 and the fact that NLOGSPACE is in $\mathcal{NC}$ ([9]). □

Finally, we show that Algorithm 1.1 (see Section 1.5.3) runs in polynomial time.

Theorem 2.10 Algorithm 1.1 runs in polynomial time.
Proof. Each containment in the algorithm is an instance of the 2-containment problem. □
2.3.3 Rule sequencability

Consider the safe, Datalog, linear rules

\[ r_1 : p(\vec{X}) := p(\vec{U}_0), a_1(\vec{U}_1), \ldots a_k(\vec{U}_k). \]
\[ r_2 : p(\vec{X}) := p(\vec{W}_0), b_1(\vec{W}_1), \ldots b_l(\vec{W}_l). \]

where \( \vec{X} \) is a vector of distinct variables. Define \( \epsilon \) to be the following rule.

\[ \epsilon : p(\vec{X}) := p(\vec{X}). \]

Recall that \( r_1 \) is sequencable under \( r_2 \) if \( (r_1 + r_2)^* \subseteq r_2^* \). Rule sequencability is not known to be decidable. However, the problem is at least as hard as any problem in \( \mathcal{NP} \), as the following theorem shows.

**Theorem 2.11** Let \( r_1 \) and \( r_2 \) be rules as above, with the additional restrictions that no predicate appears more than three times in the body of \( r_1 \) or more than once in the body of \( r_2 \), and that all predicates have arity at most four. Detecting rule sequencability is \( \mathcal{NP} \)-hard for rules of this form.

**Proof.** Consider an arbitrary 3SAT instance \( I \), and apply Algorithm 2.5 to obtain conjunctive queries \( C_1 : h := B_1 \) and \( C_2 : h := B_2 \). We construct rules \( r_1 \) and \( r_2 \) such that \( C_1 \subseteq C_2 \) iff \( r_1 \) is sequencable under \( r_2 \). By the discussion of the beginning of this section, we know that \( B_1 \Rightarrow B_2 \), and that \( C_1 \subseteq C_2 \) iff \( B_2 \Rightarrow B_1 \). The rules \( r_1 \) and \( r_2 \) are

\[ r_1 : p(X, Y, Z, W) := p(Y, X, Z, W), X|B_1. \]
\[ r_2 : p(X, Y, Z, W) := p(X, Y, W, Z), X|B_2. \]

where \( X, Y, Z \) and \( W \) are new, distinct variables and \( g \) is a new predicate symbol.

Note that the \( p \)-atom in the expansions \( r_1^* \) and \( r_2^* \) is \( p(X, Y, W, Z) \), so \( r_1^* \) and \( r_2^* \) are contained in \( \epsilon \) and each rule is 1-bounded.

Assume \( r_1 \) is sequencable under \( r_2 \). Then \( r_1 r_2 \) is contained in some expansion in \( r_2^* r_1^* \).

By the 1-boundedness of \( r_1 \) and \( r_2 \), \( r_1 r_2 \) must be contained in one of \( \epsilon \), \( r_1 \), \( r_2 \) and \( r_2 r_1 \) (see Figure 2.8). In each case, the head mapping induces the assignment set \( \{ X := X, Y := Y, Z := Z, W := W \} \). However, in the first three containments, the destination for the \( p \)-atom generated by the expansion is inconsistent with the head mapping, and we may conclude that \( r_1 r_2 \subseteq r_2 r_1 \).

Consider any conjunct mapping \( M : r_2 r_1 \Rightarrow r_1 r_2 \) (see Figure 2.8). As we observed, the head mapping yields the assignment \( \{ X := X \} \). Now, by definition (see the introduction to this section), the first argument of every atom in the conjunctions \( X|B_2 \) and \( X|B_1 \) is \( X \), and therefore both these conjunctions must map to the conjunction \( X|B_1 \) in \( r_1 r_2 \). Hence, the conjunct mapping \( M \) must map \( X|B_2 \) and \( X|B_1 \) into \( X|B_1 \), so \( B_2 \Rightarrow B_1 \), as required.

For the converse, assume that \( B_2 \Rightarrow B_1 \). Then the mapping \( M \) indicated in Figure 2.8 proves that \( r_1 r_2 \subseteq r_2 r_1 \), which in turn suffices to prove sequencability by Theorem 1.9. \( \Box \)

In view of the lack of a known algorithm to detect sequencability, a variety of conditions have been proposed that are sufficient (but not necessary) to detect sequencability in pairs
Figure 2.8: The construction of Theorem 2.11.
of linear rules. The most popular condition is that of commutativity, \( r_1 r_2 \subseteq r_2 r_1 \). The more general condition \( r_1 r_2^* \subseteq r_2 r_1^* \) was proposed independently by Ramakrishnan et al. ([25]) and Ioannidis ([17]); the former shows that the condition is verifiable in polynomial space. The following theorem considers the complexity of such conditions.

**Theorem 2.12** Let \( r_1 \) and \( r_2 \) be rules obeying the conditions of Theorem 2.11. Then testing each of the following conditions, each sufficient to prove the sequencability of \( r_1 \) under \( r_2 \), is \( \mathbf{NP} \)-hard.

(a) \( r_1 \subseteq r_2 \)

(b) \( r_1 = r_2 \)

(c) \( r_1 \subseteq r_2^* \)

(d) \( r_1 r_2 \subseteq r_2 r_1 \)

(e) \( r_1 r_2 = r_2 r_1 \)

(f) \( r_1 r_2 \subseteq r_2 r_1^* \).

**Proof.** Let \( T \) be a 3SAT instance, and let \( B_1 \) and \( B_2 \) be the conjunctions resulting from the application of Algorithm 2.5. We provide reductions such that conditions (a) - (f) are satisfied iff there is a conjunct mapping \( M : B_2 \Rightarrow B_1 \).

To prove (a), (b) and (c), we construct the rules

\[
\begin{align*}
r_1 &: p(X,Y) \leftarrow p(Y,X), B_1. \\
r_2 &: p(X,Y) \leftarrow p(Y,X), B_2.
\end{align*}
\]

The observation that each rule is 1-bounded, and that \( B_1 \Rightarrow B_2 \) by construction, suffices to complete the proof.

The construction of Theorem 2.11 yields \( \mathbf{NP} \)-hardness reductions for conditions (d) - (f). \( \square \)

Conditions (a), (b), (d) and (e) are each in \( \mathbf{NP} \); conditions (c) and (f) may be tested in polynomial space by the chase algorithm of Ramakrishnan et al. ([25]).

Theorem 2.10 implies that the conditions (a) through (f) can probably not be tested in polynomial time. However, conditions (a), (b), (d) and (e) reduce to the testing of containments among pairs of conjunctive queries, and Theorem 2.4 may apply to these conditions over various classes of rules that arise in practice. For example, if \( r_1 \) and \( r_2 \) each have no repetitions of predicates in their respective bodies, then this algorithm provides a polynomial-time test of conditions (a),(b),(d) and (e). Ioannidis ([16]) has also proposed an algorithm to test commutativity (condition (e)) in this restricted case.

### 2.3.4 Basis-linearizability

Consider the safe, simple recursive rule

\[
r_1 : p(\bar{X}) \leftarrow p(\bar{U}_1), \ldots, p(\bar{U}_n), e_1(\bar{W}_1), \ldots, e_k(\bar{W}_k).
\]
where $n > 1$ and $\overline{X}$ is a vector of distinct variables. Recall that $r_1$ is basis-linearizable if, for every basis rule

$$r_2 : p(\overline{X}) \leftarrow b(\overline{X}).$$

we may replace $r_1$ with the rule

$$r'_1 : p(\overline{X}) \leftarrow b(\overline{U}_1), \ldots, b(\overline{U}_{n-1}), p(\overline{U}_n), e_1(\overline{W}_1), \ldots, e_k(\overline{W}_k).$$

to obtain an equivalent program. The linear rule $r'_1$ is obtained from the nonlinear rule $r_1$ by replacing all but the last occurrence of $p$ with a corresponding occurrence of the basis predicate $b$. Recall that basis-linearizability indicates that right-linearity is the normal form for the conjunctive queries generates by the program. That is, the sirup $r_1$ is basis-linearizable iff every top-down expansion of $p(\overline{X})$ using $r_1$ is contained in a right-linear expansion.

Linearizability of this sort was investigated by Zhang et al. ([40] 4), who claim a polynomial-time decision procedure for bilinear, function-free rules with one nonrecursive subgoal (i.e., $n = 2$ and $k = 1$), although (as we will show in the next chapter) their proof is flawed. In Chapter 3, we will extend their result to include all bilinear recursions, as long as no nonrecursive predicate appears more than once in the body of the rule. We will also show that the algorithm runs in polynomial time.

Basis-linearizability is not known to be decidable in the case in which predicates are allowed to appear repetitively among the subgoals. Ramakrishnan et al. ([25]) show that detecting basis-linearizability in bilinear recursions is $\mathcal{NP}$-hard; their reduction involves a recursive predicate of arity 6, and places no bound on the number of predicate repetitions in the body of the rule. We tighten that result in the following theorem.

**Theorem 2.13** Let $r_1$ be a bilinear rule as above, with the restrictions that $p$ has arity 2, all other predicates have arity at most 5, and no predicate appears more than four times in the body of $r_1$. Then, deciding basis-linearizability is $\mathcal{NP}$-hard for rules of this form.

**Proof.** Let $I$ be a 3SAT instance to which Algorithm 2.5 has been applied to produce conjunctions $B_1$ and $B_2$. We construct a rule $r_1$ that is basis-linearizable iff there is a conjunct mapping $M : B_2 \Rightarrow B_1$. Note that $B_1 \Rightarrow B_2$ by construction. The rule is

$$r_1 : p(X,Y) \leftarrow p(X,U), p(T,Y), e(X,Y), e(V,Y), f(X,U), f(V,U), X|R|B_1, V|S|B_2.$$

where $X, Y, U, T, V, R$ and $S$ are new and distinct variables.

If the rule $r_1$ is basis-linearizable, then the tree $T_1$ in Figure 2.9 is contained in a right-linear tree (a top-down expansion in which only $p(T,Y)$ is expanded through $r_1$). By convention, the empty rule

$$e : p(X,Y) \leftarrow p(X,Y).$$

is a right-linear tree of depth 0.

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4This paper has recently been published in TOH 14(1), but the proof has been omitted.
Since \( p(X, Y) \) is not a leaf in \( T_1 \), every destination for \( p(X, Y) \) among the leaves of \( T_1 \) is inconsistent with the head mapping, and we may conclude that \( T_1 \not\geq \epsilon \); that is, \( T_1 \) is contained in a right-linear tree \( T_2 \) in which the head is expanded using rule \( r_1 \).

Now, the head mapping from \( T_2 \) into \( T_1 \) induces the assignments \( \{ X := X, Y := Y \} \). Hence, the atom \( p(X, U) \) must have destination \( p(X, U') \). and every conjunct mapping from \( T_2 \) into \( T_1 \) must induce the assignment \( U := U' \). The only destinations for \( e(V, Y) \) consistent with these assignments force \( V := X \) or \( V := V' \), and the only such destinations for the atom \( f(V, U) \) force the assignments \( V := V' \) or \( V := X \). Hence, every conjunct mapping \( M : T_2 \Rightarrow T_1 \) must induce the assignment \( V := X \), forcing the mapping \( V|S|B_2 \Rightarrow X|R|B_1 \) or \( V|S|B_2 \Rightarrow X|R'|B_1' \); in either case, we may conclude \( B_2 \Rightarrow B_1 \).

For sufficiency, assume that \( B_2 \Rightarrow B_1 \). Then, the conjunct mappings in the previous paragraph, along with the partial mappings \( p(T, Y) \rightarrow p(T, Y) \) and \( X|R|B_1 \rightarrow X|R|B_1 \), suffice to prove basis-linearizability by Theorem 1.18. \( \square \)

Finally, we justify our claim that Algorithm 1.2 (in Section 1.5.3) runs in polynomial time.

**Theorem 2.14** Algorithm 1.2 runs in polynomial time.

**Proof.** Each containment test in the algorithm is an instance of the 2-containment problem. \( \square \)
Chapter 3

A decision procedure for basis-linearizability

3.1 Introduction

Consider the safe and function-free ("Datalog") logic program $P$ with a single doubly-recursive ("bilinear") rule of the form

$$r_1 : \ p(X_1, \ldots, X_m) \ : \ = \ \ p_{(1)}(\vec{Y}), p_{(2)}(\vec{Z}), e_1(\vec{U}_1), \ldots, e_N(\vec{U}_N).$$

and a single basis rule of the form

$$r_2 : \ p(X_1, \ldots, X_m) \ : \ = \ b(X_1, \ldots, X_m).$$

where we have subscripted the recursive occurrences of $p$ for ease of reference. We will refer to atoms in the body of the recursive rule by their principal functors, using the subscripts to disambiguate the recursive atoms; that is, the term "$p_{(1)}" will be used to refer to $p_{(1)}(\vec{Y})$ (the first recursive $p$-atom in the body of $r_1$), and the term "$e_i" to refer to the atom $e_i(\vec{U}_i)$.

We assume that the rules $r_1$ and $r_2$ satisfy the following requirements.

1. The variables appearing in the head are distinct. Recall that these variables variables are termed distinguished, and that all other variables are termed nondistinguished.

2. The rules are range-restricted or safe; that is, every distinguished variable appears in the rule body.

3. The base predicate $b$ and the subgoals $e_i$ are EDB predicates, and these predicates are distinct. Recall from Chapter 1 that EDB relations are stored by extension in the database, and that the predicate $p$ is termed intensional or IDB.

Recall that $P$ is termed linearizable by basis iff right-linearity is a normal form for the proof trees (or conjunctive queries) generated by the program. That is, $P$ is basis-linearizable iff $P$ is equivalent to the following linear program $Q$. 
$r_1 : \ p(X_1, \ldots, X_m) \leftarrow b(\bar{Y}), p(\bar{Z}), e_1(\bar{U}_1), \ldots, e_N(\bar{U}_N)$.  \\
$r_2 : \ p(X_1, \ldots, X_m) \leftarrow b(X_1, \ldots, X_m)$. \\

$Q$ is obtained from $P$ by replacing the first recursive occurrence of $p$ in the body of $r_1$ (that is, the atom $p(\bar{Y})$) with the base atom $b(\bar{Y})$.

**Example 3.1** We repeat here the program of Example 1.1, computing the transitive closure of $b$.

$r_1 : \ p(X, Y) \leftarrow p(X, U), p(U, Y)$.  \\
$r_2 : \ p(X, Y) \leftarrow b(X, Y)$.

$p(X, U)$, the first recursive atom in $r_1$, is referred to as $p_{(1)}$, and $p(U, Y)$ as $p_{(2)}$. Recall that we proved this program to be basis-linearizable in Section 1.5.2; that is, the program is equivalent to the following linear program.

$r_1' : \ p(X, Y) \leftarrow b(X, U), p(U, Y)$.  \\
$r_2 : \ p(X, Y) \leftarrow b(X, Y)$.

The gains of performing the transformation are obtained from the use of query evaluators specific to linear recursions.  \\

In this chapter, we present a decision procedure for the recognition of basis-linearizability in bilinear recursions of the form of $P$. The running time of the algorithm is polynomial in the size of the program $P$.

### 3.1.1 Related results

Consider the program $P$ of the preceding section. As we showed in Chapter 2, if repetitions are allowed in the EDB subgoals of the recursive rule in this program, then the detection of basis-linearizability is $NP$-hard; in fact, the decidability of basis-linearizability for such programs is open. In this chapter, we show that if no such repetitions are allowed, then basis-linearizability may be detected in polynomial time; hence, in some sense, our result represents a boundary between tractability and intractability. Finally, as we will show in the next chapter, if we consider programs with a single bilinear rule, an unbounded number of linear rules and 5 basis rules, then the detection of basis-linearizability becomes undecidable.

This chapter is an extension of the work of Zhang, Yu and Troy ([40] ) who proposed the problem of basis-linearizability in the restricted case $N \leq 1$; that is, in the case in which the recursive rule has at most one EDB subgoal. They claim a polynomial time algorithm for this case; however, the proof of correctness of their algorithm is flawed, and we will touch upon this flaw in Section 3.5.3. Their algorithm also ignores so-called deletion-linearizable recursions, on the grounds that such programs may be linearized in a different way (see Section 3.4).

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1. In fact, it can be performed in linear time.  
2. This result has recently been published in TODS ([41]), but the proof has been omitted.
3.2. **THE ALGORITHM**

The algorithm of [40] does not extend in an obvious way to the programs that we consider (in which \(N\) is unbounded). That is, the representation of \(e_1, \ldots, e_N\) as their "join" (a single atom), followed by an application of the algorithm of [40], is insufficient to detect basis-linearizability. The following example illustrates this point.

**Example 3.2** Consider the program

\[
\begin{align*}
    r_1 & : \ p(X, Y) :- p(X, U), p(U, Y), c(U), d(Y). \\
    r_2 & : \ p(X, Y) :- b(X, Y).
\end{align*}
\]

where \(b, c\) and \(d\) are distinct EDB predicates. This program is basis-linearizable, as the algorithm of Section 3.2 shows. Assume that we represent the EDB predicates \(c\) and \(d\) by their Cartesian product, in some new EDB predicate \(e\). Then, we obtain the program

\[
\begin{align*}
    r_1 & : \ p(X, Y) :- p(X, U), p(U, Y), e(U, Y). \\
    r_2 & : \ p(X, Y) :- b(X, Y).
\end{align*}
\]

which is not basis-linearizable, as the algorithm of Section 3.2 also shows. □

The proof of [40] also does not extend directly to the proof of correctness of our algorithm. Both their proof and ours rely heavily on the idea of safety; that is, on the requirement that every distinguished variable appears in the rule body. In the case \(N = 1\), every distinguished variable \(X_i\) must appear among the arguments of \(p_{(1)}, p_{(2)}\) or the single EDB subgoal \(e_1\) by the assumption of safety; however, if \(N\) is unbounded, then \(X_i\) may appear as the only argument to some "new" EDB predicate \(e_j\).

### 3.2 The Algorithm

In this section, we present an algorithm that decides whether the program \(\mathcal{P}\) is basis-linearizable, and show that the algorithm is polynomial in the size of \(\mathcal{P}\).

Let us say that a nondistinguished variable that appears only in the arguments of the atom \(t\) in \(r_1\) is said to be **local** to \(t\); all other arguments are termed **nonlocal**.

Recall that we will refer to atoms in the body of the rules in \(\mathcal{P}\) by their principal functors, using subscripts to disambiguate the recursive \(p\)-atoms.

**Definition 3.1** We say that \(p_{(1)}\) is an **adjunct** to \(p_{(2)}\) in \(\mathcal{P}\) if there is a partial mapping \(p_{(1)} \to p_{(2)}\) that induces an assignment set that is the identity on nonlocal variables in \(p_{(1)}\). That is, \(p_{(1)}\) is obtainable from \(p_{(2)}\) by replacing 0 or more occurrences of each variable in \(p_{(2)}\) with a new, local variable. If \(p_{(1)}\) is an adjunct, then \(\mathcal{P}\) is said to be **deletion-linearizable**. □

The intuitive importance of adjuncts is that they may be deleted from the recursive rule to produce an equivalent, linear program, as we will show in Section 3.4.

**Definition 3.2** Define \(r_1 - p_{(1)}\) to be the rule \(r_1\) in which \(p_{(1)}\) has been deleted, and let \(\mathcal{P} - p_{(1)}\) be the resulting program. If \(p_{(1)}\) is an adjunct to \(p_{(2)}\), then every distinguished
variable appearing among the arguments of \( p(1) \) also appears in \( p(2) \), so we conclude that this deletion preserves safety. □

For any atom \( t \) in the rule \( r_1 \), or in any top-down expansion, let us use the notation \( t[i] \) to refer to the \( i \)th argument of \( t \). We will always reserve the keyword \( X_i \) to refer to the \( i \)th distinguished variable in the head of the recursive rule.

**Definition 3.3** The *home* position of any distinguished variable \( X_i \) is the \( i \)th position in any \( p \)-atom. □

**Definition 3.4** \( p(1) \) is said to be a *trivial* adjunct to \( p(2) \) if \( p(1) \) is an adjunct, \( p(1) \) contains no nonlocal nondistinguished variables and, whenever the distinguished variable \( X_i \) appears in \( p(1) \), then \( p(2)[i] \) is \( X_i \) (that is, \( X_i \) appears in its home position in \( p(2) \)). □

**Example 3.3** Consider the program \( P \) defined as below.

\[
\begin{align*}
    r_1 & : p(X,Y,W,Z) \leftarrow p(U,X,A,B), p(X,X,A,W), e(Y,W,Z). \\
    r_2 & : p(X,Y,W,Z) \leftarrow b(X,Y,W,Z).
\end{align*}
\]

The nondistinguished variables \( U \) and \( A \) are local to \( p(1) \) (that is, to the atom \( p(U,X,A,B) \)). The atom \( p(1) \) is an adjunct to the atom \( p(2) \) (that is, the atom \( p(X,X,A,W) \)); in fact, \( p(1) \) is a trivial adjunct since \( X \) appears in its home position in \( p(2) \). The rule \( r_1 \rightarrow p(1) \) is presented below.

\[
r_1 \rightarrow p(1) : p(X,Y,W,Z) \leftarrow p(X,X,A,W), e(Y,Z).
\]

Note that this rule is safe. □

Recall from Chapter 1 that top-down expansions generated by \( P \) are written in a way that preserves the left-to-right order of the subgoals in every rule, and that an expansion or proof tree is termed *right-linear* if only the rightmost \( p \)-atom in the recursive rule is ever recursively expanded. Finally, recall that a top-down expansion generated by \( P \) is termed *open* if only the recursive rule is used in constructing the expansion.

**Example 3.4** The expansions \( T_1, T_2, T_3 \) and \( T_4 \) of Figure 3.1 are all open. \( T_1 \) is the minimal violation of right-linearity in \( P \), and the expansions \( T_2, T_3 \) and \( T_4 \) are the right-linear expansions of depth 0, 1 and 2 respectively. □

We will use the terms *tree* and *expansion* interchangeably. As we mentioned in Chapter 1, these expansions may all be constructed in time that is polynomial in the size of \( P \).

Now, let \( f \) be a containment mapping (equivalently, \( M \) a conjunct mapping) from \( T_2 \), \( T_3 \) or \( T_4 \) into \( T_1 \). Recall from Section 1.5.2 that the mapping \( f \) (or \( M \)) is termed *acceptable* if, under the mapping, the \( p(2) \)-child of the root of \( T_1 \) is the destination of no \( p(1) \)-leaf.
Figure 3.1: Expansions used in the algorithm.
Example 3.5 Consider the transitive-closure program of Example 3.1. The containment mapping \( f \) defined by \( f(X) = X, f(Y) = Y, f(U) = U', f(U') = U \) is an acceptable mapping from \( T_4 \) into \( T_1 \), as indicated in Figure 3.2. □

We now state the main results of this chapter.

