Non-Confluent NLC Graph Grammar Inference by Compressing Disjoint Subgraphs

Hendrik Blockeel\textsuperscript{1,2} and Robert Brijder\textsuperscript{1}

\textsuperscript{1} Leiden Institute of Advanced Computer Science, Universiteit Leiden, The Netherlands, rbrijder@liacs.nl
\textsuperscript{2} Department of Computer Science, Katholieke Universiteit Leuven, Belgium, hendrik.blockeel@cs.kuleuven.be

Abstract. Grammar inference deals with determining (preferable simple) models/grammars consistent with a set of observations. There is a large body of research on grammar inference within the theory of formal languages. However, there is surprisingly little known on grammar inference for graph grammars. In this paper we take a further step in this direction and work within the framework of node label controlled (NLC) graph grammars. Specifically, we characterize, given a set of disjoint and isomorphic subgraphs of a graph $G$, whether or not there is an NLC graph grammar rule which can generate these subgraphs to obtain $G$. This generalizes previous results by assuming that the set of isomorphic subgraphs is disjoint instead of non-touching. This leads naturally to consider the more involved “non-confluent” graph grammar rules.

1 Introduction

Grammar inference, also called grammar induction, is a general line of research where one is concerned with determining a “simple” grammar that is consistent with a given set of possible and impossible outcomes. Hence, one “goes back” in the derivation: instead of determining the generative power of a grammar, one determines the grammar given the generated output. This topic is well-studied for formal languages, especially with respect to context-free languages, see e.g. [6, 4], however, relatively little is known for graph grammars.

The topic of inference of graph grammars is considered in [5] and uses their so-called Subdue scheme developed in [2]. In [1] a rigorous approach of grammar inference within the framework of node label controlled (NLC) graph grammars [3], a natural and well-studied class of graph grammars, is initiated. There it is characterized, given a set $S$ of non-touching isomorphic graphs of a graph $G$, whether or not there is a graph grammar consisting of one rule able to generate the graphs of $S$ to obtain $G$. We continue this research and generalize this result for the case where these graphs are disjoint instead of non-touching. Such a generalization requires one to deal with a number of issues. Most notably, one has to deal with non-confluency issues: the generated graph depends on the order in which touching subgraphs are generated.
2 Notation and Terminology

We consider (simple) graphs \( G = (V, E) \), where \( V \) is a finite set of nodes and \( E \subseteq \{ \{x, y\} \mid x, y \in V, x \neq y \} \) is the set of edges – hence no loops or parallel edges are allowed. We denote \( V(G) = V \) and \( E(G) = E \). For \( S \subseteq V \), the induced subgraph of \( G \) is \((S, E')\) where \( E' \subseteq E \) and for each \( e \in E \) we have \( e \in E' \) if \( e \subseteq S \). We consider only induced subgraphs, and therefore we sometimes just write “subgraph” instead of induced subgraph. The neighborhood of \( S \subseteq V \) in \( G \), denoted by \( N_G(S) \), is \( \{ v \in V \setminus S \mid \{s, v\} \in E \text{ for some } s \in S \} \). If \( S = \{x\} \) is a singleton, then we also write \( N_G(x) = N_G(S) \). A labelled graph is a triple \( G = (V, E, l) \) where \( (V, E) \) is a graph and \( l : V \to L \) is a node labelling function, where \( L \) is a finite set of labels. As usual, graphs are considered isomorphic if they are identical modulo the identity of the vertex. It is important to realize that for labelled graphs, vertices identified by an isomorphism have identical labels. In graphical depictions of labelled graphs we will always represent the vertices by their labels.

Subgraphs \( G_1 \) and \( G_2 \) are called disjoint if \( V(G_1) \) and \( V(G_2) \) are disjoint. They are called touching if \( V(G_1) \cup N_G(V(G_1)) \) and \( V(G_2) \cup N_G(V(G_2)) \) are not disjoint.