**Theorem 3.1** \( \mathcal{P} \) is basis-linearizable iff at least one of the following is true.

1. \( p_{(1)} \) is a trivial adjunct to \( p_{(2)} \) in \( \mathcal{P} \);
2. \( p_{(1)} \) is an adjunct, and \( \mathcal{P} - p_{(1)} \) is 1-bounded; or
3. There is an acceptable mapping from one of \( T_2, T_3 \) and \( T_4 \) into \( T_1 \). □

The proof of this theorem is an extensive combinatorial analysis, and will occupy the remainder of this chapter. Before we begin this proof, let us observe that the algorithm implied by Theorem 3.1 is polynomial in the size of \( \mathcal{P} \).

**Theorem 3.2** The procedure of Theorem 1 is in NLOGSPACE.

**Corollary 1.** The procedure of Theorem 1 is in \( \text{AC} \).

**Corollary 2.** The procedure of Theorem 1 is polynomial.

**Proof.** Determining whether \( p_{(1)} \) is an adjunct, or a trivial adjunct, is easily determined in LOGSPACE, so Condition (1) is in LOGSPACE. \( \mathcal{P} - p_{(1)} \) is a linear sirup with no repeated
3.3. PROOF OUTLINE

EDB subgoals; by Theorem 2.9, Condition (2) is in NLOGSPACE. By a case analysis on the destinations of the $p_{(1)}$-atom in $T_3$ and $T_4$, Condition (3) may be tested through nine 2-containment tests, each of which may be accomplished in NLOGSPACE by Theorem 2.4. Hence, the algorithm is in NLOGSPACE. Corollary 2 follows by [9], and Corollary 3 immediately follows. □

3.3 Proof Outline

In Section 3.4, we will investigate the behaviour of programs in which $p_{(1)}$ is an adjunct to $p_{(2)}$, and show that in this case, the recursive atom $p_{(1)}$ is redundant in the recursive rule $r_1$. Section 3.5 contains the proof of Theorem 3.1.

3.4 Adjuncts

Let us assume that $p_{(1)}$ is an adjunct to $p_{(2)}$ in $P$. It turns out that, in this case, the atom $p_{(1)}$ is redundant in the recursive rule $r_1$; hence, we call such programs deletion-linearizable. We will prove this fact in the remainder of this subsection. As before, by the form of the basis rule, we will restrict our attention to proof trees (ground or otherwise) in which the basis rule is never used. That is, we adopt the convention that $p$ itself is both an EDB and an IDB relation. In this subsection, we will consider ground or instantiated expansions: that is, trees in which all variables have been replaced by constants.

An important property of adjuncts is treated in the following lemma.

**Lemma 3.1** If $p_{(1)}$ is an adjunct to $p_{(2)}$, then any $p$-fact that unifies with $p_{(2)}$ also unifies with $p_{(1)}$, and the unifications agree on the values of all nonlocal variables in $p_{(1)}$.

**Proof.** Let $f$ represent the assignment set induced by the partial mapping $p_{(1)}(\tilde{Y}) - p_{(2)}(\tilde{Z})$, and assume that $p(a_1, \ldots, a_m)$ unifies with $p_{(2)}(\tilde{Z})$ under the substitution $\tau$. The function $\tau(f)$ is then a substitution under which $p_{(1)}$ unifies with $p(a_1, \ldots, a_m)$. Since $f$ is the identity on nonlocal variables, $\tau$ and $\tau(f)$ agree on these variables. □

**Definition 3.5** Let $T$ be a proof tree (or expansion) generated by $P$. The right strut of $T$ is the proof tree (or expansion) obtained from $T$ by discarding all $p_{(1)}$-atoms. □

**Lemma 3.2** If $p_{(1)}$ is an adjunct, then for any tree $T$ generated by $P$ from any database $D$, the right strut of $T$ is a proof tree generated by $P - p_{(1)}$ from $D$ and yielding the same fact as $T$.

**Corollary.** $P \subseteq P - p_{(1)}$.

**Proof.** Straightforward induction on the depth of the right strut of $T$. □

**Example 3.6** Consider the program $P$ of Example 3.3, in which $p_{(1)}$ is an adjunct to $p_{(2)}$. The right strut of the expansion of Figure 3.3 (a) is shown in Figure 3.3 (b). □
Lemma 3.3 Consider any database $D$, and assume that $p_{(1)}$ is an adjunct. For $n \geq 1$, if $S$ is a proof tree of depth $n$ generated by $\mathcal{P} - p_{(1)}$ from $D$, then there is a complete tree $R$ of depth $n$ that is generated by $\mathcal{P}$ from $D$ such that $S$ is the right strut of $R$.

Corollary 1. $\mathcal{P} - p_{(1)} \subseteq \mathcal{P}$.

Corollary 2. $\mathcal{P} \equiv \mathcal{P} - p_{(1)}$.

Proof. The proof is a straightforward induction on $n$, using Lemma 3.1. For the basis ($n = 1$), let $S$ be the proof tree

$$
p(\bar{a})
\begin{array}{c}
p(2)(\bar{b})
\end{array}
\begin{array}{c}
e_1(\bar{e}_1)
\end{array}
\begin{array}{c}
\ldots
\end{array}
\begin{array}{c}
e_N(\bar{e}_N)
\end{array}
$$

By Lemma 3.1, $\mathcal{P}$ generates the proof tree $R$ defined as

$$
p(\bar{a})
\begin{array}{c}
p(1)(\bar{b})
\end{array}
\begin{array}{c}
p(2)(\bar{b})
\end{array}
\begin{array}{c}
e_1(\bar{e}_1)
\end{array}
\begin{array}{c}
\ldots
\end{array}
\begin{array}{c}
e_N(\bar{e}_N)
\end{array}
$$

For the induction, assume the truth of the hypothesis for $1 \leq i < n$. Let $S$ be a tree of depth $n$ as in Figure 3.4, in which the top level of the expansion is the ground query

$$
p(\bar{a}) := p_{(2)}(\bar{b}), e_1(\bar{e}_1), \ldots, e_N(\bar{e}_N).
$$

and where $p_{(2)}(\bar{b})$ is generated from $\mathcal{P} - p_{(1)}$ by a tree $I$ of depth $n - 1$. By hypothesis, $\mathcal{P}$ generates a complete tree $J$ of depth $n - 1$ from the leaves of $I$, establishing the fact $p(\bar{b})$, for which $I$ is a right strut. By Lemma 3.1, $\mathcal{P}$ generates a complete proof tree of depth $n$ establishing the fact $p(\bar{a})$, such that the first level of the proof tree is the query

$$
p(\bar{a}) := p_{(1)}(\bar{b}), p_{(2)}(\bar{b}), e_1(\bar{e}_1), \ldots, e_N(\bar{e}_N).
$$

and where the subtrees establishing $p_{(1)}$ and $p_{(2)}$ are both $J$ (see Figure 3.4).

The proof of Corollary 1 is immediate. Corollary 2 is proved using Lemma 3.2.  \(\square\)
Figure 3.1: The induction
3.5 Proof

This section will be devoted to the proof of Theorem 3.1.

Recall that an expansion is termed open if the basis rule is never used in constructing the expansion, and closed iff there are no \( p \)-leaves in it; that is, the basis rule is used to “close off” all intensional atoms in the latter case. Recall also that an expansion or proof tree is termed right-linear if only the \( p(2) \)-atom in the recursive rule is ever recursively expanded (see Figure 3.6.)

By definition, \( \mathcal{P} \) is basis-linearizable iff every non-right-linear closed expansion is contained in some closed right-linear expansion (see Section 1.4.3). However, the form of the basis rule permits us to deal exclusively with open expansions; that is, the application of the basis rule to an open expansion amounts to the “renaming” of every \( p \)-leaf in the open expansion to the EDB predicate \( b \), and every closed expansion is obtainable in this manner. Thus, \( \mathcal{P} \) is basis-linearizable iff every open expansion is contained in a right-linear, open expansion. We may now think of the basis-linearizability of the sirup \( r_1 \) as the right-linearity of the proof trees generated by \( r_1 \) from every database, for every set of initialisation rules. The proof of correctness of Theorem 3.1 will be based exclusively on open expansions.

The outline of the proof is as follows.

3.5.1 Proof outline

1. In Section 3.5.2, we will show that the conditions of Theorem 3.1 are sufficient to show that each non-right-linear expansion is contained in a right-linear expansion; that is, that these conditions suffice to prove basis-linearizability in \( \mathcal{P} \).

2. Section 3.5.3 is the heart of this chapter. In this section, we prove that the conditions
3.5. PROOF

of Theorem 3.1 are necessary for \( \mathcal{P} \) to be basis-linearizable. The proof of necessity proceeds as follows, under the assumption of basis-linearizability in \( \mathcal{P} \). Note that, in this case, the minimal violation of right-linearity (expansion \( T_1 \) in Figure 3.6) must be contained in some right-linear expansion (\( T_5 \) in Figure 3.6).

(a) If \( p_{(1)} \) is an adjunct to \( p_{(2)} \), then \( p_{(1)} \) is trivial or \( \mathcal{P} - p_{(1)} \) is one-bounded.

(b) Assume that the minimal violation of right-linearity (expansion \( T_1 \) in Figure 3.7) is contained in a right-linear expansion of depth at most 1 (one of \( T_2 \) and \( T_3 \) in Figure 3.7); then, the containment is provable by an acceptable containment mapping.

(c) Assume that \( T_1 \) is contained in a right-linear expansion of depth at least 2 (see Figure 3.8). Then one of the following must hold.

- \( p_{(1)} \) is an adjunct to \( p_{(2)} \).
- \( T_1 \) is contained in a right-linear expansion of depth at most 1.
- \( T_1 \) is contained in the right-linear of depth 2, and the containment is provable by an acceptable mapping. In fact, the mapping must have the form shown in Figure 3.9.

3.5.2 Sufficiency

In this section, we prove that the conditions of Theorem 3.1 are each sufficient to prove basis-linearizability in \( \mathcal{P} \). The sufficiency of Condition 3 follows by Theorem 1.8. Consider Conditions 1 and 2.

Recall our convention that \( t[i] \) refers to the \( i \)th argument of the atom \( t \), and that \( p_{(1)} \) is
Figure 3.7: Assume $T_1 \subset T_2$ or $T_1 \subset T_3$

Figure 3.8: Assume $T_1 \subset T_5$. 
said to be a trivial adjunct to \( p(2) \) if \( p(1) \) is an adjunct, \( p(1) \) contains no nonlocal nondistinguished variables and, whenever the distinguished variable \( X_i \) appears in \( p(1) \), then \( p(2)[i] \) is \( X_i \) (that is, \( X_i \) appears in its “home” position in \( p(2) \)). Throughout this chapter, \( X_i \) will always be used to refer to the \( i \)th distinguished variable in the head of the recursive rule.

Consider any tree \( T \). We assume that every nondistinguished variable \( U \) in \( r_1 \) is renamed by “priming” at each successive level of the expansion; that is, the version of \( U \) in sibling atoms in \( T \) is renamed to the new variable obtained by superscripting \( U \) with a “\( i \)” \( i \) times for some \( i \) (written \( U^{(i)} \)). If \( T \) is a linear expansion (that is, at most one \( p \)-atom is recursively expanded at any level), then the version of \( U \) at depth \( i \) in the expansion is \( U^{(i-1)} \). Figure 3.6 illustrates this convention.

Let \( q = q^1 \) represent the version of the atom \( q \) at depth 1 in a tree \( T \). If \( s \) is an atom in \( T \), then \( p(s)_j \) represents the atom \( s \) in the subtree \( T \) of some tree \( S \) that is rooted at the atom \( p(s)_j \). By convention, \( p(s)_j \) is the \( p(s)_j \)-atom obtained by expanding \( p(s)_j^{(i-1)} \) through the recursive rule \( r_1 \).

**Example 3.7** Consider the transitive-closure program of Example 3.1. The right-linear expansion of depth 3 has leaves and arguments as shown in Figure 3.10. ⊓⊔

**Trivial adjuncts** satisfy the following property.

**Lemma 3.4** Assume that \( p(1) \) is a trivial adjunct to \( p(2) \) in \( \mathcal{P} \). For all right-linear expansions \( T \) of depth \( n \), for all integers \( i, j < n \), and for all \( l \):

1. If \( p(1)[l] \) is the distinguished variable \( X_k \), then \( p(2)^l p(1)[l] \) is also \( X_k \); and

2. Any \( p \)-atom that unifies with \( p(2)^l p(1) \) unifies with \( p(2)^j p(1) \), and the unifications yield the same substitutions for all variables that are nonlocal to either of these two atoms in the conjunctive query represented by \( T \).
Proof. Assume \( p_{(1)}[l] \) is \( X_k \). Since \( p_{(1)} \) is a trivial adjunct, \( p_{(2)}[k] \) is \( X_k \). A straightforward induction on \( r \geq 1 \) shows that \( p_{(2)}^r[k] \) is \( X_k \), which immediately implies 1.

To prove 2, we note that the only nonlocal variables that appear in \( p_{(1)} \) are distinguished variables, which (by 1) appear in the same positions in \( p_{(2)}^r p_{(1)} \) and \( p_{(2)}^r p_{(1)} \). All other variables in \( p_{(1)} \) are local in \( r_1 \), and their primed versions therefore appear in only one atom in \( T \) (that is, \( U^{(1)} \) appears only in the atom \( p_{(2)}^r p_{(1)} \)).

Example 3.8 Consider the rule \( r_1 \) in Example 3.3. Figure 3.11 depicts an expansion using this rule. Note that \( X \) persists in its home position.

Lemma 3.5 Assume that \( p_{(1)} \) is a trivial adjunct to \( p_{(2)} \), and let \( S \) be a proof tree of depth \( k \) generated by \( \mathcal{P} - p_{(1)} \) from a database \( D \). Then \( \mathcal{P} \) generates a right-linear proof tree \( R \) of depth \( k \) from \( D \) such that \( S \) is its right strut (see Figure 3.12).

Corollary. If \( p_{(1)} \) is a trivial adjunct to \( p_{(2)} \), then \( \mathcal{P} \) is basis-linearizable.

Proof. \( S \) has only one \( p \)-leaf, say \( p_{(2)}^k \). We may eliminate all other \( p \)-facts from \( D \) without altering the fact produced by \( S \). By Lemma 3.3, \( \mathcal{P} \) generates a complete tree \( I \) with depth \( k \) from \( D \); hence, in \( I \), the atom \( p_{(2)}^k p_{(1)} \) unifies with the single \( p \)-fact in \( D \). By Lemma 3.4, all the atoms \( p_{(2)}^r p_{(1)} \) may be consistently unified with this \( p \)-fact to construct a right-linear proof tree \( R \) of depth \( k \) that is generated by \( \mathcal{P} \) from \( D \) (see Figure 3.12).

The corollary is proved by observing that, by Lemma 3.2, every proof tree generated by \( \mathcal{P} \) from a database \( D \) is also generated by \( \mathcal{P} - p_{(1)} \) from \( D \).

Lemma 3.6 Assume that \( p_{(1)} \) is an adjunct, and that \( \mathcal{P} - p_{(1)} \) is 1-bounded. Then \( \mathcal{P} \) is basis-linearizable.
Figure 3.11: Persistence of $X$.

Figure 3.12: Trees $S$ and $R$
Proof. Consider any database \( D \), and any proof-tree \( S \) of depth \( k \) generated by \( \mathcal{P} \) that establishes a fact \( p(\bar{a}) \). By Lemma 3.2, there is a proof tree \( I \) of depth \( k \) generated by \( \mathcal{P} - p_{(1)} \) that also establishes this \( p \)-fact. If \( \mathcal{P} \) is 1-bounded, then either \( p(\bar{a}) \in D \) or \( p(\bar{a}) \) is generated by \( \mathcal{P} - p_{(1)} \) using a tree \( J \) of depth 1. Applying Lemma 3.3 completes the proof.

\[ \square \]

3.5.3 Necessity

This section will be devoted to the proof of necessity of the conditions in Theorem 3.1. If \( \mathcal{P} \) is basis-linearizable, then every non-right-linear open expansion generated by \( \mathcal{P} \) is contained in a right-linear expansion (i.e., that \( T_1 \subset T_5 \) in Figure 3.13). We will focus our attention on containment mappings that must exist from right-linear expansions into the minimal violation of right-linearity (\( T_1 \) in Figure 3.13).

First, we will prove that if \( \mathcal{P} \) is basis-linearizable and \( p_{(1)} \) is an adjunct, then \( p_{(1)} \) is a trivial adjunct or \( \mathcal{P} - p_{(1)} \) is one-bounded.

Next, we will show that if \( T_1 \) is contained in a right-linear expansion of depth at most 1 under an unacceptable containment mapping (see Figure 3.14), then \( p_{(1)} \) is an adjunct to \( p_{(2)} \).

The remaining subsections concerns mappings that cannot exist from long right-linear trees into \( T_1 \). Specifically, we will show that if \( T_1 \) is contained in a right-linear tree \( T_5 \) of depth at least 2 (see Figure 3.15), then one of the following holds.

1. \( p_{(1)} \) is an adjunct to \( p_{(2)} \).

2. \( T_1 \) is contained in an expansion of depth at most 1.
Figure 3.14: Unacceptable mapping from $T_3$ into $T_1$.

Figure 3.15: Assume $T_1 \subset T_5$
3. $T_5$ has depth 2, and the containment mapping is acceptable. In fact, the mapping is of the form shown in Figure 3.16.

This procedure completes our proof. While reading these subsections, keep in mind the fact that if $f$ is a containment mapping from some tree $S$ into some tree $T$, the notation $f(q) = w$ implies that $q$ is a leaf in $S$ and $w$ is a leaf in $T$.

**Notation** We will use the following notation to describe the arguments of $p$-atoms in the rule body. The expression

$$p_i(\overline{A \vec{X}})$$

denotes the situation that some variable $A$ appears in position $i$ in $p_i$, the distinguished variable $X_i$ appears in position $j$ and the distinguished variable $X_j$ appears in position $k$. Unless otherwise stated, $A$ is an arbitrary variable (perhaps $X_i$), and any or all of $\{i,j,k\}$ may be equal.

**Necessity of conditions 1 and 2**

Assume that $\mathcal{P}$ is basis-linearizable. We will prove that, if $p_{(1)}$ is an adjunct to $p_{(2)}$ in $\mathcal{P}$, then either $\mathcal{P} - p_{(1)}$ is one-bounded or $p_{(1)}$ is trivial. Recall that nondistinguished variables in $r_1$ will be consistently renamed in each tree by priming.

**Lemma 3.7** If $f$ is a containment mapping from any tree $S$ into any tree $T$, then $f(X_i) = X_i$ for every distinguished variable $X_i$.

**Proof.** Both trees have the root $p(X_1, \ldots, X_m)$. $\square$

Assume that $p_{(1)}$ is an adjunct to $p_{(2)}$. Consider the expansion $T_6$ of Figure 3.17(b); since $\mathcal{P}$ is assumed to be basis-linearizable, the top-down expansion described by $T_6$ in
Figure 3.17: $T_8 \subset T_6 \subset T_9$
Figure 3.17 is contained in some right-linear expansion $T_9$. Assume, now, that $\mathcal{P} - p_{(1)}$ is not one-bounded; we will show that $p_{(1)}$ is a trivial adjunct to $p_{(2)}$. By Lemma 3.3, the right strut $T_8$ of $T_6$ is contained in $T_6$, and we may conclude that $T_8$ is contained in $T_9$ (see Figure 3.17). Thus, $T_8 \subset T_9$, and $T_9$ has height at least two since $\mathcal{P} - p_{(1)}$ is assumed not to be 1-bounded.

Let $f$ be a containment mapping from $T_9$ into $T_8$. Note that the only $p$-leaf in $T_8$ is $p_{(2)}[p_{(2)}]$, and this leaf must be the destination of every $p$-leaf in $T_9$.

**Lemma 3.8** If $p_{(1)}[j]$ is $X_i$, then $p_{(2)}[i]$ is $X_i$.

*Proof.* By the definition of an adjunct, $p_{(2)}[j]$ is $X_i$. The picture is

$$p_{(1)}( X_i ) \quad p_{(2)}( \overset{i}{C} X_i )$$

The mapping $f(p_{(1)}) = p_{(2)}[p_{(2)}]$ forces $f(X_i) = C$. Since $f$ preserves distinguished variables, $C = X_i$. □

**Lemma 3.9** No nonlocal nondistinguished variable appears in $p_{(1)}$.

*Proof.* Assume that the nonlocal nondistinguished variable $A$ appears in position $i$ in $p_{(1)}$; by the definition of an adjunct, $p_{(2)}[i] = A$. The picture is

$$p_{(1)}( A ) \quad p_{(2)}( A )$$

Examine the lowest two levels of the tree $T_9$, which we assume has depth $n + 1$ for some $n > 0$. The destination for $p_{(2)}^{(n-1)}p_{(1)}$ forces $f(A^{(n-1)}) = A'$.

By safety, $X_i$ appears in the rule body. By Lemma 3.8, $X_i$ cannot appear in $p_{(1)}$. Assume that it appears in position $k$ in some $e_q$. Then, the $k$th argument of $p_{(2)}^{(n-1)}e_q$ is $A^{(n-1)}$. However, the $k$th argument of $e_q$ is $X_i$ by assumption, and the $k$th argument of $p_{(2)}e_q$ is therefore $A$ (see Figure 3.11 for an illustration). Further, these two atoms are the only possible destinations for $p_{(2)}^{(n-1)}e_q$ because of our assumption of no repeated EDB predicates in the recursive rule. Hence, the possible destinations for $p_{(2)}^{(n-1)}e_q$ forces $f(A^{(n-1)})$ to be a nonprimed variable, which is a contradiction. Hence, $X_i$ must appear in $p_{(2)}$ only, say in position $j \neq i$. The picture is

$$p_{(1)}( A ) \quad p_{(2)}( A X_i )$$

But then, the $j$th argument of $p_{(2)}^{(n+1)}$ is $A^{(n-1)}$, and the $j$-th argument of $p_{(2)}p_{(2)}$ is $A \neq A'$, a contradiction. □

By Lemmas 3.8 and 3.9, $p_{(1)}$ must be a trivial adjunct to $p_{(2)}$. 


Minimal programs

Let us say that \( \mathcal{P} \) is minimal iff the minimal violation of right-linearity (\( T_1 \) in Figure 3.18) is contained in a right-linear expansion of depth at most 1 (that is, in one of the expansions \( T_2 \) and \( T_3 \) in the same figure).

Assume that \( \mathcal{P} \) is basis-linearizable and minimal. We will show that if \( p_{(1)} \) is not an adjunct to \( p_{(2)} \), then there is an acceptable containment mapping from \( T_2 \) or \( T_3 \) into \( T_1 \). Since any mapping from \( T_2 \) into \( T_1 \) is acceptable, we will concern ourselves only with an unacceptable containment mapping \( f \) from \( T_3 \) into \( T_1 \); that is, a mapping in which \( f(p_{(1)}) = p_{(2)} \) (see Figure 3.19).

**Lemma 3.10** Assume that a nondistinguished variable \( A \) appears in an EDB subgoal \( \epsilon_q \), and that \( f \) is a containment mapping from a right-linear tree \( T_3 \) of depth at least 1 into \( T_1 \). Then \( f(A) = A \) or \( f(A) = A' \).

**Proof.** Assume that \( A \) appears in the \( k \)th position in \( \epsilon_q \). Since \( T_3 \) has depth at least 1, the atom \( \epsilon_q \) appears as a leaf. Because there are no repetitions of any EDB predicate in the subgoals of the recursive rule, the only \( \epsilon_q \)-atoms in \( T_1 \) are \( \epsilon_q \) and \( p_{(1)} \epsilon_q \); the \( k \)th argument of the former is \( A \) and the \( k \)th argument of the latter is \( A' \).

\[
\begin{align*}
\epsilon_q( A ) & \quad \epsilon_q( A ) \quad p_{(1)} \epsilon_q( A' ) \\
in T_3 & \quad in T_1 & \quad in T_1
\end{align*}
\]
Considering all possible destinations in $T_1$ for the $e_q$-leaf in $T_5$ suffices to complete the proof.

Recall our convention that $t[i]$ refers to the $i$th argument of the atom $t$.

**Lemma 3.11** Assume that $P$ is minimal, and that $f$ is a containment mapping from $T_3$ into $T_1$ under which the destination of $p_{(1)}$ is $p_{(2)}$ (see Figure 3.19). Then $p_{(1)}$ is an adjunct to $p_{(2)}$.

*Proof.* Assume that a distinguished variable $X_i$ appears in some position $j$ in $p_{(1)}$. By Lemma 3.7 and the assumed mapping $f(p_{(1)}) = p_{(2)}$, $p_{(2)}[j]$ is $X_i$. To complete the proof, we show that if any nondistinguished nonlocal variable $A$ appears in any position $i$ in $p_{(1)}$, then $A$ also occupies position $i$ in $p_{(2)}$. Assume the existence of a nondistinguished variable $A$ in the $i$th argument position in $p_{(1)}$, such that $A$ appears in $p_{(2)}$, or in some $e_q$.

If $A$ appears as an argument to some $e_q$, then by Lemma 3.10, $f(A)$ is $A$ or $A'$. Since no primed variable appears in $p_{(2)}$, the mapping $f(p_{(1)}) = p_{(2)}$ forces $p_{(2)}[i] = A$.

Assume now that $A$ appears in the $j$th position in the arguments of $p_{(2)}$. The picture is

$$p_{(1)}(i \quad j \quad B) \quad p_{(2)}(i \quad j \quad A)$$

Now, $B$ cannot be distinguished, otherwise by previous discussion, $A$ would also have to be distinguished. By the assumed mapping on $p_{(1)}$, we have $f(A) = C'$. Since the $j$th arguments of $p_{(1)}p_{(1)}$ and $p_{(1)}p_{(2)}$ are both primed variables, we conclude that $f(p_{(2)}) = p_{(2)}$. Then $f(A) = A$ and $C' = A$. □
3.5. PROOF

Connectivity

It turns out that if $\mathcal{P}$ is basis-linearizable and not minimal, then the p-atoms $p_1$ and $p_2$ in the body of the recursive rule must be connected. The primary tools used in the remainder of the proof are connectivity and safety.

Two atoms in the body of the recursive rule $r_1$ are said to be *directly connected* if they share a nondistinguished variable; *connectivity* is defined as the transitive closure of the direct connectivity relation. Similarly, two nondistinguished variables are connected if they appear in a pair of connected atoms. The special case of connectivity between the recursive atoms $p_1$ and $p_2$ is formally defined below; the formality is necessary to the results of the remainder of this chapter.

**Definition 3.6** Assume that the nondistinguished variable $A$ appears in the arguments of $p_1$, and that the nondistinguished variable $B$ appears in the arguments of $p_2$. We say that $A$ and $B$ are *directly connected* if $A = B$. The atoms $p_1$ and $p_2$ are said to be directly connected if they share a nondistinguished variable $A$. We say that $A$ and $B$ are *indirectly connected* if $A \neq B$, and if for $n > 0$, there are nondistinguished variables $U_1, \ldots, U_{n+1}$ and distinct EDB subgoals $e_{k_1}, \ldots, e_{k_n}$ such that

1. $A = U_1$.
2. $B = U_{n+1}$.
3. For $1 \leq i \leq n$, the variables $U_i$ and $U_{i+1}$ appear in the arguments of $e_{k_i}$.

The sequence $< e_{k_1}, \ldots, e_{k_n} >$ is termed a *connection sequence* between $A$ and $B$, and the sequence $< U_1, \ldots, U_{n+1} >$ is termed the *corresponding variable sequence*. 

\[ \Box \]

As we mentioned earlier, nondistinguished variables in $r_1$ will be consistently renamed in each tree by *priming*. That is, if $A$ is a nondistinguished variable, then its occurrences in any tree will be $A^{(i)}$ where $i$ is an integer indicating superscripts of $i$ ""s. Further, occurrences of the nondistinguished variables $A$ and $B$ in sibling atoms will bear the same superscript. If the tree is linear, then $A^{(i)}$ is the occurrence of $A$ at depth $i - 1$ in the tree.

Let $f$ be a containment mapping from a right-linear expansion $R$ of depth at least $1$ into an expansion $S$. Recall that if $f$ is a mapping from some tree $S$ into some tree $T$, the notation $f(q) = w$ implies that $q$ is a leaf in $S$ and $w$ is a leaf in $T$.

**Lemma 3.12** Assume that the nondistinguished variables $V$ and $W$ appear in the arguments of some EDB predicate $e_q$. For any $i$, assume that $f$ is a containment mapping from a right-linear tree $R$ of depth at least $(i + 1)$ into an expansion $S$, and let $V^{(i)}$ and $W^{(i)}$ be the respective occurrences of $V$ and $W$ at depth $(i + 1)$ in $R$. Then, there is some $j$ such that $f(V^{(i)}) = V^{(j)}$ and $f(W^{(i)}) = W^{(j)}$.

**Proof.** Assume that $V$ and $W$ appear in the positions $k$ and $l$ in $e_q$, respectively. The $k$th and $l$th arguments of the $e_q$-atom at depth $(i + 1)$ in $R$ are $V^{(i)}$ and $W^{(i)}$ respectively.
Since there are no EDB repetitions in the recursive rule, every $e_q$-atom in $S$ has $k$th and $l$th arguments $V^{(j)}$ and $W^{(j)}$ respectively, for some $j$. □

**Lemma 3.13** Assume that $R$ is a right-linear tree of depth $m$, $S$ is any expansion and $f$ if a containment mapping from $R$ into $S$. Assume that the nondistinguished variable $A$ in $p_{(1)}$ is connected to the variable $B$ in $p_{(2)}$. Then for $0 \leq i < m$, exactly one of the following is true.

1. $A = B$ and $f(A^{(i)}) = f(B^{(i)})$.

2. $A \neq B$, and there is some $j$ such that $f(A^{(i)}) = A^{(j)}$ and $f(B^{(i)}) = B^{(j)}$.

**Proof.** If $A$ and $B$ are directly connected, then $A = B$ and (1) above is true. If $A$ and $B$ are indirectly connected, then $A \neq B$.

Let

$$< e_{k_1}, \ldots, e_{k_n} >$$

be a connection sequence between $A$ and $B$, and let

$$< U_1, \ldots, U_{n+1} >$$

be the corresponding variable sequence. Recall that $A = U_1$ and $B = U_{n+1}$. We show that (2) above is true.

Consider the possible destinations for the atom $p_{(2)}^{i} e_{k_1}$, which contains the variables $A^{(i)} = U_1^{(i)}$ and $U_2^{(i)}$. By Lemma 3.12, there is some $j$ such that $f(A^{(i)}) = A^{(j)}$ and $f(U_2^{(i)}) = U_2^{(j)}$. If $U_2 = B$, then the result follows. Otherwise, the variables $U_2^{(i)}$ and $U_3^{(i)}$ appear in the leaf $p_{(2)}^{i} e_{k_2}$; the use of Lemma 3.12 and the single-valuedness of $f$ shows that $f(U_3^{(i)}) = U_3^{(j)}$. An inductive repetition suffices to complete the proof. □

Note that the assumption that there are no EDB repetitions in the body of the recursive rule is essential to the proof of Lemmas 3.12 and 3.13.

In the remainder of this subsection, we will show that if $P$ is basis-linearizable, but $p_{(1)}$ and $p_{(2)}$ are not connected, then $P$ is minimal. Recall that that $P$ is termed minimal if the small non-right-linear tree $T_1$ is contained in a right-linear tree of height at most one (that is, in one of $T_2$ and $T_3$).

**Lemma 3.14** If $P$ is basis-linearizable and not connected, then $P$ is minimal.

**Proof.** Assume that $f$ is a containment mapping from some right-linear tree $T_5$ of height $n > 1$ into $T_3$. We construct a containment mapping $g$ from $T_3$ into $T_1$. We define the destinations of $g$ as follows: $g$ preserves the destination of $p_{(1)}$, and of any $e_q$ connected to $p_{(1)}$; all other atoms in $r_1$ are mapped to "themselves" under $g$. More formally, we partition nondistinguished variables into two classes. A nondistinguished variable is termed *tied* if it appears in $p_{(1)}$ or in any predicate that is connected to $p_{(1)}$, and *free* otherwise. We define $g$ as under.
3.5. **Proof**

\[ g(V) = \begin{cases} 
V & \text{if } V \text{ is distinguished} \\
f(V) & \text{if } V \text{ is tied} \\
V & \text{if } V \text{ is free} 
\end{cases} \]

It is easily seen that \( g \) is a containment mapping from the depth-1 expansion \( T_3 \) into \( T_1 \) (see Figure 3.20). \( \square \)

**Non-minimal programs**

Finally, let us turn our attention to the case in which the minimal violation of right-linearity (\( T_1 \) in Figure 3.21) is contained in a right-linear expansion \( T_5 \) of depth at least 2 (see Figure 3.21).

Assume that \( \mathcal{P} \) is basis-linearizable, and that \( f \) is a containment mapping from \( T_5 \) into \( T_1 \). By a case analysis on the possible destinations for the leaf \( p_{(1)} \) (at depth 1) in the right-linear tree \( T_5 \), we will show the following.

1. If \( f(p_{(1)}) = p_{(1)}p_{(1)} \) and \( \mathcal{P} \) is not minimal, then \( T_5 \) has depth 2, \( f(p_{(2)}p_{(1)}) = p_{(3)}p_{(2)} \) and \( f(p_{(2)}p_{(2)}) = p_{(2)} \); i.e., \( f \) is an acceptable containment mapping. (Recall that an expression of the form \( f(t) = s \) means that \( t \) is a leaf in the containing tree, and \( s \) is a leaf in the contained tree). Figure 3.22 describes this claim.

2. If \( f(p_{(1)}) = p_{(1)}p_{(2)} \) or \( f(p_{(1)}) = p_{(2)} \) (see Figure 3.23), then \( p_{(1)} \) is an adjunct to \( p_{(2)} \) or \( \mathcal{P} \) is minimal.
Let us end this section with some observations on the nature of the containment mapping $f$.

**Lemma 3.15** If the nondistinguished variable $A$ appears in some $e_q$, then $f(A) = A$ or $f(A) = A'$, and $f(A') = A$ or $f(A') = A'$.

*Proof.* Assume the presence of the atom

\[ e_q(\tilde{A}) \]

in $r_1$. Since $T_5$ is of depth at least 2, the two leaves

\[ e_q(\tilde{A}) \quad p_{(2)}e_q(\tilde{A'}) \]

must appear in it. Since there are no subgoal repetitions in $r_1$, the only $e_q$-atoms in $T_1$ are of the form

\[ e_q(\tilde{A}) \quad p_{(1)}e_q(\tilde{A'}) \]

\[ \square \]

**Lemma 3.16** Assume that the following variables appear in the indicated positions in $r_1$:

\[ p_{(1)}(\tilde{C}) \quad p_{(2)}(\tilde{A}) \quad e_q(\tilde{X}_i) \]

Then $f(A)$ is $X_i$ or $C$.

*Proof.* Since $T_5$ is of height at least 2, the atom $p_{(2)}e_q$ exists in $T_5$, with form $e_q(\tilde{A})$. The only $e_q$-atoms in $T_1$ are of the form $e_q(\tilde{C})$ and $e_q(\tilde{A})$. \[ \square \]
Figure 3.22: The case \( f(p_{(1)}) = p_{(1)}p_{(1)}. \)
The case \( f(p_{(1)}) = p_{(1)} p_{(2)} \) Assume that \( \mathcal{P} \) is basis-linearizable. Then the minimal violation \( T_1 \) of right linearity (see Figure 3.24) is contained in a right-linear expansion \( T_5 \). Assume that \( T_5 \) has depth at least 2, and that \( f \) is a containment mapping from \( T_5 \) into the minimal violation \( T_1 \), such such that \( f(p_{(1)}) = p_{(1)} p_{(1)} \) (see Figure 3.24(a)). We will show that \( \mathcal{P} \) is minimal, or that \( f(p_{(2)} p_{(1)}) = p_{(2)} \), \( T_5 \) has height 2 and \( f(p_{(2)} p_{(2)}) = p_{(2)} \) (see Figure 3.24(b)).

If \( p_{(1)} \) and \( p_{(2)} \) are not connected, then \( \mathcal{P} \) is minimal by Lemma 3.14. Assume that \( p_{(1)} \) and \( p_{(2)} \) are connected. The mapping \( f(p_{(1)}) = p_{(1)} p_{(1)} \) yields the following results.

Definition 3.7 We say that \( p_{(1)} \) is invariant if whenever any distinguished variable \( X_i \) appears in it, then \( p_{(1)}[i] \) is \( X_i \). That is, \( X_i \) (also) appears in its "home" position in \( p_{(1)} \).

Lemma 3.17 Assume that \( p_{(1)} \) is invariant. If \( X_i \) appears in any position \( j \) in \( p_{(1)} \), then \( p_{(1)}[j] = X_i \).

Proof. By invariance, \( p_{(1)}[i] = X_i \), and our result follows immediately.

Lemma 3.18 If \( f(p_{(1)}) = p_{(1)} p_{(1)} \), then \( p_{(1)} \) is invariant, and \( f(A) = A' \) for all distinguished variables \( A \) in \( p_{(1)} \). Further, any variable \( B \) in \( p_{(2)} \) that is connected to a variable \( A \) in \( p_{(1)} \) also satisfies \( f(B) = B' \).

Proof. Assume that \( X_i \) appears in position \( j \neq i \) in \( p_{(1)} \). The picture is

\[
p_{(1)}( i, j, X_i )
\]

The \( j \)th argument of \( p_{(1)} p_{(1)} \) is \( C \). By the assumed mapping \( f(p_{(1)}) = p_{(1)} p_{(1)} \), \( f(X_i) = C \); since \( f(X_i) = X_i \), our result follows. Otherwise, if \( X_i \) appears in \( p_{(1)} \), then it occupies position \( i \). Hence, \( p_{(1)} \) is invariant.
Figure 3.24: The case $f(p_{(1)}) = p_{(1)}p_{(1)}$. 

(a) Assumption.

(b) Conclusion.
If the nondistinguished variable \( A \) appears in the \( i \)th position in \( p_{(1)} \), then \( A' \) appears in the \( i \)th position in \( p_{(1)}p_{(1)}' \); hence, \( f(A) = A' \). If a nondistinguished variable \( B \) appearing in \( p_{(2)} \) is connected to \( A \), then \( f(B) = B' \) by Lemma 3.13. □

**Proving that** \( f(p_{(2)}p_{(1)}) = p_{(1)}p_{(2)} \). We now prove that \( f(p_{(2)}p_{(1)}) = p_{(1)}p_{(2)} \). Recall that \( f \) is a containment mapping from a right-linear expansion \( T_5 \) of depth at least 2 into the minimal violation \( T_1 \), such that \( f(p_{(1)}) = p_{(1)}p_{(1)} \).

**Definition 3.8** Define a **Class 1** variable to be a distinguished variable \( X_j \) that appears only among the arguments of \( p_{(2)} \) (that is, \( X_j \) does not appear in the arguments of \( p_{(1)} \) or any \( e_q \)). Define a **Class 2** variable to be a Class 1 variable \( X_j \) that appears in some position \( k \neq j \) in the arguments of \( p_{(2)} \), but does not appear in position \( j \) (its “home” position). Define a **Class 3** variable to be a Class 2 variable \( X_k \), such that the \( k \)th argument of \( p_{(2)} \) is some Class 2 variable \( X_j \). That is, the arguments of \( p_{(2)} \) are as follows, where \( C \neq X_j \) and \( X_j \neq X_k \).

\[
p_{(2)}( \hat{C} \hat{X}_j \hat{X}_k )
\]

For \( 1 \leq i \leq 3 \), an argument position \( l \) is termed **Class j** iff \( p_{(2)}[l] \) is a Class \( j \) variable. □

**Lemma 3.19** Let \( l \) be a Class 3 position. Then \( X_i \) is a Class 3 variable.

**Proof.** Assume that \( X_k \) is a Class 3 variable appearing as the \( l \)th argument of \( p_{(2)} \). By definition, \( k \neq l \). The picture is as follows, where \( X_j \) and \( X_k \) appear only in \( p_{(2)} \), \( j \neq k, k \neq l \) and \( C \neq X_j \).

\[
p_{(2)}( \hat{C} \hat{X}_j \hat{X}_k )
\]

By safety, \( X_i \) appears in \( p_{(1)} \), \( p_{(2)} \) or some \( e_q \). Since \( X_k \) does not appear in \( p_{(1)} \) and \( X_k \neq X_i \), \( X_i \) cannot appear in any \( e_q \) by Lemma 3.16. Assume, now that \( X_i \) appears in \( p_{(1)} \); by invariance, it must occupy position \( l \). Since \( T_5 \) has depth at least 2, one of the atoms \( p_{(2)}p_{(2)} \) or \( p_{(2)}p_{(2)}p_{(1)} \) must appear as a leaf, and the \( l \)th argument of each of these atoms is \( X_j \). Since \( X_j \) does not appear in \( p_{(1)} \), it cannot appear in either of the leaves \( p_{(1)}p_{(1)} \) or \( p_{(1)}p_{(2)} \) in \( T_1 \); further, the \( l \)th argument of \( p_{(2)} \) is \( X_k \), which is distinct from \( X_j \) by assumption. Hence, neither of the atoms \( p_{(2)}p_{(2)} \) and \( p_{(2)}p_{(2)}p_{(1)} \) has a legal destination in \( T_1 \). Hence, by safety, \( X_i \) must appear only in \( p_{(2)} \) and our result follows. □

**Lemma 3.20** For all \( i \), \( i \) is a Class 3 position iff \( X_i \) is a Class 3 variable.

**Proof.** The “only if” follows from Lemma 3.19. For the converse, note that by definition, if there are \( k \) Class 3 variables then there are at least \( k \) Class 3 positions; our result follows by Lemma 3.19 and by pigeonholing, recalling the fact that all distinguished variables are distinct. □

**Lemma 3.21** The arguments of \( p_{(1)} \) and \( p_{(2)} \) cannot be of the form

\[
p_{(1)}( \hat{A} ) \quad \quad p_{(2)}( \hat{J} \hat{X}_j )
\]
where \( A \) and \( B \) are connected nondistinguished variables and \( X_j \) appears only in \( p_{(2)} \).

**Proof.** Assume the converse. Since \( B \) is nondistinguished, \( j \neq k \); that is, \( X_j \) is a Class 2 variable. By Lemma 3.18, \( f(B) = B' \), and \( p_{(1)} \) is invariant. By safety, \( X_k \) must appear in \( p_{(1)}, p_{(2)} \) or some \( e_q \).

Since \( X_j \) does not appear in \( p_{(1)} \), Lemma 3.16 prohibits \( X_k \) from appearing in any \( e_q \). If \( X_k \) appears only in \( p_{(2)} \), then it is a Class 3 variable; by Lemma 3.20, \( k \) must be a Class 3 position, and \( X_j \) a Class 3 variable; but \( p_{(1)}[j] \) is nondistinguished, a contradiction. Hence, \( X_k \) must appear in the arguments of \( p_{(1)} \), and must occupy position \( k \) by invariance. The picture is

\[
p_{(1)}( \overline{A} \overline{X_k} ) p_{(2)}( \overline{B} \overline{X_j} )
\]

Now, one of \( p_{(2)}p_{(2)} \) and \( p_{(2)}p_{(2)}p_{(1)} \) must appear as a leaf in \( T_5 \), and \( B \) appears as the \( k \)th argument of each of these leaves. However, the \( k \)th argument of each leaf in \( T_1 \) is a nonprimed variable, contradicting the fact that \( f(B) = B' \). \( \square \)

**Lemma 3.22** Assume that the arguments of \( p_{(1)} \) and \( p_{(2)} \) are as follows

\[
p_{(1)}( \overline{A} ) p_{(2)}( \overline{B} )
\]

where \( A \) and \( B \) are connected nondistinguished variables. Then \( p_{(1)}[j] \) is \( X_j \).

**Proof.** By Lemma 3.18 and connectivity, \( f(B) = B' \). By safety, \( X_j \) must appear in the body. However, by Lemma 3.16, it cannot appear in \( e_q \). By Lemma 3.21, \( X_j \) cannot appear only in \( p_{(2)} \). Hence, \( X_j \) must appear in \( p_{(1)} \), and the result follows by invariance. \( \square \)

**Lemma 3.23** Let \( f \) be a containment mapping from a right-linear expansion \( T_5 \) of depth at least 2 into the minimal violation \( T_1 \), and assume that \( \mathcal{P} \) is not minimal. Then \( f(p_{(2)}p_{(1)}) = p_{(1)}p_{(2)} \).

**Proof.** Since \( \mathcal{P} \) is not minimal, \( p_{(1)} \) and \( p_{(2)} \) must be connected. By Lemma 3.22, we must have the following situation, where \( A \) and \( B \) are connected nondistinguished variables.

\[
p_{(1)}( \overline{A} \overline{X_j} ) p_{(2)}( \overline{B} )
\]

By Lemma 3.18, \( f(A) = A' \) and \( f(B) = B' \). Now, the \( j \)th argument of \( p_{(2)}p_{(1)} \) is \( B \), but the \( j \)th arguments of the leaves \( p_{(1)}p_{(1)} \) and \( p_{(2)} \) in \( T_1 \) are not \( B' \); that is, the \( p \)-leaves in \( T_1 \) are as below.

\[
p_{(1)}p_{(1)}( \overline{j} \overline{X_j} ) p_{(1)}p_{(2)}( \overline{j} \overline{B'} ) p_{(2)}( \overline{j} \overline{B} )
\]

Hence, \( f(p_{(2)}p_{(1)}) = p_{(1)}p_{(2)} \). \( \square \)
$T_5$ has height 2 Recall that a Class 1 variable is a distinguished variable that appears only in the arguments of $p_{(2)}$, and that any position in $p_{(2)}$ that is occupied by a Class 1 variable is a Class 1 position. It turns out that for all $i$, $X_i$ is a Class 1 variable iff $i$ is a Class 1 position.

Lemma 3.24 For all $i$, if $i$ is a Class 1 position, then $X_i$ is a Class 1 variable.

Corollary. $i$ is a Class 1 position iff $X_i$ is a Class 1 variable.