Define, for disjoint \( W_1, W_2 \subseteq V \), \( K_{W_1, W_2} = \{(x_1, x_2) \mid x_1 \in W_1, x_2 \in W_2\} \) to be the set of all tuples with the left element from \( W_1 \) and the right element from \( W_2 \). Define \( u((x_1, x_2)) \) to be the underlying set \( \{x_1, x_2\} \), and define \( \pi_i((x_1, x_2)) = x_i \) for \( i \in \{1, 2\} \). Often, for function \( f : X \to Y \) we write \( f(D) = \{f(x) \mid x \in D\} \) for \( D \subseteq X \).

3 NLC Graph Grammars

Typically, a graph grammar transforms a graph \( G \) by replacing an (induced) subgraph \( H \) by another graph \( H' \) where \( H' \) is embedded in the remaining part \( G \setminus H \) of the original graph in a way prescribed by a so-called graph grammar embedding relation. The node label controlled (NLC) graph grammars are the simplest class of these grammars, where \( H \) is a single node. Note that for the grammars the exact identities of the nodes are not important as multiple copies of \( H' \) may be inserted. Hence, we consider labelled graphs where the embedding relation is defined w.r.t. node labels instead of nodes. In this section we recall informally the notions and definitions concerning NLC grammars used in this paper, and refer to [3] for a gentle and more detailed introduction to these grammars.

A NLC graph grammar is a system \( Q \) consisting of a set of node labels \( L \), an embedding relation \( E \subseteq L^2 \), and a set of productions \( P \) where a production is of the form \( N \to S \) where \( N \in L \) and \( S \) is a (labelled) graph. In this paper we will focus on the case \( |P| = 1 \). Hence \( Q \) can be denoted as a rule \( r = N \to S/E \) (if \( L \) is understood from the context of considerations). Given a graph \( G \), \( r \) can be applied to any node \( v \) labelled by \( N \). The result of applying \( r \) to \( v \) in \( G \) is that \( v \) is removed from \( G \) along with the edges adjacent to \( v \), and (a copy of) \( S \) is
added to \( G \), and an edge \( e = \{ x, y \} \) is added to \( G \) iff \( x \in V(S) \), \( y \in N_G(S) \) and \((l(x), l(y)) \in E\) (recall that \( l \) is the labelling function). To avoid confusion with embedding relations, the set of edges of a graph \( G \) are written in the remainder as \( E(G) \) and not as \( E \).

![Fig. 1: The derivation of a graph \( G \) (left-hand side) to \( G' \) (right-hand side).](image)

**Example 1.** Let \( G \) be the graph on the left-hand side of Figure 1. Consider the grammar rule \( r = N \rightarrow S/E' \), where \( S \) is the graph

![Diagram of graph S](image)

and \( E' = \{(a, b), (b, a), (c, c), (a, N), (c, N)\} \). (Note that formally we have only defined \( S \) up to isomorphism, however as we have seen this is not an objection.) Then Figure 1 depicts one possible derivation from \( G \) to a graph \( G' \) (on the right-hand side of the figure) for which no rule is applicable anymore. Note that there is one other possible derivation to a “terminal” graph \( G'' \) (i.e., a graph without vertices labelled by \( N \)): to obtain \( G'' \) we choose first the right-hand vertex labelled by \( N \) (the one not connected to the vertex labelled by \( b \)) in \( G \) in the derivation. Note that \( G' \) and \( G'' \) are different graphs. We assume that the set of labels \( L \) is \( \{a, b, c, N\} \). This example will be our running example of this paper.

In [1] the inference of NLC grammars with exactly one rule \( r = N \rightarrow S/E \) are studied where moreover \( S \) does not contain a vertex labelled by \( N \) and \( E \) does not contain a tuple containing \( N \). This is sufficient for the case where the subgraphs isomorphic to \( S \) are non-touching. To consider the case where the subgraphs are disjoint, we allow \( E \) to contain tuples containing \( N \). However, we do require that \( S \) remains without vertices labelled by \( N \). Therefore there is no “real” recursion: no vertices labelled by \( N \) can be introduced in any derivation.
4 Known results: Non-touching graphs

In this section we recall some notions and a result from [1] which we will need in
subsequent sections. First we define in this context the notion of compatibility.

**Definition 2.** Let $G$ be a graph and $S$ be an induced subgraph of $G$. We say
that $E \subseteq L \times L$ is **compatible for** $S$ (in $G$) if there is a graph $F$ such that
an application of NLC grammar rule $N \rightarrow S'/E$ to $F$ “creates” $S$ and obtains graph
$G$. Note: $S'$ is (isomorphic to) $S$.

**Example 3.** Reconsider our running example. Hence we again let $G'$ be the graph
at the right-hand side of Figure 1. Moreover we let $S_1$ and $S_2$ be the subgraphs
of $G'$ of the form

```
  a --- a
  |    |
  b    c
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where $S_1$ is the one connected to the a vertex labelled by $b$ and $S_2$ is the other
one. Note that $S_1$ and $S_2$ are disjoint and touching in $G'$. We have that, e.g.,
$E_1 = \{(b,a),(c,c)\}$, $E_2 = \{(b,a),(c,c),(a,b)\}$ or $E_3 = \{(b,a),(c,c),(c,b),(b,b)\}$
is compatible for $S_2$ in $G'$. The middle graph of the figure is a graph $F$ such
that an application of the NLC grammar rule $N \rightarrow S'/E$ to $F$ “creates” $S_2$ and
obtains graph $G'$.

To characterize the notion of compatibility, the notions of **inset** and **outset**
for arbitrary $Q \subseteq V^2$ (where $V$ is the set of edges of $G$) are crucial.

**Definition 4.** Let $Q \subseteq V^2$, and let $P_Q = \{In_Q, Out_Q\}$ be the partition
of $Q$ where, for $x \in Q$, $x \in In_Q$ iff $u(x) \in E(G)$. We define the elements of
$\{In_Q, Out_Q\}$ as the **inset**, denoted by $I_Q$, and **outset**, denoted by $O_Q$, of $Q$,
respectively.

Let $S$ be an induced subgraph of $G$. Then the **inset** (outset, resp.) of $S$, denoted
by $I_S$ ($O_S$, resp.), is defined to be the inset (outset, resp.) of $Q = K_{V(S),N_G(V(S))}$.

The following lemma, given and proven in [1], characterizes compatibility for
a single graph $S$ in terms of the inset and outset of $S$: the inset are tuples that
should be in $E$, while the outset are tuples that should not be in $E$.

**Lemma 5.** Let $S$ be an induced subgraph of $G$, and let $E \subseteq L \times L$. Then $E$ is
compatible for $S$ iff $I_S \subseteq E \subseteq L^2 \setminus O_S$ (i.e., $E$ separates $I_S$ from $O_S$).

Hence, there is a compatible $E$ for $S$ in $G$ iff $I_S \cap O_S = \emptyset$.

**Example 6.** Reconsider again our running example. Then $I_{S_2} = \{(b,a),(c,c)\}$
and $O_{S_2} = \{(a,a),(a,c),(c,a),(b,c)\}$ (w.r.t. $G'$). Since $I_{S_2} \cap O_{S_2} = \emptyset$, there is a
compatible $E$ for $S_2$ in $G'$. We have that $I_{S_2} \subseteq E \subseteq L^2 \setminus O_{S_2}$ holds for, e.g., $E_1$,
$E_2$ and $E_3$ in Example 3.

We consider now sequences of subgraphs to be generated by a single graph
rule. Note that these graphs must necessarily be mutually isomorphic.
Definition 7. Let $G$ be a graph and $S_1, S_2, \ldots, S_n$ be induced subgraphs of $G$ isomorphic to $S$. We say that $E \subseteq L \times L$ is compatible for $(S_1, S_2, \ldots, S_n)$ (in $G$) if there are graphs $G_0, \ldots, G_n$ such that $G_n = G$ and for each $i \in \{1, \ldots, n\}$, $G_i$ is obtained from $G_{i-1}$ by applying NLC grammar rule $N \rightarrow S/E$ that “creates” $S_i$.