Proof. Assume that $i$ is a Class 1 position; that is, $p_{(2)}[i]$ is a variable $X_k$ that appears only in $p_{(2)}$. If $k = i$ then the result follows. Assume $k \neq i$. By safety, $X_i$ appears in $p_{(1)}$, some $e_q$ or $p_{(2)}$. By Lemma 3.16 and since $X_k$ (by assumption) does not appear in $p_{(1)}$, $X_i$ cannot appear in any $e_q$. If $X_i$ appears in $p_{(1)}$, then by invariance it occupies position $i$. But then, the $i$th argument of $p_{(2)}p_{(1)}$ is $X_k$, which by assumption does not appear in $p_{(1)}$ (and therefore does not appear in $p_{(1)}p_{(2)}$); hence, $f(p_{(2)}p_{(1)}) \neq p_{(1)}p_{(2)}$, contradicting Lemma 3.23. Therefore, $X_i$ must appear only in $p_{(2)}$.

To prove the corollary, we proceed as follows. By definition, if there are $k$ Class 1 variables, then there are at least $k$ Class 1 positions. By the preceding result, the number of Class 1 variables is no smaller than the number of Class 1 positions; thus, the number of Class 1 variables is the same as the number of Class 1 positions. The corollary now follows by the preceding result and pigeonholing. □

Now, we show that if $A$ and $B$ are connected nondistinguished variables, then $f(A') = A$ and $f(B') = B$. The idea is that we know that $p_{(2)}p_{(1)}[i] = A'$, and that $f(p_{(2)}p_{(1)}) = p_{(1)}p_{(2)}$; hence, we need only discover the value of $p_{(1)}p_{(2)}[i]$.

Lemma 3.25 Let $f$ be a containment mapping as before, and assume the following picture

$$p_{(1)}( \overset{i}{\hat{A}} ) \quad p_{(2)}( \overset{j}{\hat{B}} )$$

where $A$ and $B$ are connected nondistinguished variables. Then, either $A = B$ and $p_{(1)}p_{(2)}[i]$ is $X_j$, or $p_{(1)}p_{(2)}[i]$ is $A$.

Proof. By Lemma 3.23, we have the picture

$$p_{(1)}( \overset{i}{A} \overset{j}{X_j} ) \quad p_{(2)}( \overset{j}{B} )$$

Now, the $j$th argument of the atoms $p_{(2)}p_{(2)}$ and $p_{(2)}p_{(2)}p_{(1)}$ is $B'$, and one of these atoms appears as a leaf in $T_5$. The $j$th arguments of the leaves in $T_1$ are $X_j$, $B'$ and $B$, so $f(B')$ is one of $X_j$, $B'$ and $B$. By connectivity (Lemma 3.13), if $f(B') = X_j$, then $A = B$ and $f(A')$ is $X_j$; if $f(B') = B$ then $f(A') = A$; and if $f(B') = B'$ then $f(A') = A'$.

Consider the case $f(B') = B'$; then, by connectivity, we must have $f(A') = A'$. Now, we know by Lemma 3.23 that $f(p_{(2)}p_{(1)}) = p_{(1)}p_{(2)}$, and that $A'$ appears as the $i$th argument of the former. If $p_{(1)}p_{(2)}[i]$ is $A'$, then the variable $A$ appears in the $i$th position in $p_{(1)}$ and $p_{(2)}$. The picture is

$$p_{(1)}( \overset{i}{\hat{A}} ) \quad p_{(2)}( \overset{i}{A} )$$
3.5. **PROOF**

By safety, \(X_i\) must appear in the rule body. By Lemma 3.16, if \(X_i\) appears in any \(e_\eta\), then \(f(A)\) is one of \(X_i\) and \(A\), contradicting Lemma 3.18. By invariance (since \(A\) is nondistinguished), \(X_i\) does not appear in \(p_{(1)}\). However, \(X_i\) cannot appear only in \(p_{(2)}\), since it would be a Class 1 variable and \(p_{(2)}[i]\) is not Class 1. Hence, \(f(B') \neq B'\) and our result follows.

**Lemma 3.26** Assume the following arguments for \(p_{(1)}\) and \(p_{(2)}\)

\[
p_{(1)}( A^i ) \quad p_{(2)}( A^j )
\]

where \(A\) is a nondistinguished variable. Then \(p_{(1)}p_{(2)}[i] \neq X_j\).

**Proof.** Assume the converse. Then by assumption and invariance, the picture is

\[
p_{(1)}( A^i \ X_j \ X_j^k ) \quad p_{(2)}( X_k^i \ A^j )
\]

where \(i \neq j, i \neq k\) since \(A\) is nondistinguished.

By Lemma 3.18, \(f(A) = A'\), and Lemma 3.23 requires that \(f(p_{(2)}p_{(1)}) = p_{(1)}p_{(2)}\); since the \(j\)th argument of \(p_{(2)}p_{(1)}\) is \(A\), we conclude that \(p_{(1)}p_{(2)}[k] = A'\) and \(p_{(2)}[k] = A\).

Now, by invariance, \(X_i\) cannot appear in \(p_{(1)}\). If \(X_i\) appears in any \(e_\eta\), then by Lemma 3.16, we must have \(f(X_k) = A\) or \(f(X_k) = X_i\), a contradiction since \(i \neq k\). Hence, \(X_i\) appears only in \(p_{(2)}\), say in position \(l\) distinct from \(i, j\) and \(k\). We now have the picture

\[
p_{(1)}( A^i \ X_j \ X_j^k ) \quad p_{(2)}( X_k^i \ A^j \ A^k \ X_i^l )
\]

where \(i \neq j, i \neq k, i \neq l, j \neq l\). However, by the corollary to Lemma 3.24 and since \(X_i\) is Class 1, \(p_{(2)}[i] (X_k)\) must also be Class 1; but \(p_{(2)}[k]\) is nondistinguished (and hence not Class 1), contradicting Lemma 3.24. \(\Box\)

**Lemma 3.27** Assume that the \(p\)-atoms in \(P\) are of the form

\[
p_{(1)}( A^i ) \quad p_{(2)}( B^j )
\]

where \(A\) and \(B\) are connected nondistinguished variables. Then \(f(A') = A\) and \(f(B') = B\).

**Proof.** By Lemmas 3.23, 3.25 and 3.26, and by connectivity. \(\Box\)

**Lemma 3.28** \(T_5\) has height 2.

**Proof.** Assume that \(A\) and \(B\) are connected nondistinguished variables appearing in \(p_{(1)}\) and \(p_{(2)}\) respectively. The picture is

\[
p_{(1)}( A^i ) \quad p_{(2)}( B^j )
\]
By Lemma 3.22, $p_{(1)}[i] = X_j$. Further, by Lemmas 3.23 and 3.27, $p_{(2)}[i] = X_l$ for some $l$ such that $p_{(1)}[l] = A$. Thus, we have the picture

$$p_{(1)}( i \ A \ X_j \ A ) \quad p_{(2)}( i \ X_l \ B )$$

where $A$ and $B$ are connected, and where $X_l \neq X_j$. We assume $T_5$ has height at least 3, and force a contradiction.

Now, $p_{(2)}p_{(2)}p_{(1)}[i] = A''$ and $p_{(2)}p_{(2)}p_{(1)}[j] = B'$. The mapping $f(B') = B$ forces $f(p_{(2)}p_{(2)}p_{(1)}) = p_{(2)}$, yielding $f(A'') = X_l$. By connectivity, $A = B$. But then the $j$th argument of each of $p_{(2)}p_{(2)}p_{(2)}$ and $p_{(2)}p_{(2)}p_{(2)}p_{(1)}$ is $A''$, and $X_l$ does not appear in position $j$ in any leaf in $T_1$; that is, $T_5$ cannot have depth 3 or depth greater than 3, a contradiction. $\square$

Hence, $p_{(2)}p_{(2)}$ is a leaf in $T_5$. Let $A$ and $B$ be as in the proof of the preceding theorem. By Lemma 3.27, $f(B') = B$. Now, $B'$ appears in the $j$th position in $p_{(2)}p_{(2)}$ (in $T_5$) and $p_{(2)}$ (in $T_1$). However, the $j$th arguments of $p_{(1)}p_{(1)}$ and $p_{(1)}p_{(2)}$ are $X_j$ and $B'$ respectively. Hence, we may conclude that $f(p_{(2)}p_{(2)}) = p_{(2)}$.

**Cyclic programs** Before we proceed to the cases $f(p_{(1)}) = p_{(1)}p_{(2)}$ and $f(p_{(1)}) = p_{(2)}$, we will investigate the behavior of cyclic programs. Recall that a Class 2 variable is a distinguished variable $X_j$ that appears only among the arguments of $p_{(2)}$, such that $p_{(2)}[j] \neq X_j$; that is, $X_j$ appears "out of position." Recall also that a position $i$ is termed Class 2 iff $p_{(2)}[i]$ is a Class 2 variable. We say that the program $P$ is cyclic if for all $j$, if $X_j$ is a Class 2 variable, then $j$ is a Class 2 position.

Assume that the arguments of the $p$-atoms in $P$ are as follows, where $A$ and $B$ are connected nondistinguished variables (not necessarily distinct). $C$ and $D$ are arbitrary nondistinguished variables and $i$ need not be distinct from $j$.

$$p_{(1)}( i \ A \ D ) \quad p_{(2)}( i \ C \ B )$$

We will show that if $P$ is cyclic and basis-linearizable, and has such arguments, then $P$ is minimal. For this purpose, we will investigate the containment of the complete expansion of depth 2 (expansion $T_6$ in Figure 3.25) in a right-linear expansion; that is, for the purpose of this subsection, we will not be considering the minimal violation of right-linearity.

Consider the complete expansion $T_6$ of depth 2, illustrated in Figure 3.25. We will assume that each nondistinguished variable $V$ is renamed to $V'$ in the children of $p_{(1)}$, and to $V''$ in the children of $p_{(2)}$, as indicated in the figure.

Assume that $P$ is basis-linearizable. Then, $T_6$ is contained in some right-linear expansion $T_5$ (see Figure 3.25): assume that $f$ is a containment mapping proving the containment. Since a nondistinguished variable appears in at least one position in each $p$-leaf in $T_5$, $T_6$ is clearly not contained in the depth-0 expansion.
3.5. PROOF

Figure 3.25: Trees $T_6$ and $T_5$
The following lemma shows that, if $\mathcal{P}$ is cyclic, then $T_6$ is not contained in any right-linear expansion of depth greater than 1.

**Lemma 3.29** Assume that the $p$-atoms in $\mathcal{P}$ are as described above, and that $\mathcal{P}$ is basis-linearizable and cyclic. Then the expansion $T_6$ is not contained in a right-linear expansion of depth greater than 1.

**Proof.** Assume that $f$ is a containment mapping from some right-linear expansion $T_5$ of depth at least 2 into $T_6$; we force a contradiction.

The $i$th argument of the leaf $p(1)$ in $T_5$ is $A$, and the $i$th arguments of the $p$-leaves in $T_6$ are $A', C', A''$ and $C''$; hence, $f(A)$ is one of these four variables. By connectivity, $f(B)$ is one of $A', C', A'', C''$, $B'$ and $B''$.

By safety, the distinguished variable $X_j$ must appear in the body of the recursive rule. Assume $X_j$ appears in some $e_q$, in position $k$ say. Since $T_5$ has depth at least 2, the leaf $p(2)e_q$ appears in it, with $k$th argument $B$. The only possible destinations for this leaf in $T_6$ are the atoms $p(1)e_q, p(2)e_q$ and $e_q$; however, the $k$th argument of each of these atoms is a nonprimed variable, a contradiction.

Assume that $X_j$ appears in the arguments of $p(1)$, in position $k$ say. The $k$th arguments of the leaves $p(1)p(1)$ and $p(2)p(1)$ are $D$ and $B$ respectively, both of which are nondistinguished; hence, we must have $f(p(1)) = p(1)p(2)$ or $f(p(1)) = p(2)p(2)$, and the $k$th argument of $p(1)p(2)$ or $p(2)p(2)$ must be the distinguished variable $X_j$. Hence, $p(2)[k]$ is some distinguished variable $X_i$. The picture is

\[
p(1)( A \ D \ X_j ) = p(2)( C \ B \ X_i )
\]

Now, since $T_5$ has depth at least 2, the leaf $p(2)p(1)$ must appear in it. The $k$th argument of this leaf is $B$; however, the $k$th argument of each leaf in $T_6$ is a nonprimed variable, and $p(2)p(1)$ has no legal destination.

Thus, $X_j$ must appear only in $p(2)$, in position $k$ say. Since $p(2)[j]$ is nondistinguished, $k \neq j$ and $X_j$ is Class 2, which violates the assumed cyclicity of $\mathcal{P}$ since $p(2)[j]$ is nondistinguished and hence is not Class 2.
\[\square\]

Now, consider the case in which $T_6$ is contained in the right-linear expansion $T_3$ of depth 1. Let $f$ be a containment mapping from $T_3$ into $T_6$. We say that $f$ is normalized iff the following conditions all hold.

1. The destinations of the leaves $p(1)$ and $p(2)$ in $T_3$ have the same parent in $T_6$. That is, both $p$-leaves are mapped to the same "side" of the complete tree $T_6$.

2. The destination of each $e_q$-leaf in $T_3$ is either the $e_q$-leaf at depth 1 in $T_6$, or the $e_q$-leaf in $T_6$ with the same parent as the destinations of the $p$-leaves in $T_3$. 

3.5. PROOF

The following is the analog of Lemma 3.14 in Section 3.6.3.

Lemma 3.30 Assume that the arguments of the $p$-atoms in $\mathcal{P}$ are as described above, and that $T_6 \subset T_3$. Then, the containment is provable by a normalised mapping.

Proof. Let $f$ be any mapping proving the containment; we construct a normalised mapping $g$ from $f$. If $f(p_{(1)})$ is one of $p_{(1)}p_{(1)}$ and $p_{(1)}p_{(2)}$, then $f(A)$ is one of $A'$ and $C'$; by connectivity, $f(B)$ must be $A'$, $C'$ or $B'$. However, the $j$th argument of each of $p_{(2)}p_{(1)}$ and $p_{(2)}p_{(2)}$ is a double-primed variable; hence, we must have $f(p_{(2)}) = p_{(1)}p_{(1)}$ or $f(p_{(2)}) = p_{(1)}p_{(2)}$. Similarly, if $f(p_{(1)})$ is one of $p_{(2)}p_{(1)}$ or $p_{(2)}p_{(2)}$, then $f(p_{(2)})$ must also be one of these atoms.

Partition the nondistinguished variables in $T_3$ into two classes. Tied variables are variables that appear in $p_{(1)}$ or $p_{(2)}$, or in any $e_q$ that is connected to $p_{(1)}$ or $p_{(2)}$; free variables consist of the remainder. Define the function $g$ as follows.

\[
g(V) = \begin{cases} 
V & \text{if } V \text{ is distinguished} \\
 f(V) & \text{if } V \text{ is tied} \\
 V & \text{if } V \text{ is free}
\end{cases}
\]

That is, $g$ preserves the destinations of $f$ for all atoms that are connected to $p_{(1)}$ or $p_{(2)}$, and maps all other $e_q$ to "themselves" in $T_6$ (see Figure 3.26). $g$ is a normalised containment mapping from $T_3$ into $T_6$. \(\square\)

Lemma 3.31 Assume that the arguments of $\mathcal{P}$ are as described above, and that $f$ is a containment mapping from $T_3$ into $T_6$ such that the destination of the leaf $p_{(1)}$ in $T_1$ is a
child of the atom \( p_{(1)} \) in \( T_6 \); that is, \( f(p_{(1)}) = p_{(1)}p_{(1)} \) or \( f(p_{(1)}) = p_{(1)}p_{(2)} \). Then \( P \) is minimal.

**Proof.** Construct a normalised containment mapping \( g \) from \( T_3 \) into \( T_6 \); \( g \) is a containment mapping from \( T_3 \) into the minimal violation \( T_1 \) of right-linearity. \( \Box \)

**Lemma 3.32** Assume that the arguments of \( P \) are as described above, and that \( f \) is a containment mapping from \( T_3 \) into \( T_6 \) such that the destination of the leaf \( p_{(1)} \) in \( T_1 \) is a child of the atom \( p_{(2)} \) in \( T_6 \); that is, \( f(p_{(1)}) = p_{(2)}p_{(1)} \) or \( f(p_{(1)}) = p_{(2)}p_{(2)} \). If \( P \) is basis-linearizable, then \( P \) is minimal.

**Proof.** Construct a normalised containment mapping \( g \) from \( T_3 \) into \( T_6 \); \( g \) is a containment mapping from \( T_3 \) into the right-linear tree \( T_4 \) of depth 2 (see Figure 3.27). Let \( Q \) be the set of right-linear open expansions generated by \( P \); as we mentioned in Chapter 1, \( Q \) may be considered a program. Then, \( T_4 \) is the minimal violation of one-boundedness in \( Q \); by (the discussion following) Theorem 1.7, we may conclude that the set of right-linear expansions of \( P \) is one-bounded.

Now, consider the minimal violation \( T_1 \) of right-linearity in \( P \). Since we assumed that \( P \) is basis-linearizable, \( T_1 \) is contained in some right-linear expansion. However, since the set of right-linear expansions is one-bounded, we conclude that \( T_1 \) is contained in a right-linear expansion of depth at most 1, and the result follows. \( \Box \)

The following lemma details the property of cyclic programs that will be used in the following two sections. This lemma is key in the proof that if the minimal violation \( T_1 \) of right-linearity is contained in a long right-linear expansion under an unacceptable containment mapping, then \( T_1 \) is minimal (that is, \( T_1 \) is contained in the right-linear expansion of depth 1).
Lemma 3.33 Assume that \( \mathcal{P} \) is basis-linearizable, and that the \( p \)-atoms in the recursive rule have the form

\[
p_{(1)}(i, A, j, D) \quad p_{(2)}(i, X, j, Y)
\]

where \( A \) and \( B \) are connected nondistinguished variables, and where \( X \) and \( Y \) are distinguished. Then \( \mathcal{P} \) is minimal.

Proof. Consider the complete expansion \( T_6 \) of depth 2; since \( \mathcal{P} \) is assumed to be basis-linearizable, \( T_6 \) is contained in some right-linear expansion. By discussion, and by Lemma 3.29, \( T_6 \) must be contained in the right-linear expansion \( T_3 \) of depth 1. By Lemmas 3.31 and 3.32, \( \mathcal{P} \) is minimal. \( \square \)

The result of Zhang, Yu and Troy Zhang et al. ([40]) claim a decision procedure for basis-linearizability in the restricted case in which the recursive rule has at most 1 EDB subgoal. As we mentioned in Section 3.1.1, the proof of [40] is flawed. The flaw is, essentially, the fact that they neglect the case covered by Lemma 3.32. They claim the following result.

Define the program \( \mathcal{P} \) to satisfy “Property 0” if

1. There is a partial mapping from \( p_{(1)} \) into \( p_{(2)} \) that preserves the distinguished variables in \( p_{(1)} \).

2. There are two distinct nondistinguished variables \( A \) and \( C \) that appear only in \( p_{(1)} \) and \( p_{(2)} \), in the following positions:

\[
p_{(1)}(i, A, j, C) \quad p_{(2)}(i, C, j, A)
\]

3. \( \mathcal{P} \) is not minimal.

The result of [40] is the claim that the complete tree \( T_6 \) of depth 2 is not contained in any right-linear expansion. The following program satisfies “Property 0,” and yet \( T_6 \) is contained in the depth-1, right-linear expansion \( T_3 \).

\[
\]
\[
\]

The weaker result of Lemma 3.33 suffices for our purposes.

The case \( f(p_{(1)}) = p_{(1)}p_{(2)} \) Let us return to the containment of the minimal violation \( T_1 \) of right-linearity (see Figure 3.28) in a right-linear expansion \( T_5 \) of depth at least 2. Let \( f \) be a containment mapping from \( T_5 \) into \( T_1 \) such that \( f(p_{(1)}) = p_{(1)}p_{(2)} \) (see Figure 3.28). We will show that if \( \mathcal{P} \) is basis-linearizable, then \( \mathcal{P} \) is minimal. As before, if \( p_{(1)} \) and \( p_{(2)} \) are not connected, then \( \mathcal{P} \) is minimal by Lemma 3.14. Assume that \( p_{(1)} \) and \( p_{(2)} \) are connected.

\[\text{\footnote{The paper has been published in TODS ([41]) without a proof.}}\]
Lemma 3.34 For all \( j \), if \( p_{(2)}[j] \) is nondistinguished, then so is \( p_{(1)}[j] \).

Corollary. If \( p_{(1)}[j] \) is a distinguished variable, then \( p_{(2)}[j] \) is distinguished.

Proof. The proof follows from the fact that \( f \) preserves distinguished variables. If \( p_{(2)}[j] \) is nondistinguished, then \( p_{(1)}p_{(2)}[j] \) would also be nondistinguished; hence, by Lemma 3.7 and the assumed mapping \( f(p_{(1)}) = p_{(1)}p_{(2)} \), \( p_{(1)}[j] \) must be nondistinguished.

Lemma 3.35 Assume that the arguments of the \( p \)-atoms in \( P \) are of the following form.

\[
p_{(1)}( \ T \ X_{j} \ ) \quad p_{(2)}( \ B \ C \ )
\]

Then \( f(B) \) is \( X_{i} \), \( D \) or \( C \).

Proof. The mapping \( f(p_{(1)}) = p_{(1)}p_{(2)} \) yields the fact that \( p_{(1)}p_{(2)}[k] \) is \( X_{j} \). The \( k \)th arguments of \( p_{(1)}p_{(1)} \) and \( p_{(2)} \) are \( D \) and \( C \) respectively. The \( k \)th argument of \( p_{(2)}p_{(1)} \) is \( B \); our result follows by an examination of all possible destinations for this atom.

Recall that a Class 2 variable is a distinguished variable \( X_{j} \) that appears only in \( p_{(2)} \), such that \( p_{(2)}[j] \neq X_{j} \). Recall also that a Class 2 position is an argument position in \( p_{(2)} \) that is occupied by a Class 2 variable.

Lemma 3.36 If \( k \) is a Class 2 position, then \( X_{k} \) is a Class 2 variable.

Proof. The picture is as follows, where \( C \neq X_{j} \), and where \( X_{j} \) appears only in \( p_{(2)} \).

\[
p_{(2)}( \ C \ X_{j} \ )
\]

By safety, \( X_{k} \) appears in the rule body. By Lemma 3.16, since \( X_{j} \) does not appear in \( p_{(1)} \), \( X_{k} \) does not appear in any \( e_{q} \). Assume that \( X_{k} \) appears in some position \( l \) in \( p_{(1)} \). Then,
3.5. PROOF

\( X_j \) appears in position \( l \) in \( p_2(p_1) \), and this atom is a leaf in \( T_5 \). Consider the possible destinations of this leaf. Now, \( X_j \) appears nowhere in \( p_1 \), and hence appears nowhere in \( p_1(p_1) \) or \( p_1(p_2) \); hence, \( f(p_2(p_1)) = p_2 \), and \( p_2[l] = X_j \). The picture is

\[
p_1(k \ x_j) \quad p_2(\ x_j \ x_k)
\]

The assumed mapping \( f(p_1) = p_1(p_2) \) requires that the \( l \)th position of \( p_1(p_2) \) is \( X_k \); that is, \( p_1[j] = X_k \). However, in this case, \( p_2(p_1)[j] = X_j \), and the mapping \( f(p_2(p_1)) = p_1 \) forces \( C = X_j \), contradicting our assumption that \( X_j \) is Class 2.