Note that, in general, the order of the elements $(S_1, S_2, \ldots, S_n)$ is important. E.g. a given $E$ may be compatible for $(S_1, S_2)$ while it is incompatible for $(S_2, S_1)$ (we will see such an example in the next section).

However, for a set of mutually non-touching and isomorphic subgraphs $S_i$ for $i \in \{1, \ldots, n\}$ of $G$, the order of the elements is not important. Thus, $E \subseteq L \times L$ compatible for $C = (S_1, S_2, \ldots, S_n)$ implies that $E$ is compatible for any permutation of $C$. In fact we have that, $E \subseteq L \times L$ is compatible for $S_1$, for $S_2$, \ldots, and for $S_n$ if it is compatible for $C$ (or any permutation of $C$). Therefore, in this case, Lemma 5 is trivially generalized: $E \subseteq L \times L$ is compatible for $(S_1, S_2, \ldots, S_n)$ iff $\cup_i I_{S_i} \subseteq E \subseteq L^2 \setminus (\cup_i O_{S_i})$ (as noted in [1]).

5 Two touching graphs

In this section we consider the case where a single NLC grammar rule $N \rightarrow S/E$ generates disjoint subgraphs which can (possibly) touch each other. Hence, this generalizes Lemma 5 by replacing the non-touching condition into disjointness. To this aim we allow non-terminal $N$ to be present in tuples of the embedding relation $E$ of NLC grammar rule $N \rightarrow S/E$. This introduces the issue of confluence: the order in which non-terminals are replaced by subgraphs influences the obtained graph. Example 1 illustrates this as the different graphs $G'$ and $G''$ can both be obtained from the original graph $G$.

As we will see the inset and outset between the vertices of two touching graphs turns out to be crucial.

Definition 8. Let $S_1$ and $S_2$ be touching graphs in $G$. For $Q_1 = K_{V(S_2), V(S_1) \cap N_G(S_2)}$, we denote $I_{Q_1}$ and $O_{Q_1}$ by $I_{(S_1, S_2)}$ and $O_{(S_1, S_2)}$, respectively. Moreover, for $Q_2 = K_{V(S_2), V(S_1)}$, we denote $I_{Q_2}$ and $O_{Q_2}$ by $I_{((S_1, S_2))}$ and $O_{((S_1, S_2))}$, respectively.

We now state some basic properties of the insets and outsets of Definition 8. Note first that $I_{(S_1, S_2)} = I_{((S_1, S_2))}$. In fact, it is equal to the inset of

$$K_{V(S_2) \cap \overline{N_G(S_1)}, V(S_1) \cap N_G(S_2)}.$$ 

Also note that, for node labels $x$ and $y$, we have $(x, y) \in I_{((S_1, S_2))}$ iff $(y, x) \in I_{((S_2, S_1))}$. This holds similarly for $O_{((S_1, S_2))}$; however, this does not hold in general for $O_{(S_1, S_2)}$. Moreover note that $O_{(S_1, S_2)} \subseteq O_{((S_1, S_2))}$, and

$$O_{((S_1, S_2))} \setminus O_{(S_1, S_2)} = l(K_{V(S_2), V(S_1) \cap N_G(S_2)}).$$

Finally note that $\tau_2(I_{(S_1, S_2)}) = l(V(S_1) \cap N_G(S_2))$. We will use these basic properties frequently in the remainder of this paper.
Example 9. In our running example, we have \( I_{(S_1, S_2)} = \{(b, a), (c, c)\}, O_{(S_1, S_2)} = \{(a, a), (a, c), (b, c), (c, a)\}, \) and \( O_{((S_1, S_2))} = L^2 \setminus I_{(S_1, S_2)} \) with \( L = \{a, b, c\}. \) Moreover, we have \( I_{(S_2, S_1)} = \{(a, b), (c, c)\}, O_{(S_2, S_1)} = \{(a, c), (b, b), (b, c), (c, b)\}, \) and \( O_{((S_2, S_1))} = L^2 \setminus I_{(S_2, S_1)}. \)

We now adapt the definition of inset and outset for a graph \( S, \) by incorporating the issues related to touching graphs.

**Definition 10.** Let \( S_1, \ldots, S_n \) be distinct subgraphs of \( G, \) and let \( Q = \cup_{i \in \{1, \ldots, n\}} K_{V(S_i), N_G(V(S_i)) \setminus (\cup_{j \in \{1, \ldots, n\} \setminus \{i\}} V(S_j))}. \) We denote \( I_Q \) and \( O_Q \) by \( I_{[S_1, \ldots, S_n]} \) and \( O_{[S_1, \ldots, S_n]}, \) respectively.

Note that \( I_{[S_1, S_2]} = I_{[S_2, S_1]} \) and if \( S_1 \) and \( S_2 \) are non-touching, we have \( I_{[S_1, S_2]} = I_{S_1} \cup I_{S_2}. \)

Example 11. In our running example, we have \( I_{[S_1, S_2]} = \{(a, b)\}, \) and \( O_{[S_1, S_2]} = \{(b, b), (c, b)\}. \)

Definitions 8 and 10 are to separate three types of insets and outsets. Roughly speaking, the two types of insets and outsets of Definition 8 deal with the tuples between \( S_1 \) and \( S_2, \) while the type of inset and outset of Definition 10 deals with the tuples from \( S_1 \) to the “outside world” (the vertices in the neighborhood of \( S_1 \) which do not belong to \( S_2 \)) plus the tuples from \( S_2 \) to the “outside world” (the vertices in the neighborhood of \( S_2 \) which do not belong to \( S_1 \)).

We now characterize the embedding relations \( E \) such that \( E \) is compatible for \((S_1, S_2)\) where \( S_1 \) and \( S_2 \) are touching subgraphs of \( G. \)

**Lemma 12.** Let \( S_1 \) and \( S_2 \) be touching subgraphs of \( G. \) Then \( E \subseteq L \times L \) is compatible for \((S_1, S_2)\) iff the following conditions hold:

1. \( I_{(S_1, S_2)} \subseteq E, \)
2. \( \{(x, N) \mid x \in \pi_2(I_{(S_1, S_2)})\} \subseteq E, \)
3. If \( e \in O_{((S_1, S_2))} \), then either \((\pi_2(e), N) \notin E \) or \( e \notin E \) (or both), and
4. \( I_{[S_1, S_2]} \subseteq E \subseteq L^2 \setminus (O_{[S_1, S_2]}). \)

Moreover, if this is the case, then we have \( E \cap O_{(S_1, S_2)} = \emptyset. \)

**Proof.** In the case where there are no edges between \( S_1 \) and \( S_2, \) we have, by Lemma 5, that \( E \subseteq L \times L \) is compatible for \((S_1, S_2)\) iff \( I_{S_1} \cup I_{S_2} \subseteq E \subseteq L^2 \setminus (O_{S_1} \cup O_{S_2}) \) – this is equivalent to condition (4) (since \( S_1 \) and \( S_2 \) are not-touching).

Now, since edges between \( S_1 \) and \( S_2 \) can only introduce additional constraints on \( E \) (i.e., not less constraints), we may consider only the graph \( F = N - N, \) an edge having two vertices labelled by \( N, \) and check the necessary and sufficient (additional) constraints on \( E \) to transform the graph in two steps where \( S_1 \) appears first and then \( S_2 \) such that the edges between \( S_1 \) and \( S_2 \) are identical to those between \( S_1 \) and \( S_2 \) in \( G. \)

Now, let \( x \) be a vertex of \( S_1 \) labelled by \( b, \) and \( y \) be a vertex of \( S_2 \) labelled by \( a. \) Assume first that \( x \) is connected to \( y \) in \( G. \) Now, if we apply the NLC rule to