\( \square \)

Lemma 3.37 \( i \) is a Class 2 position iff \( X_i \) is a Class 2 variable.

Proof. By Lemma 3.36 and pigeonholing, as in the proof of Lemma 3.24. \( \square \)

Lemma 3.38 \( P \) is cyclic.

Proof. By Lemmas 3.36 and 3.37. \( \square \)

Lemma 3.39 Assume the picture

\[
p_1(i \ A \ C \ x_k) \quad p_2(k \ x_k \ A)
\]

where \( A \) and \( C \) are nondistinguished and \( X_k \neq X_i \). Then \( f \) cannot exist.

Proof. By safety, \( X_i \) must appear in the rule body. By Lemma 3.16, it cannot appear in any \( \epsilon_q \). Assume it appears in \( p_1 \), in position \( l \) say. The mapping \( f(p_1(p_1)) = p_1(p_2) \) requires that \( p_1(p_2)[l] = X_i \); hence, \( p_1[l] \) is some distinguished variable \( X_m \neq X_k \) such that \( p_2[m] \) is \( X_i \). Now, the \( l \)th argument of the leaf \( p_2(p_1) \) in \( T_5 \) is \( X_k \), but \( X_k \) does not appear in position \( l \) in any leaf in \( T_1 \); that is, the \( l \)th arguments of the leaves in \( T_1 \) are as below.

\[
p_1(p_1) \quad p_1(p_2) \quad p_2(X_i) \quad p_2(X_m)
\]

Hence, \( X_i \) appears only in \( p_2 \), and is thus Class 2. By Lemma 3.37, \( k \) must be a Class 2 position, a contradiction since \( A \) is nondistinguished. \( \square \)

Lemma 3.40 Assume the picture

\[
p_1(i \ A \ C) \quad p_2(B)
\]

where \( A \) and \( B \) are connected nondistinguished variables. If \( P \) is not minimal, then \( C \neq B \). \( A = B \) and \( f(A) \) is \( X_j \) or \( C \).

Proof. By Lemma 3.34, \( C \) is nondistinguished. If \( C = B \) then \( P \) is minimal by Lemma 3.33. Assume that \( C \neq B \). By safety, \( X_j \) appears in \( p_1 \), \( p_2 \) or some \( \epsilon_q \).
CHAPTER 3. A DECISION PROCEDURE FOR BASIS-LINEARIZABILITY

If $X_j$ appears in some $e_q$, then our result follows by Lemma 3.16 and connectivity (Lemma 3.13). Assume that $X_j$ appears in no $e_q$. By Lemma 3.37, $X_j$ cannot appear only in $p_{(2)}$; hence, $X_j$ appears in $p_{(1)}$, in position $k$ say.

The assumption $f(p_{(1)}) = p_{(1)}[k]$ requires that $p_{(2)}[k]$ be some distinguished variable $X_l$ different from $X_j$ such that $p_{(1)}[l]$ is $X_j$. Since $A$ and $C$ are nondistinguished, $k \neq i$ and $k \neq j$. The situation is

\[
p_{(1)}( \begin{array}{cccc}
 1 & 0 & 1 & j \\
 0 & 1 & 0 & j \\
 0 & 0 & 1 & i \\
 0 & 0 & 0 & i \\
\end{array} ) \quad p_{(2)}( \begin{array}{cccc}
 0 & 1 & 0 & k \\
 1 & 0 & 0 & k \\
 0 & 0 & 1 & l \\
 0 & 0 & 0 & l \\
\end{array} )
\]

By Lemma 3.35, $f(B)$ is one of $X_j$, $C$ and $X_l$. Since we assumed $C \neq A$, by connectivity we must have $A = B$. We will show that $f(A) \neq X_l$ to complete the proof.

For the assumed mapping on $p_{(1)}$, $p_{(2)}[i]$ must be $X_m$ for some $m$ ($m \neq l, m \neq j$) such that $p_{(1)}[m]$ is $X_l$. The new picture is

\[
p_{(1)}( \begin{array}{cccc}
 1 & 0 & 1 & k \\
 0 & 1 & 0 & j \\
 0 & 0 & 1 & m \\
 0 & 0 & 0 & m \\
\end{array} ) \quad p_{(2)}( \begin{array}{cccc}
 0 & 1 & 0 & j \\
 1 & 0 & 0 & k \\
 0 & 0 & 1 & X_l \\
 0 & 0 & 0 & X_l \\
\end{array} )
\]

An examination of destinations for $p_{(2)}p_{(1)}$ suffices to show that we must have $f(p_{(2)}p_{(1)}) = p_{(2)}$. This mapping yields $f(A') = A$; however, in this case, neither $p_{(2)}p_{(2)}$ nor $p_{(2)}p_{(2)}p_{(1)}$ has a destination among the leaves of $T_1$.

**Lemma 3.41** Assume the picture

\[
p_{(1)}( \begin{array}{cc}
 1 & j \\
 0 & C \\
\end{array} ) \quad p_{(2)}( \begin{array}{c}
 j \\
 A \\
\end{array} )
\]

If $f(A) = C$, then $\mathcal{P}$ is minimal.

**Proof.** Assume $f(A) = C$. If $C = A$, then $\mathcal{P}$ is minimal by Lemma 3.33. Assume $C \neq A$: we will show that $f$ cannot exist. The mapping $f(p_{(1)}) = p_{(2)}$, along with Lemma 3.34, requires that $C$ is nondistinguished. The same mapping and the assumption $f(A) = C$ requires that $p_{(2)}[i]$ be some distinguished variable $X_k$ such that $p_{(1)}[k]$ is $C$. Since $A \neq C$, we conclude that $X_k \neq X_i$. The new picture is

\[
p_{(1)}( \begin{array}{ccc}
 1 & 0 & j \\
 0 & C & k \\
\end{array} ) \quad p_{(2)}( \begin{array}{cc}
 i & j \\
 X_k & A \\
\end{array} )
\]

Now, the mapping $f(p_{(1)}) = p_{(1)}p_{(2)}$ yields $f(C) = A'$; hence, $p_{(2)}[k] = A$. By Lemma 3.39, $f$ cannot exist.

**Lemma 3.42** Assume that the arguments of $p_{(1)}$ and $p_{(2)}$ are as follows, where $A$ and $C$ are nondistinguished (hence $i \neq j$).

\[
p_{(1)}( \begin{array}{ccc}
 1 & i & j \\
 0 & C & X_j \\
\end{array} ) \quad p_{(2)}( \begin{array}{ccc}
 i & j & k \\
 X_i & A & X_k \\
\end{array} )
\]
Let $T_r$ be a right-linear tree of depth $r > 1$. Then, the $k$th argument of the $p_1^{(r)}$-leaf in $T_r$ (i.e. of $p_1^{(r)}$) is some $X_i \neq X_j$.

**Proof.** Consider the set $S = \{k_1, \ldots, k_n\}$ of all positions in $p_1^{(1)}$ that are occupied by $X_j$; by assumption, this set has cardinality at least 1. Since $p_1^{(1)}[i]$ and $p_1^{(1)}[j]$ are nondistinguished, $k_q \neq i$ and $k_q \neq j$ for all $q$. The requirement $f(p_1^{(1)}) = p_1^{(1)}p_2^{(1)}$, along with the fact that $f$ is the identity on distinguished variables, shows that for each $l \in S$, $p_2^{(1)}[l]$ is $X_m$ for some $m \in S$. A straightforward induction on $1 \leq q \leq r$ shows that for any $l \in S$, there is an $m \in S$ such that the $l$th argument of $p_2^{(r)}$ is $X_m$. Our result follows. □

**Lemma 3.43** Assume that the arguments of $p_1^{(1)}$ and $p_2^{(1)}$ are as follows, where $A$ and $C$ are nondistinguished and $C \neq A$. Then $f(A) \neq X_j$.

\[ p_1^{(1)}(\begin{array}{c} i \\ A \\ \end{array} ) \quad p_2^{(1)}(\begin{array}{c} j \\ B \end{array} ) \]

**Proof.** If $f(p_1^{(1)}) = p_1^{(1)}p_2^{(1)}$ and $f(A) = X_j$, then we have the following picture where $k \neq i, k \neq j$.

\[ p_1^{(1)}(\begin{array}{c} i \\ A \\ \end{array} ) \quad p_1^{(1)}(\begin{array}{c} j \\ C \end{array} ) \quad \quad p_2^{(1)}(\begin{array}{c} k \\ X_j \end{array} ) \quad p_2^{(1)}(\begin{array}{c} j \\ A \end{array} ) \]

The $k$th argument of the leaf $p_1^{(1)}p_1^{(1)}$ in $T_1$ is the nondistinguished variable $C$. Since we assume $f(p_1^{(1)}) = p_1^{(1)}p_2^{(1)}$, the $k$th argument of $p_1^{(1)}p_2^{(1)}$ is $X_j$. The $i$th and $j$th arguments of the $p$-leaves in $T_1$ are as follows.

\[ p_1^{(1)}p_1^{(1)}(\begin{array}{c} i \\ A' \end{array} ) \quad p_1^{(1)}p_2^{(1)}(\begin{array}{c} j \\ C' \end{array} ) \quad p_2^{(1)}(\begin{array}{c} k \\ X_j \end{array} ) \quad p_2^{(1)}(\begin{array}{c} j \\ A' \end{array} ) \quad p_2^{(1)}(\begin{array}{c} i \\ X_k \end{array} ) \quad p_2^{(1)}(\begin{array}{c} j \\ A \end{array} ) \]

Let $T_5$ have depth $n + 1$, for some $n \geq 1$. Consider the lowest $p$-leaves in $T_5$; that is, the atoms $p_2^{(n)}p_1^{(1)}$ and $p_2^{(n+1)}$. By Lemma 3.42, the $k$th argument of $p_2^{(n+1)}$ is some distinguished variable distinct from $X_j$, and hence we must have $f(p_2^{(n+1)}) = p_2^{(2)}$. Now, the $i$th argument of $p_2^{(n)}p_1^{(1)}$ and the $j$th argument of $p_2^{(n+1)}$ are both $A^n$ (recall that this is the variable $A$, primed $n$ times). The mapping $f(p_2^{(n+1)}) = p_2^{(2)}$ forces $f(A^{(n)}) = A$; however, $A$ does not appear in the $i$th position of any $p$-leaf in $T_1$, and hence $p_2^{(n)}p_1^{(1)}$ has no destination in $T_1$. □

**Lemma 3.44** $\mathcal{P}$ is minimal.

**Proof.** By Lemmas 3.40, 3.41 and 3.43. □

**The case $f(p_1^{(1)}) = p_2^{(1)}$** Assume that $\mathcal{P}$ is basis-linearizable, and that the minimal violation $T_1$ of Figure 3.29 is contained in a right-linear tree $T_5$ of depth at least 2. Assume further that the containment mapping $f$ from $T_5$ into $T_1$ satisfies $f(p_1^{(1)}) = p_2^{(1)}$ (see Figure 3.29). We will show that $\mathcal{P}$ is minimal or $p_1^{(1)}$ is an adjunct to $p_2^{(1)}$, to complete the proof.

**Lemma 3.45** For all $i$ and $j$, if $p_1^{(1)}[j]$ is the distinguished variable $X_i$, then $p_2^{(1)}[j]$ is $X_i$. 

Proof. Since $f$ is a containment mapping from $T_5$ into $T_1$, and since both expansions have the root $p(X_1, \ldots, X_m)$, we conclude that $f(X_i) = X_i$ for all $i$. Our result follows because $f(p(1)) = p(2)$ by assumption.

Recall that a Class 2 variable is a distinguished variable $X_j$ that appears only in $p(2)$, such that $p(2)[j] \neq X_j$. Recall also that a Class 2 position is a position in $p(2)$ that is occupied by a Class 2 variable.

**Lemma 3.46** If $k$ is a Class 2 position, then $X_k$ is a Class 2 variable.

**Proof.** Assume the following scenario, where $C \neq X_j$ (so $j \neq k$), and where $X_j$ appears only in $p(2)$.

$$p(2)(\overline{C}^k X_j)$$

By safety, $X_k$ appears in the rule body. By Lemma 3.16, it cannot appear in any $\epsilon_q$. Assume it appears in $p(1)$, in position $l$; the mapping $f(p(1)) = p(2)$ forces $p(2)[l] = X_k$ (so $l \neq j, l \neq k$). The picture is

$$p(1)(\overline{X_k}^l) \quad p(2)(\overline{C}^k X_j^l X_k^l)$$

Now, $X_j$ appears in the $l$th position of the leaf $p(2)p(1)$ in $T_5$, but appears nowhere in the leaves $p(1)p(1)$ or $p(1)p(2)$ in $T_1$ (since $X_j$ does not appear in $p(1)$); also, the $l$th argument of $p(2)$ is $X_k \neq X_j$, so $p(2)p(1)$ has no legal destination in $T_1$. Thus, $X_k$ appears only in $p(2)$.

**Lemma 3.47** For all $i$, $i$ is a Class 2 position iff $X_i$ is a Class 2 variable.

**Corollary.** $P$ is cyclic.
3.5. **Proof**

Proof. The proof follows by Lemma 3.46 and pigeonholing. □

**Lemma 3.48** Assume that $A$ is a nondistinguished variable appearing in $p_{(1)}$. Then $f(A) \neq X_j$.

**Proof.** Assume the converse. By the assumed mapping $f(p_{(1)}) = p_{(2)}$, the picture is the following.

\[ p_{(1)}(i\ a\ j\ \epsilon\ c\ ) \quad p_{(2)}(i\ x_j\ j\ a\ ) \]

We show that $T_5$ cannot have depth 2 or greater, a contradiction since $T_5$ is assumed to have depth at least 2.

Since $A$ is nondistinguished, $i \neq j$. By Lemma 3.45, $C$ must be nondistinguished. By safety, $X_i$ must appear in the rule body.

If $X_i$ appears in any $e_q$, then by Lemma 3.16, $f(X_j)$ is $A$ or $X_i$, a contradiction. Assume that $X_i$ appears in $p_{(1)}$, in position $k$ say. Then, by Lemma 3.45, $p_{(2)}[k]$ is $X_i$. The picture is

\[ p_{(1)}(i\ a\ j\ \epsilon\ c\ X_i\ ) \quad p_{(2)}(i\ x_j\ j\ a\ X_i\ ) \]

Now, since $T_5$ has depth at least 2, the leaf $p_{(2)}[k]$ appears in it. The $k$th argument of this leaf is $X_j$. However, $X_j$ does not appear in the $k$th position in any leaf in $T_1$, a contradiction.

Hence, $X_i$ appears only in $p_{(2)}$. However, then $X_i$ is a Class 2 variable, and we conclude by Lemma 3.47 that $p_{(2)}[i]$ (that is, $X_j$) is a Class 2 variable. However, this result contradicts Lemma 3.47 because $p_{(2)}[j]$ is a nondistinguished variable, and is hence not Class 2. □

**Lemma 3.49** $p_{(1)}$ is an adjunct to $p_{(2)}$ or $\mathcal{P}$ is minimal.

**Proof.** We will show the following.

1. If a distinguished variable $X_j$ appears in the $i$th position in $p_{(1)}$, then $p_{(2)}[i]$ is $X_j$.

2. If a nondistinguished variable $A$ appears in $p_{(1)}$ (in the $i$th position, say) and in some $e_q$, then $p_{(2)}[i]$ is $A$.

3. If a nondistinguished variable $A$ appears in $p_{(1)}$ and $p_{(2)}$, then $\mathcal{P}$ is minimal.

Hence, if $\mathcal{P}$ is not minimal, then every nonlocal variable appearing in the arguments of $p_{(1)}$ appears in the same position in $p_{(2)}$; that is, $p_{(1)}$ is an adjunct to $p_{(2)}$.

To prove (1), we observe that by Lemma 3.45, every distinguished variable in $p_{(1)}$ appears in the same position in $p_{(2)}$.

To prove (2), we proceed as follows. Assume that $p_{(1)}$ shares a nondistinguished variable $A$ with an EDB subgoal $e_q$, and that $A$ is the $i$th argument of $p_{(1)}$. By Lemma 3.15, $f(A)$ is $A$ or $A'$. However, no primed variable appears in $p_{(1)}$, so the mapping $f(p_{(1)}) = p_{(2)}$ forces $p_{(2)}[i] = A$.

Finally, we prove (3). Assume, now, that a nondistinguished variable $A$ appears in position $i$ in $p_{(1)}$, and in position $j$ in $p_{(2)}$. We show that $\mathcal{P}$ is minimal. By Lemma 3.33, if
$i = j$ then $\mathcal{P}$ is minimal. Assume $i \neq j$, and let the $j$th argument of $p(1)$ be $C$. The picture is

$$p(1)(\ A \ C \ ) \quad p(2)(j \ A \ )$$

By Lemma 3.45, since $p(2)[j]$ is nondistinguished, $C$ must be nondistinguished. Further, by Lemma 3.33, if $p(2)[j]$ is nondistinguished then $\mathcal{P}$ is minimal. Assume that $p(1)[i]$ is some distinguished variable $X_k$; the mapping $f(p(1)) = p(2)$ forces $f(A) = X_k$. The picture is

$$p(1)(\ A \ C \ ) \quad p(2)(X_k \ j \ A \ )$$

By safety, $X_j$ appears in the rule body. Assume that $X_j$ appears in some $e_n$; by Lemma 3.17, we must have $f(A) = X_j$ or $f(A) = C$. Since $C$ is nondistinguished, the former must hold, so that $X_k = X_j$, contradicting Lemma 3.48. By Lemma 3.47, $X_j$ cannot appear only in $p(2)$, since in this case $X_j$ would be Class 2 but $p(2)[j] = A$ is nondistinguished. Thus, $X_j$ must appear in $p(1)$, in position $m$ say. Then, the mapping $f(p(1)) = p(2)$ forces $p(2)[m] = X_j$. The picture is

$$p(1)(\ A \ C \ X_j \ ) \quad p(2)(X_k \ j \ X_j \ m \ A \ )$$

Now, the leaf $p(2)p(1)$ must appear in $T_5$, and the $m$th argument of this leaf is $A$. The $m$th arguments of the leaves $p(1)p(1)$ and $p(1)p(2)$ in $T_1$ are each $C \neq X_k$, so we must have $f(p(2)p(1)) = p(2)$. Thus, $p(2)[m]$ must be $X_k$, so $X_k = X_j$, contradicting Lemma 3.48. □

The proof is now complete.
Chapter 4

Undecidability of the general problems

4.1 Introduction

Finally, let us turn to the decidability of basis-linearizability and sequencability. In this chapter, we will show that both these problems are undecidable for a restricted class of Datalog programs.

4.1.1 Definitions

Consider the following single-IDB, safe, Datalog program $\mathcal{P}$, in which the head of every rule is rectified (i.e., contains no repetitions of any variable). Recall that a program is single-IDB iff there is only one intensional predicate in $\mathcal{P}$.

Let $\mathcal{P}$ consist of the $n$ recursive rules

$r_1 : p(\bar{X}_0) : - p(\bar{X}_{11}), \ldots p(\bar{X}_{1k_1}), \mathcal{C}_1.$

$\vdots$

$r_i : p(\bar{X}_0) : - p(\bar{X}_{i1}), \ldots p(\bar{X}_{ik_i}), \mathcal{C}_i.$

$\vdots$

$r_n : p(\bar{X}_0) : - p(\bar{X}_{n1}), \ldots p(\bar{X}_{nk_n}), \mathcal{C}_n.$

and the $m$ nonrecursive rules

$b_1 : p(\bar{X}_0) : - \mathcal{D}_1.$

$\vdots$

$b_j : p(\bar{X}_0) : - \mathcal{D}_j.$

$\vdots$

$b_m : p(\bar{X}_0) : - \mathcal{D}_m.$

where the $\mathcal{C}_i$s and $\mathcal{D}_j$s are arbitrary conjunctions of EDB predicates.
Base-case linearizability

Recall from Section 1.4.3 that a conjunctive query generated by $P$ is right-linear if only the rightmost occurrence of $p$ is ever recursively expanded (see Figure 4.1). Recall also that $P$ is basis-linearizable iff every conjunctive query generated by $P$ is contained in a right-linear conjunctive query.

Sequencability

Recall from Section 1.4.4 that a conjunctive query generated by $P$ is termed sequenced if $r_i$ is never used to expand a $p$-atom introduced by $r_j$ in a top-down expansion generating this conjunctive query, if $i < j$ (see Figure 4.2). Recall also that $P$ is termed sequencable iff every conjunctive query generated by $P$ is contained in a sequenced query generated by $P$.

4.2 Results

We state below the main results of this chapter. In the following statements, $P$ and $Q$ are safe. Datalog programs defining a single intensional predicate, using head-rectified rules.

Result 4.1 $P \subseteq Q \ (P \equiv Q)$ is undecidable, even if

(a) $P$ and $Q$ are linear, and have no more than five basis rules; or

(b) Each of $P$ and $Q$ contains only one recursive rule and nine nonrecursive rules.

\[ \square \]

Result 4.2 The base-case linearizability of $P$ is undecidable, even if $P$ contains only one nonlinear rule and five basis rules. \[ \square \]
Figure 4.2: Sequenced query.
Result 4.3 The sequencability of $\mathcal{P}$ is undecidable, even if $\mathcal{P}$ contains only two recursive rules and nine basis rules. □

4.2.1 Related results

Shmueli ([33]) and Abiteboul ([1]) present general results that also yield undecidability results for program equivalence. Shmueli considers programs with a single recursive predicate; however, these programs have several IDB predicates, and include rules whose heads are not rectified. The assumption of head-rectification is integral to the proof of Theorem 3.1. Abiteboul’s result concerns single-IDB programs with a single recursive rule; however, those programs have rules that are not head-rectified, and contain an unbounded number of initialisation rules.

4.3 Outline

Our undecidability results involve reductions from undecidable problems for context-free grammars. In Section 4.4, we will define certain normal forms for context-free grammars, and show that the containment of such normal-form grammars is undecidable. In this section, we will also show how unsafe Datalog programs may be made safe, allowing the reductions of the subsequent sections to involve unsafe programs.

In Section 4.5, we will prove Results 4.1(a) and 4.2. Section 4.6 contains the proof of Results 4.1(b) and 4.3.

4.4 Preliminaries

In this section, we present results that will be of use in the proofs of the next two sections.

4.4.1 Context-free grammars

The results of the following sections will be based upon reductions from undecidable problems in language theory. In this subsection, we establish some preliminary results. Our treatment is concise, and assumes concepts that are explained in [15].

Definition 4.1 For any grammar $G$, a production $A \rightarrow \beta$ is termed intensional if at least one nonterminal appears in $\beta$, and extensional otherwise. □

Definition 4.2 A grammar $G$ over the alphabet $\Sigma = \{a, b\}$ is termed bounded-basis if $G$ is $\epsilon$-free and if there are only two extensional productions in $G$, which are of the form $N_a \rightarrow a$ and $N_b \rightarrow b$ where $N_a \neq N_b$, and where neither $N_a$ nor $N_b$ appears as the head of any other production. Hence, we may partition the nonterminals into intensional and extensional nonterminals, depending on whether they appear on the left-hand side of an intensional or extensional production. $N_a$ is termed the extensional nonterminal representing $a$, and $N_b$ is termed the extensional nonterminal representing $b$. □
4.4. PRELIMINARIES

Lemma 4.1 Given any linear grammar $H$ over $\Sigma = \{a, b\}$, we may effectively construct a linear, bounded-basis grammar $G$ such that $L(G) = L(H) - \{\varepsilon\}$.

Proof. Construct a linear, $\varepsilon$-free grammar $I$ for $L(H) - \{\varepsilon\}$ by determining nullable non-terminals and following the procedure of Theorem 4.3 in Section 4.4 of [15]. Assume that $S$ is the start symbol of $I$. We construct $G$ from $I$, as follows. Introduce new nonterminals $N_a$ and $N_b$, and the productions $N_a \rightarrow a$ and $N_b \rightarrow b$. Finally, consider any extensional production $A \rightarrow \alpha$. If $\alpha$ is $a$, replace the production by the unit production $A \rightarrow N_a$; if $\alpha$ is $b$, replace the production by $A \rightarrow N_b$. Otherwise, $\alpha$ is of the form $\beta a$ or $\beta b$. In the first case, replace the production by the production $A \rightarrow \beta N_a$, and in the second, replace the production by $A \rightarrow \beta N_b$. $\square$

Definition 4.3 A Modified Chomsky Normal Form (MCNF) grammar $G$ over the terminal alphabet $\Sigma = \{a, b\}$ is a grammar with the following properties.

1. $G$ is bounded-basis.

2. Each intensional nonterminal $N$ appears at the head of at most two productions. Further, if $N$ does appear as the head of two productions, then both productions are unit productions. That is, intensional productions are of three types.

(a) If $N \rightarrow M$ and $N \rightarrow K$ are productions, then these productions are or-productions.

(b) $N \rightarrow MK$ is an and-production.

(c) If $N$ appears only on the left-hand side of the production $N \rightarrow M$, then this production is a copy production.

$\square$

Lemma 4.2 For every grammar $H$ over $\Sigma = \{a, b\}$, there is an MCNF grammar $G$ generating $L(H) - \{\varepsilon\}$.

Proof. Construct a Chomsky Normal Form grammar for $L(H) - \varepsilon$, with start symbol $S$. Introduce the nonterminals $N_a$ and $N_b$, and the productions $N_a \rightarrow a$ and $N_b \rightarrow b$. Then, replace every other production of the form $N \rightarrow c$, where $c$ is a terminal, by the production $N \rightarrow N_c$. All productions other than $N_a \rightarrow a$ and $N_b \rightarrow b$ are now intensional. Replace every and-production $N \rightarrow MK$ by the two productions $N \rightarrow L$ and $L \rightarrow MK$, where $L$ is a new nonterminal. At this point, the only violations of MCNF are the presence of nonterminals $N$ such that $N \rightarrow R_1, \ldots, N \rightarrow R_{k+1}$, for $k > 1$, are the productions with $N$ on the left-hand side. Introduce new nonterminals $M_1, \ldots, M_k$; then, add the productions $N \rightarrow M_1$ and $M_k \rightarrow R_{k+1}$; finally, for $2 \leq i \leq k$, replace the production $N \rightarrow R_i$ with the two productions $M_{i-1} \rightarrow R_i$ and $M_{i-1} \rightarrow M_i$. $\square$

Lemma 4.3 Assume $\Sigma = \{a, b\}$. It is undecidable, for an arbitrary context-free grammar (CFG) $G$ over the alphabet $\Sigma$, whether $\Sigma^* \subset L(G)$. This result is true even if $G$ is linear.

\footnote{$\alpha$ is a string of terminals.}
Proof. Let $\Sigma = \{a_1, \ldots, a_m\}$; the corresponding problems over this alphabet are known to be undecidable ([15]). The size of the alphabet can be reduced to 2 by padding and encoding.

\[\square\]

Lemma 4.4 Let $G_1$ and $G_2$ be bounded-basis grammars over the alphabet $\Sigma = \{a, b\}$. Then $G_1 \subset G_2$ is undecidable. This result is true even if $G_1$ and $G_2$ are required to be linear, or if both grammars are required to be in Modified Chomsky Normal Form.

Proof. Let $G_1$ be the obvious bounded-basis, linear (or MCNF) grammar generating $\Sigma^+$. Testing whether $\epsilon \in L(G_2)$ is decidable, and our result follows by Lemmas 4.1 and 4.3 (4.2 and 4.3 if $G_2$ is MCNF). \[\square\]

Lemma 4.5 Let $G$ be a linear, bounded-basis grammar over $\Sigma = \{a, b\}$. Then, $\Sigma^+ L(G) \subset \Sigma L(G)$ is undecidable.

Proof. $\Sigma^+ \subset L(G)$ iff

1. $\Sigma \subset L(G)$ and
2. $\Sigma^+ L(G) \subset \Sigma L(G)$.

Since 1 is decidable, our result then follows by Lemma 4.4.

\[\square\]

4.4.2 Datalog programs

The following lemma will be of use in the following sections.

Lemma 4.6 Let $C$ and $D$ be the conjunctive queries

$C : p(\vec{X}) :\neg \mathcal{C}$.

$D : p(\vec{X}) : \mathcal{D}, f(Z)$.

where $\mathcal{C}$ and $\mathcal{D}$ are conjunctions of EDB predicates, $Z$ is a distinguished variable (i.e. $Z$ appears in $\vec{X}$) and $f(Z)$ does not appear in $\mathcal{C}$. Then $C \not\subset D$.

Proof. Every containment mapping $g : D \rightarrow C$ must satisfy $g(Z) = Z$, since $g(p(\vec{X}))$ must be $p(\vec{X})$. However, then $g(f(Z))$ does not appear in the body of $C$. \[\square\]

Safety

Recall that a rule is termed safe if every variable appearing in the rule head (a distinguished variable) appears in the rule body, and a program is termed safe if every rule in the program is safe. The constructions of the following sections will deal with programs that are unsafe. However, these programs may be made safe without altering the results of these sections, as follows.

Let

\[r : p(\vec{X}) : \neg \mathcal{C}.'\]
be a (not necessarily safe) conjunctive query (or rule), and let $e$ be a predicate not appearing in $r$. Then the notation $safe(r,e)$ represents the query obtained from $r$ by adding conjunctions $e(A)$ to the body of $r$ for every variable $A$ that appears in $r$. Similarly, the notation $safe(P,e)$ represents the replacement of every rule $r$ in the program $P$ with the rule $safe(r,e)$ for some predicate $e$ that appears nowhere in $P$.

**Example 4.1** If $r$ is the rule

$$r: p(X,Y) :- b(X,U).$$

then $safe(r,e)$ is the rule

$$p(X,Y) :- b(X,U), e(X), e(Y), e(U).$$

**Lemma 4.7** For any conjunctive queries $r$ and $s$ and any predicate $e$ that appears nowhere in $r$ or $s$, there is a containment mapping $f: s \rightarrow r$ iff there is a containment mapping $g: safe(s,e) \rightarrow safe(r,e)$.

**Proof.** The containment mapping $g: safe(s,e) \rightarrow safe(r,e)$ is a containment mapping from $s$ into $r$. For the converse, assume that $f$ is a containment mapping from $s$ into $r$. Consider any atom $e(A)$ in $safe(s,e)$: by construction, $A$ appears in $s$, and therefore $f(A)$ appears in $r$. Also by construction, $e(f(A))$ appears in $safe(r,e)$, and $f$ is therefore a containment mapping from $safe(s,e)$ into $safe(r,e)$.

**Lemma 4.8** Let $P$ be a program, and let $e$ be a predicate not appearing in $P$. Then, $P$ generates the top-down expansion $r$ iff $safe(P,e)$ generates the top-down expansion $safe(r,e)$.

**Corollary.** Let $P$ and $Q$ be programs, and assume that $e$ does not appear in $P$ or $Q$. Then, $P \subseteq Q$ iff $safe(P,e) \subseteq safe(Q,e)$.

**Proof.** Straightforward induction on the number of rule applications in $P$. The corollary follows by Lemma 4.7 and the theorem of Sagiv and Yannakakis (Theorem 1.2).

For the remainder of this chapter, we will consider unsafe programs with the understanding that these programs will be made safe as in the above lemma.

### 4.5 Linear Logic Programs

In this section, we prove Result 4.1(a) and Result 4.2. The basic idea is the simulation of bounded-basis grammars using single-DB programs with head-rectified rules and a bounded number of basis rules.

---

2The predicate $e$ essentially represents the DOM relation ([36])
4.5.1 The construction

Let $G$ be an $e$-free grammar over $\Sigma = \{a_1, \ldots, a_k\}$ with nonterminals $\{N_1, \ldots, N_m\}$. We will construct a program $P$, defining the IDB predicate $p$, to simulate $G$. The EDB for $P$ will consist of binary predicates $\{a_1, \ldots, a_k\}$ and a unary predicate $f$.

Let $X, Y, W$ and $Z$ be new variable names; the head of each rule in $P$ is

$$p(X, Y, W, Z, N_1, \ldots, N_m)$$

Note that each rule head is rectified (i.e. contains no repeated variables). Let $< N_i >$ denote an $m$-vector in which the $i$th component is $W$, and all other components are $Z$. Further, let us use the notation

$$p(< A, B > < N_i >>)$$

to represent the $p$-atom

$$p(A, B, W, Z, < N_i >>)$$

**Example 4.2** Let $G$ be a linear grammar over $\Sigma = \{a, b\}$ with start symbol $S$ and the productions

$$S \rightarrow aS \quad S \rightarrow bB \quad B \rightarrow b.$$  

$G$ clearly generates $a^*bb$. The head of each rule in $P$ is the atom $p(X, Y, W, Z, S, B)$, and $p(< U, Y > < B >>)$ denotes the atom $p(U, Y, W, Z, Z, W)$. □

**Definition 4.4** We define a transformation from symbols in $G$ (terminal or nonterminal) to atomic formulae, as follows. Let $U$ and $V$ be distinct variables. For any terminal $a_i$, the $\{U, V\}$-atom corresponding to $a_i$ is the atom $a_i(U, V)$. The $\{U, V\}$-atom corresponding to a nonterminal $N_i$ is the atom $p(< U, V > < N_i >>)$. This transformation may be extended to strings, as follows. Let $s = s_1 \ldots s_n$ be a nonempty string of terminals and nonterminals in $G$. Assume that $U_1, \ldots, U_{n+1}$ are distinct variables. We define the $\{U_1, \ldots, U_{n+1}\}$-chain corresponding to $s$ to be the conjunction $c = c_1, \ldots, c_n$ where for all $i$, $c_i$ is the $\{U_i, U_{i+1}\}$-atom corresponding to $s_i$. □

**Example 4.3** Let $G$ be the grammar of Example 4.2. The $\{X, U\}$-atom corresponding to the terminal $b$ is $b(X, U)$, and the $\{X, U, Y\}$-chain corresponding to the string $bB$ is the conjunction $b(X, U), p(< U, Y > < B >>)$, or $b(X, U), p(U, Y, W, Z, Z, W)$. □

**Definition 4.5** Let $s = s_1 \ldots s_n$ be a (possibly empty) string of terminals and nonterminals, let $C$ and $\Gamma$ be conjunctions of atomic formulae, and let $C$ be the conjunctive query (or rule)

$$C : p(\tilde{H}) \leftarrow \Gamma, C.$$ 

Let $D$ and $E$ be variables appearing in $C$. $\Gamma$ is termed a chain from $D$ to $E$, embedded in $C$ and representing $s$ iff one of the following is true.
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1. \( s = \epsilon, \Gamma \) is the empty conjunction **true** and \( D = E \).

2. \( s = s_1 \) (a terminal or nonterminal), \( D \) and \( E \) are distinct and \( \Gamma \) is the \( \{D, E\} \) atom corresponding to \( s_1 \).

3. \( s = s_1 \ldots s_n \) with \( n > 1 \), \( D \) and \( E \) are distinct and \( \Gamma \) is the \( \{D, U_1, \ldots, U_{n-1}, E\} \)-chain corresponding to \( s \) for some distinct variables \( U_1, \ldots, U_{n-1} \) distinct from \( D \) and \( E \), and not appearing in \( \bar{H} \) or among the arguments of the conjuncts in \( C \).

If \( s \) is a nonempty string of terminals and \( D \) and \( E \) appear in \( \bar{H} \), then \( \Gamma \) is a **binary chain** ([33]). □

**Example 4.4** Consider the conjunctive query

\( C_1 : p(X, Y, W, Z) :- a(X, U_1), b(U_1, U_2), a(U_2, Y), f(W), f(Z). \)

The conjunction \( a(X, U_1), b(U_1, U_2), a(U_2, Y) \) is a binary chain from \( X \) to \( Y \) representing the terminal string \( aba \) and embedded in \( C_1 \). □

Binary chains may be used to simulate strings in a language, as follows.

**Lemma 4.9** Consider the conjunctive queries

\( C_1 : p(\bar{H}) :- \Gamma_1, C_1. \)

\( C_2 : p(\bar{H}) :- \Gamma_2, C_2. \)

where \( \Gamma_1, \Gamma_2, C_1 \) and \( C_2 \) are conjunctions of EDB predicate occurrences. Let \( X \) and \( Y \) be distinguished variables (i.e. they appear in \( \bar{H} \)). Let \( \Gamma_1 \) be a binary chain from \( X \) to \( Y \), embedded in \( C_1 \) and representing the terminal string \( t = t_1 \ldots t_l \), and let \( \Gamma_2 \) be a binary chain from \( X \) to \( Y \), embedded in \( C_2 \) and representing the terminal string \( s = s_1 \ldots s_n \). Assume that there is a containment mapping \( g \) from

\( p(\bar{H}) :- C_2. \)

into

\( p(\bar{H}) :- C_1. \)

Then, there is a containment mapping \( h : C_2 \rightarrow C_1 \) iff \( n = l \) and the strings \( t_1 \ldots t_l \) and \( s_1 \ldots s_n \) are identical.

**Proof.** Assume that \( \Gamma_1 \) and \( \Gamma_2 \) are as below.

\( \Gamma_1 : t_1(X, U_1), \ldots, t_l(U_{i-1}, Y). \)

\( \Gamma_2 : s_1(X, V_1), \ldots, s_l(V_{n-1}, Y). \)
Assume that the strings are identical. Let \( h \) be the identity mapping on distinguished variables (the variables in \( \bar{H} \)), and define \( h(V_i) = U_i \) for all \( i \). The function \( f \) defined by

\[
f(A) = \begin{cases} 
    h(A) & \text{if } h \text{ is defined on } A \\
    g(A) & \text{if } g \text{ is defined on } A
\end{cases}
\]

is a containment mapping from \( C_2 \) into \( C_1 \).

For the converse, assume that \( h \) is a containment mapping from \( C_2 \) into \( C_1 \). Then \( h(X) = X \) and \( h(Y) = Y \), since \( X \) and \( Y \) are distinguished.

If \( n = 0 \), then \( \Gamma_2 = s_1(X,Y) \). Since \( h \) is the identity of distinguished variables, and since \( s_1 \) does not appear in \( C_1 \) by assumption, we may conclude that \( \Gamma_2 = h(s_1(X,Y)) = s_1(X,Y) \).

Consider any \( n > 0 \). If \( l = 0 \) (that is, \( \Gamma_1 = t_1(X,Y) \)), then \( h(s_1(X,V_1)) \) must be \( t_1(X,Y) \), and \( h(V_1) = Y \), a contradiction since \( Y \) does not appear as the first argument of any atom in \( \Gamma_1 \) (so \( s_2(V_1,V_2) \) has no destination in \( \Gamma_1 \)). If \( l > 0 \), then the only atom in \( \Gamma_1 \) whose first argument is \( X \) is \( t_1(X,U_1) \). Thus, \( h(s_1(X,V_1)) = t_1(X,U_1) \), yielding \( s_1 = t_1 \) and \( h(V_1) = U_1 \). An inductive repetition on \( l \) may be used to show that \( l = n \), and \( s_1 \ldots s_n = t_1 \ldots t_n \). \( \square \)

**Example 4.5** Let the conjunctive queries \( C_1 \) and \( C_2 \) be as follows.

\[
C_1 : p(X,Y,W,Z) \dashv a(X,U_1), b(U_1,U_2), a(U_2,Y), f(W), f(Z).
\]

\[
C_2 : p(X,Y,W,Z) \dashv a(X,V_1), b(V_1,V_2), a(V_2,Y), f(W), f(Z).
\]

Then, the mapping \( h \) defined by \( h(X) = X, h(Y) = Y, h(W) = W, h(Z) = Z, h(V_1) = U_1, h(V_2) = U_2 \) is a containment mapping from \( C_2 \) into \( C_1 \). However, there is no containment mapping from \( C_3 \) or \( C_4 \) into \( C_1 \), where \( C_3 \) and \( C_4 \) are defined as follows.

\[
C_3 : p(X,Y,W,Z) \dashv b(X,V_1), b(V_1,V_2), a(V_2,Y), f(W), f(Z).
\]

\[
C_4 : p(X,Y,W,Z) \dashv a(X,V_1), a(V_1,Y), f(W), f(Z).
\]

The transformation from \( G \) to \( \mathcal{P} \) is effected by the following algorithm.

**Algorithm 4.1**

INPUT: an \( \epsilon \)-free grammar \( G \) with nonterminals \( N_1, \ldots, N_m \).

OUTPUT: a single-IDB program \( \mathcal{P} \) to simulate \( G^{3} \).

1. The head of every rule is \( p(X,Y,W,Z,N_1, \ldots, N_m) \).

2. Consider every production

\[
d_i : \ N_j \rightarrow \beta
\]

in \( G \), where \( \beta \) is of length \( n \). Let \( \{U_1, \ldots, U_{n-1}\} \) be a set of new and distinct variables.

and let \( \gamma \) be the \( \{X, U_1, \ldots, U_{n-1}, Y\} \)-chain representing \( \beta \). We construct the rule

\[
r_i : p(X,Y,W,Z,N_1, \ldots, N_m) \vdash \gamma, f(N_j), f(W).
\]

\( ^3 \)The manner of the simulation will be discussed later.
3. Add a single basis rule

\[ \begin{align*}
\text{b} &: p(X, Y, W, Z, N_1, \ldots, N_m) :& f(Z).
\end{align*} \]

If \( G \) is linear, then \( P \) is linear. Further, if \( G \) has \( k \) extensional productions, then \( P \) has \( k + 1 \) initialisation rules.

**Example 4.6** Consider the linear grammar \( G \) of Example 4.2. Our construction produces the following rules.

\[ \begin{align*}
p(X, Y, W, Z, S, B) :&= a(X, U), p(U, Y, W, Z, W, Z), f(S), f(W). \\
p(X, Y, W, Z, S, B) :&= b(X, V), p(V, Y, W, Z, Z, W), f(S), f(W). \\
p(X, Y, W, Z, S, B) :&= b(X, Y), f(B), f(W). \end{align*} \]

The importance of the variables \( W \) and \( Z \) is that they are persistent; that is, they appear in their "home" positions in every \( p \)-atom resulting from a top-down expansion in \( P \).

**Lemma 4.10** Let \( P \) be a single-IDB program defining the predicate \( p \), and let \( X_i \) be the \( i \)th variable in the head of every rule. Assume that the \( i \)th argument of every \( p \)-atom in the body of every rule is \( X_i \). Then the \( i \)th argument of every \( p \)-leaf in any top-down expansion of \( p \) using the rules in \( P \) is \( X_i \).

**Proof.** By induction on the number \( n \) of rule applications in the expansion. \( \square \)

The intention of our construction is that the rules of \( P \) mimic derivations in \( G \), to produce binary chains to represent every string in \( L(G) \). The idea is illustrated in Figure 4.3. In the figure, the variable \( A \) may be a new nondistinguished variable, or the distinguished variable \( X \). Similarly, \( B \) may be a nondistinguished variable, or the distinguished variable \( Y \). \( U \) is a new nondistinguished variable.

**Example 4.7** Figure 4.4 shows how a binary chain representing the string \( bb \) is generated by the program of Example 4.4. \( \square \)

However, these rules also may be used to mimic "illegal" derivations in the grammar. That is, the production \( N_i \rightarrow a_k N_j \) cannot be used to expand the nonterminal \( N_i \), if
Lemma 4.11 Let $C$ be an illegal conjunctive query generated by $\mathcal{P}$. Then $C \subset b$, where $b$ is the nonrecursive rule added in step 3 of the algorithm.

Proof. Both conjunctive queries have the root $p(X, Y, W, Z, N_1, \ldots, N_m)$, and the identity mapping on variables in the root is a containment mapping from $b$ into $C$. \qed

The simulation of $G$ by $\mathcal{P}$ is formalised in the next three lemmas.

Lemma 4.12 Let $S$ be the legal top-down expansion

$$S : p(X, Y, W, Z, N_1, \ldots, N_m) := A, p(<U_a, V_1>, N) \leadsto N_{i'}, f(V_{i'}).$$
where $U_a$ and $V_1$ are distinct, $A$ is a chain from $X$ to $U_a$ representing some string $\alpha$ in $S$, and $\Gamma$ is a chain from $V_1$ to $Y$ representing some string $\gamma$ in $S$, and the conjunction

$$(A, p(<U_a, V_1>> <N_j>>), \Gamma)$$

is a chain from $X$ to $Y$ representing $\alpha N_j \gamma$ in $S$.

Construct the top-down expansion $T$ by expanding the indicated $p$-atom through some rule $r_k$ constructed by Algorithm 4.1 from the production $d_k : N_m \rightarrow \beta$. Then

1. If $N_m \neq N_j$, $T$ is illegal; and
2. If $N_m = N_j$, then $T$ is of the form

$$T : p(X, Y, W, Z, N_1, \ldots, N_m) := \Delta, f(N_i), f(W).$$

where $\Delta$ is a chain from $X$ to $Y$, representing $\alpha \beta \gamma$ and embedded in $T$.

**Proof.** By the construction of the rule $r_k$ by Algorithm 4.1, $r_k$ is of the form

$$r_k : p(X, Y, W, Z, N_1, \ldots, N_m) := B, f(N_m), f(W).$$

where $B$ is a $\{X, R_1, \ldots, R_n, Y\}$-chain corresponding to $\beta$ and the $R_i$ are distinct variables not appearing in the rule head.

If $N_m \neq N_j$, then (since the $N_m$-argument of $p(<U_a, V_1>> <N_j>>)$ is $Z$), the body of $T$ contains the conjunct $f(Z)$, and $T$ is therefore illegal. However, if $N_m = N_j$, then by the persistence of $W$, the only $f$-atoms added are copies of $f(W)$. Assume that the $R_i$ are renamed to new variables $D_i$ in the expansion; then the children of the indicated $p$-atom in $S$ forms a chain from $U_a$ to $V_1$, representing $\beta$ in $T$. Setting $\Delta = (A, B, \Gamma)$ completes the proof. \Box

**Lemma 4.13** If $\beta$ is a sentential form derived from the nonterminal $N_i$ by $G$, then

$$T : p(X, Y, W, Z, N_1, \ldots, N_m) := B, f(N_i), f(W).$$

is a top-down expansion in legal($\mathcal{P}$), where $B$ is a chain from $X$ to $Y$ representing $\beta$ and embedded in $T$.

**Corollary.** Assume $a_{i_1} a_{i_2} \ldots a_{i_k} \in yield(N_i)$. Then legal($\mathcal{P}$) generates the conjunctive query

$$C : p(X, Y, W, Z, N_1, \ldots, N_m) := B, f(N_i), f(W).$$

where $B$ is a binary chain representing $a_{i_1} \ldots a_{i_k}$.

**Proof.** Assume $N_i \vdash \beta$. We prove our result by induction on $n$. If $n = 1$, then $N_i \rightarrow \beta$ is a production and our result follows by construction. Assume the truth of the hypothesis for $i < n$, where $n > 1$. Assume that $N_i \vdash \delta$; then $\delta$ is of the form $\alpha \beta \gamma$, where $N_i \vdash^{1} \alpha N_j \beta$, and where $d_k : N_j \rightarrow \beta$ is a production. By our inductive hypothesis, $\mathcal{P}$ generates a legal top-down expansion
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\[ S : p(X, Y, W, Z, N_1, \ldots, N_m) := A, p(< U_a, V_1 > < N_j > ), \Gamma, f(N_i), f(W). \]

where \((A, p(U_a, V_1) < N_j >, \Gamma)\) is a chain from \(X\) to \(Y\), embedded in \(S\) and representing \(\alpha N_j \gamma\). \(A\) is a chain from \(X\) to \(U_a\) representing \(\alpha\) in \(S\), and \(\Gamma\) is a chain from \(V_1\) to \(Y\) representing \(\gamma\) in \(S\). We construct \(T\) by expanding the indicated \(p\)-atom through the rule \(r_k\) corresponding to the production \(d_k\), and our result follows by Lemma 4.12. \(\square\)

**Lemma 4.14** Let \(T\) be a top-down expansion in \(\text{legal}(\mathcal{P})\). Then \(T\) is of the form

\[ T : p(X, Y, W, Z, N_1, \ldots, N_m) := B, f(N_i), f(W). \]

where \(B\) is a chain from \(X\) to \(Y\), embedded in \(T\) and representing a sentential form \(\beta \in \text{yield}(N_i)\) for some \(N_i\).

**Corollary** Let \(C\) be a conjunctive query in \(\text{legal}(\mathcal{P})\). Then \(C\) is of the form

\[ p(X, Y, W, Z, N_1, \ldots, N_m) := B, f(N_i), f(W). \]

where \(B\) is a binary chain representing some string \(a_{i_1} \ldots a_{i_k} \in \text{yield}(N_i)\).

**Proof.** Let \(T\) be a top-down expansion in which \(n\) rules are applied. We prove our result by induction on \(n\).

If \(n = 1\), then the rule applied is of the form

\[ r_k : p(X, Y, W, Z, N_1, \ldots, N_m) := B, f(N_i), f(W). \]

where \(B\) is a chain representing some string \(\beta\) and

\[ d_k : N_i \rightarrow \beta \]

is a production in \(G\).

Assume the truth of the hypothesis for \(i < n\), where \(n > 1\). Let the following be a legal top-down expansion generated by \(n\) rule applications.

\[ T : p(X, Y, W, Z, N_1, \ldots, N_m) := \Delta. \]

\(T\) must be generated by the expansion of some \(p\)-atom in some legal top-down expansion \(S\) (generated by \(n - 1\) rule applications) through some rule \(r_k\). By our inductive hypothesis, \(S\) is of the form

\[ S : p(X, Y, W, Z, N_1, \ldots, N_m) := A, p(< U_a, V_1 > < N_j > ), \Gamma, f(N_i), f(W). \]

where \(N_i \Rightarrow \alpha N_j \gamma\), and where the conjunction

\[ (A, p(U_a, V_1) < N_j >, \Gamma) \]

is a chain from \(X\) to \(Y\), embedded in \(S\) and representing \(\alpha N_j \gamma\) (so that \(A\) is a chain from \(X\) to \(U_a\) representing \(\alpha\) in \(S\) and \(\Gamma\) is a chain from \(V_1\) to \(Y\) representing \(\gamma\) in \(S\)). Consider
the rule \( r_k \) that is used to expand the indicated \( p \)-atom in \( S \) to obtain \( T \). By construction, the rule \( r_k \) is of the form

\[
\tau_k : p(X, Y, W, Z, N_1, \ldots, N_m) := B, f(N_m), f(W).
\]

such that

\[
d_k : N_m \rightarrow \beta
\]

is a production in \( G \). By Lemma 4.12 and the assumed legality of \( T \), we must have \( N_m = N_j \); hence \( N_i \Rightarrow \alpha \beta \gamma \) and our result follows by Lemma 4.12. \( \square \)

4.5.2 Using the construction

Let \( G_1 \) be an \( \varepsilon \)-free grammar over \( \Sigma = \{a_1, \ldots, a_k\} \), with start symbol \( N_1 \) and intensional nonterminals \( N_1, \ldots, N_m \). Let \( G_2 \) be an \( \varepsilon \)-free grammar over \( \Sigma \), with start symbol \( M_1 \) and nonterminals \( M_1, \ldots, M_l \). Without loss of generality, we assume that the nonterminals of \( G_1 \) and \( G_2 \) are distinct.

Let \( S \) be a new nonterminal. Construct an \( \varepsilon \)-free grammar \( G_3 \) (with start symbol \( S \)) as the union of all the productions in \( G_1 \) and \( G_2 \), and add the two productions \( s_1 \) and \( s_2 \) described below.

\[
s_1 : S \rightarrow N_1
\]

\[
s_2 : S \rightarrow M_1
\]

\( L(G_3) \) is clearly \( L(G_1) \cup L(G_2) \).

Let \( G_4 \) be the \( \varepsilon \)-free grammar obtained from \( G_3 \) by deleting the production \( s_1 \). \( L(G_4) \) is clearly the same as \( L(G_2) \); we have merely introduced a unit production to change the start symbol. Note that for any \( N_i \) or \( M_i \), the yield of this nonterminal is the same for \( G_3 \) and \( G_4 \); that is, the only nonterminal for which the yields may differ in \( G_3 \) and \( G_4 \) is the start symbol \( S \).

Apply Algorithm 4.1 to \( G_3 \) and \( G_4 \) to create programs \( P \) and \( Q \) respectively, ensuring that the rule head in each case is \( p(X, Y, W, Z, S, N_1, \ldots, N_k, M_1, \ldots, M_l) \); that is, the nonterminals of \( G_3 \) and \( G_4 \) appear in the same positions in the heads of all rules in \( P \) and \( Q \). Hence, every rule in \( Q \) also appears in \( P \), and we may conclude that \( Q \subset P \).

**Lemma 4.15** \( P \subset Q \) iff \( L(G_1) \subset L(G_2) \).

**Corollary.** \( P \equiv Q \) iff \( L(G_1) \subset L(G_2) \).

**Proof.**

By the construction of \( G_3 \) and \( G_4 \), the strings generated by any nonterminal \( N \neq S \) are the same for \( G_3 \) and \( G_4 \).

Assume that \( L(G_1) \subset L(G_2) \). Then \( L(G_3) \subset L(G_4) \) by the construction of \( G_3 \) and \( G_4 \), and any string generated by any nonterminal in \( G_3 \) is also generated by the same nonterminal in \( G_4 \). Consider any conjunctive query \( C \) generated by \( P \); if \( C \) is illegal, then \( C \) is contained in the basis rule \( b \) of \( Q \). If \( C \) is legal, then by Lemma 4.14, assumption. Lemma 4.13 and Lemma 4.9, \( C \) is contained in some legal conjunctive query \( D \) generated by \( Q \).
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For the converse, assume that \( \mathcal{P} \subseteq \mathcal{Q} \). Then every legal conjunctive query \( \mathcal{C}_\mathcal{P} \) generated by \( \mathcal{P} \) is contained in some legal conjunctive query \( \mathcal{C}_\mathcal{Q} \) generated by \( \mathcal{Q} \), and Lemmas 4.13, 4.14 and 4.9 suffice to complete the proof. \( \square \)

**Theorem 4.1** Let \( \mathcal{P} \) and \( \mathcal{Q} \) be safe, linear, single-IDB programs with head-rectified rules and five basis rules. Then \( \mathcal{P} \subseteq \mathcal{Q} \) (\( \mathcal{P} \equiv \mathcal{Q} \)) is undecidable.

**Proof.** Let \( G_1 \) and \( G_2 \) be linear bounded-basis grammars over the alphabet \( \Sigma = \{ a_1, a_2 \} \) and apply the construction of the preceding lemma; our result follows by Lemmas 4.15 and 4.4. Safety is imposed as in Section 4.4. Note that, if \( G_1 \) and \( G_2 \) are bounded-basis, then Lemma 4.15 holds even if \( G_1 \) and \( G_2 \) have the same extensional nonterminals, and the number of basis rules can therefore be reduced to three. \( \square \)

Now, let \( G_1 \) be the following linear grammar over \( \Sigma = \{ a_1, a_2 \} \).

\[
\begin{align*}
d_1 &: N_1 \rightarrow a_1 N_1 \\
d_2 &: N_1 \rightarrow a_2 N_1 \\
d_3 &: N_1 \rightarrow a_1 \\
d_4 &: N_1 \rightarrow a_2
\end{align*}
\]

\( G_1 \) generates \( \{ a_1 + a_2 \}^+ \). Let \( G_2 \) be a linear, bounded-basis grammar over \( \Sigma \), with nonterminals \( M_1, \ldots, M_l \) and start symbol \( M_1 \). We assume without loss of generality that \( N_1 \) is distinct from each \( M_i \). Construct the grammar \( G_3 \) with new start symbol \( S \) by taking the union of the productions in \( G_1 \) and \( G_2 \), and adding the production

\[
s : S \rightarrow N_1 M_1.
\]

\( G_3 \) generates \( \Sigma^+ L(G_2) \). Apply Algorithm 4.1 to \( G_3 \) to produce the program \( \mathcal{P} \). Note that \( \mathcal{P} \) has five basis rules and only one nonlinear rule (corresponding to the production \( s \)).

Consider the legal conjunctive queries in \( \mathcal{P} \). Since \( S \) appears on the left-hand side of only the production \( s \) and does not appear on the right-hand side of any production, the nonlinear rule \( r \), representing the production \( s \) is used only in the simulation of strings in \( \text{yield}(S) \), and the rule can only be used at the root of a top-down expansion involved in such a simulation.

**Theorem 4.2** Let \( \mathcal{P} \) be a safe, head-rectified, single-IDB program with five basis rules and one nonlinear rule. The base-case linearizability of \( \mathcal{P} \) is undecidable.

**Proof.** Let \( G_3 \) be the grammar of the preceding discussion, and let \( \mathcal{P} \) be the result of applying Algorithm 4.1 to \( G_3 \). Any illegal conjunctive query generated by \( \mathcal{P} \) is contained in the basis rule \( b \). Every legal conjunctive query representing a string in \( \text{yield}(N_1) \) or \( \text{yield}(M_i) \) is linear, and hence right-linear. The legal conjunctive queries representing strings in \( \text{yield}(S) \) simulate \( \Sigma^+ L(G_2) \), and the right-linear subset of these queries simulates \( \Sigma L(G_2) \); our result follows by Lemma 4.5. Safety is imposed as in Section 4.1. \( \square \)
4.6 Single-recursive-rule programs

In this section, we present a construction whereby an arbitrary Modified Chomsky Normal Form (MCNF) grammar may be simulated using a head-rectified, single-IDB program with a single recursive rule and a bounded number of basis rules. The construction may be used to show that sequencability is undecidable, even for programs with only two recursive rules. In addition, the construction can be used to prove the undecidability of equivalence (or containment) of programs with a single recursive rule.

4.6.1 The construction

Let \( H \) be an MCNF grammar over \( \Sigma = \{a_1, a_2\} \), with nonterminals \( N_1, \ldots, N_m \), start symbol \( N_3 \) and extensional productions \( N_1 \rightarrow a_1 \) and \( N_2 \rightarrow a_2 \). We construct a program \( \mathcal{P} \), with one nonrecursive rule, to simulate \( H \).

The program \( \mathcal{P} \) defines the IDB predicate \( p \), and the head of each rule is

\[
p(R, X, Y, W, Z, G, A, B, N_1, \ldots, N_m)
\]

As before, \( << N_i >> \) denotes an \( m \)-vector in which the \( i \)th component is \( W \), and in which all other components are \( Z \). The expression

\[
p(< K, L > < M > < R, T > < < N_i >>)
\]

will be used to represent the \( p \)-atom

\[
p(Z, K, L, W, Z, M, R, T, < < N_i >>)
\]

That is, the first argument is always \( Z \), and the 4th and 5th are always \( W \) and \( Z \) respectively (so that \( W \) and \( Z \) appear in their “home” positions). The EDB predicates in \( \mathcal{P} \) are \( a_1, a_2, f, g \) and \( h \).

The variables in the head of each rule have the following purposes:

1. \( R \) is a switch that is relevant only to the proof that sequencability is undecidable. The \( R \)-position in the arguments of each \( p \)-atom in the body of the recursive rule will be occupied by the variable \( Z \), described below.

2. \( X \) and \( Y \) are the end-points of binary chains representing strings in \( L(H) \), as in the preceding section.

3. \( W \) and \( Z \) are guard variables. as in the preceding section. They are used to weed out illegal conjunctive queries generated by the programs (i.e., queries representing impossible derivations in the grammar).

4. \( G \) is a guard position. Intuitively, a \( p \)-atom may be legally expanded through the recursive rule if its \( G \)-th argument is \( W \), but not if its \( G \)-th argument is \( Z \).

5. \( A \) and \( B \) are used to allow a choice in expanding one of two or-productions, in a manner to be described.
CHAPTER 4. UNDECIDABILITY OF THE GENERAL PROBLEMS

6. $N_1, \ldots, N_m$ represent the corresponding nonterminals in the grammar.

The rules of $\mathcal{P}$ are constructed as follows.

Algorithm 4.2
INPUT: an MCNF grammar $G$ with nonterminals $N_1, \ldots, N_m$, where $N_1$ is the extensional nonterminal representing $\alpha_1$ and $N_2$ is the extensional nonterminal representing $\alpha_2$.
OUTPUT: a head-rectified, single-IDB program $\mathcal{P}$ with one recursive rule $r$ and 9 basis rules $i_1 \ldots i_9$.

1. The head of each rule is $p(R, X, Y, W, Z, G, A, B, N_1, \ldots, N_m)$.

2. $\mathcal{P}$ has the following 9 basis rules:

   $$p(R, X, Y, W, Z, G, A, B, N_1, \ldots, N_m) :=$$

   $$i_1 : a(X, Y), f(N_1), f(G).$$
   $$i_2 : b(X, Y), f(N_2), f(G).$$
   $$i_3 : f(Z).$$
   $$i_4 : g(G).$$
   $$i_5 : g(W).$$
   $$i_6 : f(U), g(U).$$
   $$i_7 : h(A, B), f(G).$$
   $$i_8 : h(U, V), h(V, W).$$
   $$i_9 : h(U, U).$$

3. The body of the recursive rule $r$ for $\mathcal{P}$ has the atoms $f(W), f(G), g(Z), g(N_1), g(N_2)$ and $h(E, F)$, where $E$ and $F$ are nondistinguished variables that appear nowhere else in the program. The body of $r$ also has $p$-atoms for each intensional production in the grammar, as follows:

   (a) Let $J \rightarrow K$ be a copy production, and let $U_J$ be a new nondistinguished variable. Then, the recursive rule contains the atom

   $$p(<X, Y <<- J <<- U_J, U_J <<- K >>)$$

   This atom (and any version of it in a top-down expansion) is called a copy-atom representing $K$ in the production.

   (b) Let $J \rightarrow K$ and $J \rightarrow L$ be a pair of or-productions, and let $T_J, U_J$ and $V_J$ be new nondistinguished variables. Then, the body of $r_\mathcal{P}$ contains the atoms

   $$p(<X, Y <<- J <<- T_J, U_J <<- K >>)$$
   $$p(<X, Y <<- J <<- V_J, V_J <<- L >>)$$
The first of these is the or-atom representing \( K \) in the first production, and the second is the or-atom representing \( L \) in the second production. Versions of these two atoms in a top-down expansion such that both atoms have the same parent are called sibling or-atoms. The idea is that we need never recursively expand both these \( p \)-atoms, since either one (but not both) may be expanded using initialisation rule \( i_7 \).

\( (c) \) Let \( J \rightarrow KL \) be an and-production, and let \( T_J, U_J \) and \( V_J \) be new nondistinguished variables. \( r_P \) has the two \( p \)-atoms

\[
\begin{align*}
p(\langle X, T_J \rangle \langle J \rangle \langle U_J, U_J \rangle \langle K \rangle) \\
p(\langle T_J, Y \rangle \langle J \rangle \langle V_J, V_J \rangle \langle L \rangle)
\end{align*}
\]

The first of these atoms is called the and-atom representing \( K \) in the production, and the second is called the and-atom representing \( L \) in the production. Versions of these atoms that have the same parent are called sibling and-atoms. The idea is that both atoms are (recursively) expanded, to create chains from \( X \) to \( T_J \), and from \( T_J \) to \( Y \).

\( \square \)

**Example 4.8** The following MCNF grammar \( G \) over \( \Sigma = \{c, d\} \) generates \( \Sigma^+ \).

\[
\begin{align*}
S & \rightarrow TT \\
T & \rightarrow S \\
T & \rightarrow H \\
H & \rightarrow C \\
H & \rightarrow D \\
C & \rightarrow c \\
D & \rightarrow d
\end{align*}
\]

The corresponding program is

\[
\begin{align*}
r & : p(R, X, Y, W, Z, G, A, B, C, D, S, T, H) :- \\
p(R, X, Y, W, Z, G, A, B, C, D, S, T, H) & \\
f(W), f(G), g(Z), g(C), g(D), h(E, F).
\end{align*}
\]

\[
\begin{align*}
p(Z, X, Y, W, Z, G, A, B, S, T, C, D) & :- \\
i_1 & : c(X, Y), f(C), f(G). \\
i_2 & : d(X, Y), f(D), f(G). \\
i_3 & : f(Z). \\
i_4 & : g(G). \\
i_5 & : g(W). \\
i_6 & : f(U), g(U). \\
i_7 & : h(A, B), f(G). \\
i_8 & : h(U, V), h(V, W).
\end{align*}
\]
\( i_0 : h(U, U) \).

In the recursive rule, the first two \( p \)-atoms represent the and-production \( S \rightarrow TT \): hence, these atoms are and-atoms. The next two \( p \)-atoms represent the or-productions \( T \rightarrow S \) and \( T \rightarrow H \), and are therefore or-atoms. Similarly, the 5th and 6th \( p \)-atoms are or-atoms representing the or-productions \( H \rightarrow C \) and \( H \rightarrow D \). The initialisation rules \( i_1 \) and \( i_2 \) represent the extensional productions \( C \rightarrow c \) and \( D \rightarrow d \) respectively.

\[ \square \]

Intuition

The intention is that the program \( \mathcal{P} \) simulate the strings in the grammar \( G \), by generating binary chains to represent the strings in \( L(G) \). The basic ideas are as follows.

Illegal expansions As in the previous section, we detect illegal top-down expansions through the existence of the atom \( f(Z) \) in the expansion. The idea is as follows. Consider any top-down expansion using only the recursive rule; as in the previous section, the variables \( W \) and \( Z \) are persistent in the \( p \)-atoms of the expansion. At each stage of the expansion, \( p \)-atoms in the body of the recursive rule are "activated" by placing \( W \) in the guard (6th) position of the atom, or "deactivated" by placing \( Z \) in this position. If the guard position of a \( p \)-atom is \( Z \), then the application of the recursive rule will introduce the atom \( f(Z) \), and the expansion is illegal; hence, such atoms must be terminated by a basis rule in all legal expansions. The activation of atoms in the body of the recursive rule enforces the fact that legal expansions correspond to derivations in the grammar.

Example 4.9 Consider the grammar and program of Example 4.8. Assume that at some stage, the atom corresponding to the production \( T \rightarrow H \) has been activated: that is, the atom is of the form


Applying the recursive rule to this atom yields atoms of the form

\[ f(W), f(W'), g(Z), g(C'), g(D), h(E, F). \]

Note that the first four atoms are deactivated (with \( Z \) in position 6), and the last two atoms are activated (with \( W \) in position 6). Note also that the atoms that are activated are precisely the atoms representing productions whose head is \( H \), as required by the fact that the atoms corresponding to the production \( T \rightarrow H \) has been expanded. Finally, note that the 5th atom (the first to be activated) represents the production \( H \rightarrow C \), and the arguments representing the nonterminals in this atom is \( << C >> \). Similarly, note that the
6th atom (the second to be activated) represents the production $H \rightarrow D$, and the arguments representing the nonterminals in this atom is $<< D >>$. \hfill $\Box$

**Or-productions** Another wrinkle is the fact that if an or-production is used in a derivation in the grammar, then there are two activated atoms in the simulating expansion. The idea, here, is that either one of these atoms may be terminated by the initialisation $i_7$, but not both (otherwise the result is contained in the initialisation rule $i_8$).

**Example 4.10** Consider the expansion of Example 4.9, in which the or-atoms corresponding to the or-productions $H \rightarrow C$ and $H \rightarrow D$ have been activated. Either one of these atoms may be terminated by rule $i_7$. However, if both are terminated in this way, then the result contains the atoms $h(I_6, I_7), h(I_7, I_8)$, and the result is contained in $i_8$. \hfill $\Box$

**The simulation**

We say that a conjunctive query (or top-down expansion) generated by the program is illegal if it is contained in one of the initialisation rules $i_1 \ldots i_9$, and legal otherwise. No interesting top-down expansions are contained in $i_1$ or $i_2$, as the following lemma shows.

**Lemma 4.16** Let $T$ be a top-down expansion in which the recursive rule $r$ is used. Then $T \not\subset i_1$ and $T \not\subset i_2$.

**Proof.** The root of $T$ is expanded using $r$, since $r$ is the only recursive rule in the program. $T$, $i_1$ and $i_2$ have the same root (the rule head that is common to all rules), and any containment mapping $c$ from $i_1$ or $i_2$ into $T$ must satisfy $c(N_1) = N_1$ and $c(N_2) = N_2$. Now, $f(N_1)$ appears in the body of $i_1$ and $f(N_2)$ appears in the body of $i_2$. However, neither $N_1$ nor $N_2$ appears in the body of $r$, and hence neither $f(N_1)$ nor $f(N_2)$ appears in $T$. Thus, there is no containment mapping $c$ from $i_1$ or $i_2$ into $T$. \hfill $\Box$

The following lemmas show us that most of the initialisation rules may never be used in any interesting top-down expansion.

**Lemma 4.17** Let $T$ be a top-down expansion in which one of the basis rules $i_3, i_5, i_6, i_8$ and $i_9$ is used. Then $T$ is illegal.

**Corollary.** Only the rules $r, i_1, i_2$ and $i_7$ are used in any legal top-down expansion.

**Proof.** The head of $T$ is the rule head that is common to all rules. By Lemma 4.10, $W$ and $Z$ appear in their "home" positions in every $p$-atom in $T$. Hence, if $i_j$ is used in $T$, then $T$ is contained in $i_j$. \hfill $\Box$

**Lemma 4.18** Assume that $T$ is a legal top-down expansion that includes a $p$-atom in which the 6th argument (the "home" position for $G$) is $W$. Then one of $r, i_1, i_2$ and $i_7$ must be used to expand such a $p$-atom.

**Proof.** By Lemma 4.17, one of $r, i_1, i_2, i_4$ and $i_7$ must be used to expand this $p$-atom. However, if $i_4$ is used, then $g(W)$ appears in the body of $T$, and $T$ is contained in $i_5$. \hfill $\Box$
Lemma 4.19 Assume that $T$ is a legal top-down expansion that includes a $p$-atom in which the 6th argument (the “home” position for $G$) is $Z$. Then only $i_4$ is used to expand any such atoms.

**Proof.** By Lemma 4.17, rules $i_3, i_5, i_6, i_8$ and $i_9$ may not be used in the expansion. If one of $r, i_1, i_2$ and $i_7$ is used, then $f(Z)$ appears in the body of $T$, and $T \subseteq i_3$. \(\square\)

Lemma 4.20 In any legal top-down expansion $T$, no copy-atom or and-atom is expanded using initialisation rule $i_7$.

**Proof.** Assume the converse; then the body of $T$ contains the atom $h(G, G)$ for some variable $G$, and $T$ therefore is contained in initialisation rule $i_9$. \(\square\)

Lemma 4.21 In any legal top-down expansion $T$, no two sibling or-atoms are expanded using rule $i_7$.

**Proof.** Otherwise, $T$ is contained in initialisation rule $i_8$. \(\square\)

Lemma 4.22 Let $T$ be a legal top-down expansion in which $s$ and $t$ are two sibling or-atoms (or sibling and-atoms). If $s$ is expanded through the initialisation rule $i_4$, then so is $t$.

**Proof.** Since $s$ and $t$ are siblings, both have the same 6th argument (the argument in the home position for $G$), say $S$. If $s$ is expanded through $i_4$, then $g(S)$ appears in the body of $T$. Since $T$ is assumed to be legal, Lemma 4.17 requires that one of the rules $r, i_1, i_2, i_4$ and $i_7$ is used to expand $t$; however, if any rule but $i_4$ is used, then $f(S)$ is a conjunct in the body of $C$ and $T$ is contained in rule $i_6$ (and is therefore illegal). \(\square\)

Lemma 4.23 In any top-down expansion $T$, $i_7$ may only be used to expand one of two sibling or-atoms, and the sibling or-atom is expanded using one of $r, i_1$ and $i_2$.

**Proof.** By Lemmas 4.21 and 4.22. \(\square\)

Lemma 4.24 Let $T$ be a legal top-down expansion in which some atom

\[ p(< I_1, I_2, I_3, I_4, I_5, I_6, I_7 >> < N_k, N_l >>) \]

(with arbitrary $I_j$) is expanded through the recursive rule $r$. Then $N_k \neq N_1$ and $N_k \neq N_2$.

**Proof.** Assume the converse; then, the body of the recursive rule has the atom $g(W)$, and $T$ is contained in $i_5$. \(\square\)

Lemma 4.25 Let $T$ be a legal top-down expansion in which some atom

\[ p(< I_1, I_2, I_3, I_4, I_5, I_6, I_7 >> < N_k, N_l >>) \]

(with arbitrary $I_j$) is expanded through the initialisation rule $i_j$, where $j \in \{1, 2\}$. Then $N_k = N_j$.

**Proof.** Assume the converse. Then $f(Z)$ appears in the body of $T$, and $T \subseteq i_3$. \(\square\)
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Lemma 4.26 Let $T$ be a conjunctive query generated by $P$ in which the recursive rule $r$ is used at least twice. Then every $p$-atom at depth $n > 1$ in $T$ has as 6th argument (the argument in the "home" position of $G$) either $W$ or $Z$.

Proof. By Lemma 4.10, $W$ and $Z$ appear in their home positions in every $p$-atom in $T$. By construction, every variable in the home position for any $N_i$ in any $p$-atom in $T$ is $W$ or $Z$, and the "guard" position is therefore occupied by $W$ or $Z$ in any child of such an atom. □

Let us say that a conjunctive query is restricted if whenever one of two sibling or-atoms is expanded through $r$, $i_1$ or $i_2$, then its sibling atom is expanded through $i_7$.

Lemma 4.27 Every legal conjunctive query $C$ is contained in a conjunctive query $D$ that is both legal and restricted.

Proof. Let us assume that one of the sibling or-atoms

$$p(< U, V > < S > < I_1, I_2 > < < N_i > >)$$

and

$$p(< U, V > < S > < I_2, I_3 > < < N_j > >)$$

is expanded through $r$, $i_1$ or $i_2$ in the top-down expansion $T$ establishing the conjunctive query $C$. Since $C$ is legal, the root of $T$ is expanded using rule $r$, and $C$ therefore contains an atom of the form $h(E, F)$. By Lemma 4.26 and Lemma 4.19, $S$ is $W$ or $G$, and by construction $f(S)$ appears in the body of $C$. By Lemmas 4.18 and 4.22, the sibling atom is expanded through one of $r$, $i_1$, $i_2$, and $i_7$. If $i_7$ is not used, then since the distinguished variables $A$ and $B$ appear nowhere in the bodies of $r$, $i_1$ or $i_2$, the variables $I_1$, $I_2$ and $I_3$ appear nowhere in the fringe of $T$ (i.e., in the body of $C$). Thus, we may construct a new conjunctive query $C'$ from $C$, by expanding the first or-atom through rule $i_7$ to produce the atoms $f(S)$ and $h(I_1, I_2)$ for variables $I_1$ and $I_2$ that appear nowhere else in the new conjunctive query $C'$. $C$ is contained in $C'$ because $f(S)$ and an atom of the form $h(E, F)$ appears in $C$. An inductive repetition suffices to remove all violations of restrictiveness in $C$, while preserving the legality of $C$. □

For any distinct variables $U$ and $V$, define a $\{U, V\}$-atom corresponding to an intensional nonterminal $N_i$ to be any $p$-atom

$$p(< U, V > < W > < H, I > < < N_i > >)$$

for any variables $H$ and $I$, and let chains be defined as in the preceding section. Note that, depending on the variables $H$ and $I$ in any $p$-atom, a string of terminals and nonterminal has many corresponding chains.

Definition 4.6 Define a top-down expansion $T$ to be closed if $T$ is legal and restricted, and if the following hold.

1. Any $p$-atom in which the 6th argument (the argument representing the guard ($G$) is the distinguished variable $Z$ is expanded through $i_4$; that is, no such $p$-atom is a leaf.
2. Consider any two sibling or-atoms neither of which is expanded using \( i_4 \). Then one of these atoms is expanded using rule \( i_2 \).

3. No \( p \)-atoms at depth 1 in the tree are leaves; that is, every \( p \)-child of the root is expanded through some rule.

By Lemmas 4.19, 4.18, 4.22 and 4.26, every top-down expansion establishing a legal, restricted conjunctive query is closed. \( \Box \)

The following Lemmas formalise the simulation of the grammar \( G \) by the program \( P \).

**Lemma 4.28** Let

\[
p(<U,V><S><I_1,I_2><N_i>)
\]

be an atom in a closed top-down expansion \( R \), where \( S \) is one of \( W \) and \( G \), where \( U \neq V \), and where \( I_1 \) and \( I_2 \) are arbitrary. If this \( p \)-atom is expanded using one application of one of \( r, i_1 \) and \( i_2 \) to produce a closed top-down expansion \( T \), then the subtree rooted at this \( p \)-atom contains the following.

1. The atom \( f(S) \), and 0 or more occurrences of the atoms \( f(W) \) and \( g(Z) \).

2. 0 or more occurrences of atoms \( h(P,Q) \) for distinct variables \( P \) and \( Q \).

3. A chain from \( U \) to \( V \) representing \( \gamma \), where \( \gamma \) is a production.

**Proof.** By Lemma 4.25, the rule \( i_k \) \((k \in \{1,2\})\) may be used only if \( N_i = N_k \); the subtree then contains the atoms \( f(S) \), \( f(W) \) and \( a_k(U,V) \). Recall that the extensional productions are of the form \( N_1 \to a_1 \) and \( N_2 \to a_2 \).

Assume that \( r \) is used. By Lemma 4.24, \( N_i \neq N_1 \) and \( N_i \neq N_2 \); that is, \( N_i \) is an intensional nonterminal. Application of \( r \) yields the atoms \( f(S) \) and \( f(W) \), two copies of \( g(Z) \) (since \( N_i \neq N_1 \) and \( N_i \neq N_2 \)), and an atom of the sort \( h(E',F') \) where \( E' \) and \( F' \) are distinct, new variables obtained by renaming \( E \) and \( F \) in the top-down expansion. Consider the \( p \)-atoms that are generated by this application of \( r \). By construction, the 6th position of any atom representing a production \( N_j \to \beta \) is \( Z \), if \( N_j \neq N_i \); hence, by Lemma 4.19, every such atom must be expanded using rule \( i_4 \) (yielding the atom \( g(Z) \)). Also by construction, the 6th argument of the atom(s) representing any production \( N_i \to \gamma \) is \( W \). There are three cases.

1. \( N_i \to N_k \) is a copy-production. By construction, the corresponding atom in the indicated application of \( r \) is

\[
p(<U,V><W><J_1,J_1><N_k>)
\]

and our result follows.
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2. \( N_i \rightarrow N_k \) and \( N_i \rightarrow N_l \) are or-productions. By construction, the corresponding atoms in the indicated application of \( r \) are

\[
\begin{align*}
p(<U,V><W><J_1,J_2><N_k>) \\
p(<U,V><W><J_2,J_3><N_i>)
\end{align*}
\]

for some nondistinguishing variables \( J_1, J_2 \) and \( J_3 \) that appear nowhere else in \( T \) (since these variables are renamed in the expansion). By Lemma 4.18, and since \( T \) is assumed closed, one of these atoms must be expanded through \( i_7 \) to add the atoms \( f(W) \) and \( h(I_1,I_2) \) (or \( h(I_2,I_3) \)) to \( T \). Our result follows.

3. \( N_i \rightarrow N_k N_l \) is an and-production, and the corresponding atoms in the indicated application of \( r \) are

\[
\begin{align*}
p(<U,I><W><J_1,J_1><N_k>) \\
p(<I,V><W><J_2,J_2><N_i>)
\end{align*}
\]

where \( I \) is a renaming of the variable \( T_{N_i} \) to a new variable that appears nowhere else in the expansion. Our result follows.

\[ \square \]

Lemma 4.29 Let

\[
p(<U,V><S><I_1,I_2><N_i>)
\]

be an atom in a closed top-down expansion \( R \), where \( S \) is one of \( W \) and \( G \), where \( U \neq V \), and where \( I_1 \) and \( I_2 \) are arbitrary. If \( N_i \rightarrow \gamma \) is a production in the grammar \( G \), then there is a closed top-down expansion \( T \) obtained by expanding this \( p \)-atom using exactly one application of \( r, i_1 \) or \( i_2 \), but with an arbitrary number of uses of other rules, such that the subtree rooted at this \( p \)-atom contains the following atoms.

1. The atom \( f(S) \), and 0 or more occurrences of the atoms \( f(W) \) and \( g(Z) \).

2. 0 or more occurrences of atoms \( h(P,Q) \) for distinct variables \( P \) and \( Q \).

3. A chain from \( U \) to \( V \) representing \( \gamma \).

Proof. If \( i = 1 \) or \( i = 2 \), then we may apply \( i_1 \) or \( i_2 \) to the indicated \( p \)-atom to obtain the result.

Assume that \( N_i \) is an intensional nonterminal. Expand the indicated \( p \)-atom through the recursive rule \( r \). Then the "non-\( p \)" children of the indicated \( p \)-atom are \( f(S) \), \( f(W) \), \( g(Z) \), and \( h(E',F') \) where \( E' \) and \( F' \) are distinct, new variables obtained by renaming \( E \) and \( F \) in the top-down expansion. Consider the \( p \)-atoms that are generated by this application of \( r \). By construction, the 6th position of any atom representing a production \( N_j \rightarrow \beta \) is \( Z \), if \( N_j \neq N_i \); hence, every such atom may be expanded using rule \( i_4 \) (yielding the atom \( g(Z) \), which appears as a child of the root.) Also by construction, the 6th argument of the atom(s) representing any production \( N_i \rightarrow \gamma \) is \( W \). There are three cases.
1. \( N_i \rightarrow N_k \) is a copy-production. By construction, the corresponding atom in the indicated application of \( r \) is

\[
p(<U,V><W><J_1,J_1><N_k>)
\]

and our result follows.

2. \( N_i \rightarrow N_k \) and \( N_i \rightarrow N_i \) are or-productions. By construction, the corresponding atoms in the indicated application of \( r \) are

\[
p(<U,V><W><J_1,J_2><N_k>)
p(<U,V><W><J_2,J_3><N_i>)
\]

for some nondistinguished variables \( J_1, J_2 \) and \( J_3 \) that appear nowhere else in \( T \) (since these variables are renamed in the expansion). Without loss of generality, assume that \( \gamma \) is \( N_k \). Then, the latter atom may be expanded through \( i_1 \) to add the atoms \( f(W) \) and \( h(I_2, I_3) \) to \( T \). Our result follows.

3. \( N_i \rightarrow N_k N_i \) is an and-production. Then, the corresponding atoms in the indicated application of \( r \) are

\[
p(<U,I><W><J_1,J_1><N_k>)
p(<I,V><W><J_2,J_2><N_i>)
\]

where \( I \) is a renaming of the variable \( T_{N_i} \) to a new variable that appears nowhere else in the expansion. Our result follows.

\[\Box\]

For any nonterminal \( J \) in \( G \), recall that \( \text{yield}(J) \) represent all the strings generated by \( J \) (i.e., the strings that would be generated if \( J \) were the start symbol of \( G \)).

Lemma 4.30 Let \( T \) be a closed top-down expansion generated by \( \mathcal{P} \). Then the body of \( T \) consists of the atoms \( f(W), f(G), g(Z), g(N_1) \) and \( g(N_2) \); atoms of the form \( h(U,V) \), where \( U \) and \( V \) do not appear in the root; and for \( 3 \leq i \leq m \), either \( g(N_i) \), or \( f(N_i) \) and a chain representing some string \( \delta \) of terminals and nonterminals such that \( N_i \Rightarrow \delta \).

Corollary. Let \( C \) be a conjunctive query generated by \( \mathcal{P} \), established by a closed top-down expansion \( T \). Then the body of \( C \) consists of the atoms \( f(W), f(G), g(Z), g(N_1) \) and \( g(N_2) \); atoms of the form \( h(U,V) \), where \( U \) and \( V \) do not appear in the root; and for \( 3 \leq i \leq m \), either \( g(N_i) \), or \( f(N_i) \) and a chain representing some terminal string \( \delta \) such that \( N_i \Rightarrow \delta \).

Proof. Let \( T \) be a closed top-down expansion in \( G \). Since \( T \) is assumed closed, the root is expanded through the recursive rule \( r \). For any intensional nonterminal \( N_i \), consider all the atoms representing productions of the form \( N_i \rightarrow \alpha \). The proof proceeds by induction on \( n \), the number of applications of \( r \cdot i_1 \) or \( i_2 \) to atoms representing productions of which \( N_i \) is the head.

If \( n = 1 \), then by Lemma 4.22, rule \( i_4 \) is used to expand all such atoms, and the atom \( g(G) \) is introduced.
4.6. SINGLE-RECURSIVE-RULE PROGRAMS

If \( n = 2 \), then rule \( r \) is used and the result follows by Lemma 4.28; note that the 6th argument (the "home" position for \( G \)) in any \( p \)-atom at depth 1 is \( G \) by construction. The induction also follows by Lemma 4.28.

To prove the corollary, we observe that in any conjunctive query (with EDB's at the leaves), if \( h(U, V) \) is obtained by the expansion of an or-atom through \( i_7 \), then the occurrence of \( U \) (or \( V \)) in the sibling or-atom disappears when \( r, i_1 \) or \( i_2 \) is used to expand the latter, since the distinguished variables \( A \) and \( B \) do not appear in the body of these rules. \( \Box \)

The converse is also true.

**Lemma 4.31** Assume that \( N_i \models \delta \), where \( i > 2 \). Then, \( \mathcal{P} \) generates a closed top-down expansion \( T \), as follows. The body of \( T \) consists of the atoms \( f(W), f(G), g(Z), g(N_1) \) and \( g(N_2) \); atoms of the form \( h(U, V) \), where \( U \) and \( V \) do not appear in the root; and either \( g(N_i) \), or \( f(N_i) \) and a chain representing \( \delta \).

**Corollary.** Assume that \( N_i \Rightarrow \delta \), where \( \delta \) is a string of terminals and \( i > 2 \). Then, \( \mathcal{P} \) generates a closed top-down expansion \( T \) generating a conjunctive query \( C \), as follows. The body of \( C \) consists of the atoms \( f(W), f(G), g(Z), g(N_1) \) and \( g(N_2) \); atoms of the form \( h(U, V) \), where \( U \) and \( V \) appear nowhere else in \( C \); and either \( g(N_i) \), or \( f(N_i) \) and a binary chain representing \( \delta \).

**Proof.** Assume that \( N_i \models \delta \). Our proof proceeds by induction on \( n \), the depth of the sentential forms derived by \( N_i \) in \( G \). The basis (\( n = 1 \)) follows by Lemma 4.29 (since the 6th position in any child of the root is \( G \), if \( r \) is used to expand the root), and the induction also follows by Lemma 4.29.

The corollary is proved as in the previous lemma. \( \Box \)

### 4.6.2 Using the construction

Let \( G_1 \) be an arbitrary MCNF grammar over the alphabet \( \Sigma = \{a_1, a_2\} \), with extensional nonterminals \( N_1 \) and \( N_2 \) representing \( a_1 \) and \( a_2 \) respectively, start symbol \( K_1 \) and nonterminals \( K_1, \ldots, K_n \). Let \( G_2 \) be an arbitrary MCNF grammar over the same alphabet, with the same extensional nonterminals representing the same terminals, and with start symbol \( L_1 \) and nonterminals \( L_1, \ldots, L_m \). Create a new start symbol \( S \); construct the new grammar \( G_3 \) with start symbol \( S \), with productions that are the union of the productions in \( G_1 \) and \( G_2 \), and with the new productions

\[
\begin{align*}
s_1 : & \quad S \rightarrow K_1 \\
s_2 : & \quad S \rightarrow L_1
\end{align*}
\]

Let \( G_4 \) be the grammar obtained from \( G_3 \) by deleting the production \( s_1 \), but with the same start symbol. Clearly, \( G_3 \) and \( G_4 \) have the same nonterminals, and \( \text{yield}(M) \) is the same in both grammars, for \( M \neq S \). Also, \( L(G_3) = L(G_1) \cup L(G_2) \) and \( L(G_4) = L(G_2) \); hence, \( L(G_4) \subseteq L(G_3) \), and \( L(G_2) \subseteq L(G_4) \) if \( L(G_1) \subseteq L(G_2) \).

Apply Algorithm 4.2 to \( G_3 \) and \( G_4 \) to produce \( \mathcal{P} \) and \( \mathcal{Q} \) respectively, making sure that the order of nonterminals is preserved in the rule heads of \( \mathcal{P} \) and \( \mathcal{Q} \).
Lemma 4.32 $\mathcal{P} \subseteq \mathcal{Q} (\mathcal{P} \equiv \mathcal{Q})$ iff $L(G_1) \subseteq L(G_2)$.
Proof. By Lemmas 4.30, 4.31 and 4.9, and by construction. □

Theorem 4.3 Let $\mathcal{P}$ and $\mathcal{Q}$ be safe, single-IDB programs with a single recursive rule and nine initialisation rules. Then, the containment or equivalence of such programs is undecidable.
Proof. By Lemmas 4.32 and 4.4. □

Theorem 4.4 The sequencability of single-IDB programs is undecidable.
Proof. Let $\mathcal{P}$ and $\mathcal{Q}$ be as above. Assume that $\mathcal{P}$ has the recursive rule $r_1$ and the nine initialization rules $i_1, \ldots, i_9$, and that $\mathcal{Q}$ consists of the recursive rule $r_2$ and the same nine initialization rules. Add the atom $f(R)$ to the body of $r_1$ to obtain the rule $r'_1$, and let $T$ be the program consisting of $r'_1, r_2, i_1, \ldots, i_9$. Now, since the "home" position for $R$ is occupied by the persistent variable $Z$ in every $p$-atom in either recursive rule, we may conclude that the recursive rule $r'_1$ is used at most once in any top-down expansion that is not contained in the initialization rule $i_3$, and that $r'_1$ is used to expand the root in such a case. Thus, the yield of $S$ in the program represents $L(G_1) \cup L(G_2)$, but the yield of $S$ in the sequenced program represents $L(G_2)$, and our result follows as above. □

---

4The body of the resulting expansion contains the atom $f(R)$, but this atom is irrelevant to the sequencability of $T$. 
Chapter 5

Concluding remarks

In this report, we investigate opportunities to optimize recursive Horn-clause programs through transformations to simpler, more efficiently evaluable programs. We focus our attention on optimizations that may be described in terms of normal forms for the proof trees generated by the program in question. We introduce the idea of subtree eliminations as a way to describe normal forms, and present a uniform approach to the development of sufficient conditions for the detection of the applicability of a normal form to the program. We then illustrate this approach on the detection of one-boundedness, basis-linearizability and sequencability, and show how the sufficient conditions that are generated may be tuned to the desired complexity. We also investigate the complexity of these three optimization problems; our investigation yields a characterization of the complexity of conjunctive query containment, and tight undecidability results for the detection of program equivalence. Our results are contained in Table 5.1. The programs considered are all Datalog. The expression \( \leq i \) reps means that each recursive rule in the program has at most \( i \) occurrences of any EDB predicate in the body of each recursive rule.

Whether sequencability is decidable in any interesting case is an open question. However,

<table>
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<th>Polynomial time</th>
<th>( \mathcal{NP} )-hard</th>
<th>Undecidable</th>
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<td>One-boundedness</td>
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<td>linear sirup,</td>
<td>never</td>
</tr>
<tr>
<td></td>
<td>( \leq 1 ) reps</td>
<td>( \leq 4 ) reps</td>
<td></td>
</tr>
<tr>
<td>Basis-linearizability</td>
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<td>bilinear sirup,</td>
<td>1 nonlinear rule,</td>
</tr>
<tr>
<td></td>
<td>( \leq 1 ) reps</td>
<td>( \leq 4 ) reps</td>
<td>5 basis rules.</td>
</tr>
<tr>
<td>Sequencability</td>
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<td>2 recursive rules</td>
<td>2 recursive rules,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(both linear),</td>
<td>9 basis rules.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \leq 3 ) reps,</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 basis rule</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.1: Complexity results.

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current work that the author is undertaking in conjunction with Tomás Feder seems to indicate a positive answer to that question.
Bibliography