create $S_1$, then $x$ should be connected to $N$ – thus we need $(b, N) \in E$. Indeed, without this rule $x$ will not be connected to any vertex of $S_2$ (after applying the NLC rule to create $S_2$). Now, if we subsequently apply the NLC rule to create $S_2$, then $y$ should be connected to $x$ and hence we need $(a, b) \in E$. Hence $(a, b) \in E$ and $(b, N) \in E$ results in an edge between $x$ and $y$. Conversely, if either $(b, N) \notin E$ or $(a, b) \notin E$, then $x$ is not connected to $y$. Consequently, both $(a, b) \in E$ and $(b, N) \in E$ if there is an edge between $a$/every vertex labelled by $b$ in $S_1$ and $a$/every vertex labelled by $a$ in $S_2$.

Thus, $E$ is compatible for $(S_1, S_2)$ iff $I_{((S_1, S_2))} \cup \{ (x, N) \mid x \in \pi_2(I_{((S_1, S_2))}) \} \subseteq E$ and both $(a, b) \in E$ and $(b, N) \in E$ implies $(a, b) \notin O_{((S_1, S_2))}$.

Finally, we have in this case $E \cap O_{(S_1, S_2)} = \emptyset$. Indeed, if $e \in E \cap O_{(S_1, S_2)}$, then $e \in O_{(S_1, S_2)}$ and $e \notin E$ and therefore, by condition (3), $(\pi_2(e), N) \notin E$. Now, $\pi_2(O_{(S_1, S_2)}) \subseteq \pi_2(I_{(S_1, S_2)}) = l(V(S_1) \cap N_G(S_2))$ cf. Definition 8. Consequently, by condition (2), $(\pi_2(e), N) \in E$ – a contradiction.

Intuitively, condition (4) of Lemma 12 deals with the edges of $S_1$ and $S_2$ to the “outside world”, while conditions (1) to (3) deal with the edges between $S_1$ and $S_2$. Conditions (1) and (2) state the tuples that must necessarily be in $E$, while condition (3) states requirements on which tuples must not (together) be in $E$.

Since $E \cap O_{(S_1, S_2)} = \emptyset$ by Lemma 12, we may modify conditions (1) and (3) of the previous lemma as follows:

1. $I_{(S_1, S_2)} \subseteq E \subseteq L^2 \setminus O_{(S_1, S_2)}$.
2. $I_{(S_1, S_2)} \subseteq E \subseteq L^2 \setminus O_{(S_1, S_2)}$, then either $(\pi_2(e), N) \notin E$ or $e \notin E$ (or both).

However, in this way the condition $E \cap O_{(S_1, S_2)} = \emptyset$ is explicitly assumed and not part of the result as stated in the lemma.

Remark 13. By condition (4) of the lemma, we may go even further and instead state “$e \in (K(V(S_2), V(S_1) \setminus N_G(S_2)) \setminus O_{[S_1, S_2]}$” in condition (3). Therefore in practice may be easier to check condition (3) if one considers only the (smaller) set $O_{((S_1, S_2))} \setminus (O_{(S_1, S_2)} \cup O_{(S_1, S_2)}) = l(K(V(S_2), V(S_1) \setminus N_G(S_2)) \setminus O_{(S_1, S_2)}).

Also note that, we have, for $e \in I_{(S_1, S_2)} \cup I_{(S_1, S_2)}$ (and hence $e \subseteq E$), $e \in O_{((S_1, S_2))}$ implies $(\pi_2(e), N) \notin E$.

Example 14. We continue our running example. As we have seen, an $E \subseteq L \times L$ compatible for $(S_1, S_2)$ in $G'$ allows, given the graph $G$ on the left-hand side of Figure 1, for the generation of the middle graph (in the figure) and subsequently the generation of $G'$. We will now determine, using Lemma 12 and the modified conditions below the lemma, the constraints on $E$ for it to be compatible for $(S_1, S_2)$.

Recall that $I_{(S_1, S_2)} = \{(b, a), (c, c)\}$, $O_{(S_1, S_2)} = \{(a, a), (a, c), (b, c), (c, a)\}$, $I_{[S_1, S_2]} = \{(a, b)\}$, and $O_{[S_1, S_2]} = \{(b, b), (c, b)\}$. Moreover, $\{(x, N) \mid x \in \pi_2(I_{(S_1, S_2)})$
= l(V(S_1) \cap N_G(S_2)) = \{(a, N), (c, N)\}. Hence, by conditions (1'), (2), and (4) of Lemma 12 we have
\[ \{(a, b), (b, a), (c, c), (a, N), (c, N)\} \subseteq E \]
and
\[ E \cap \{(a, a), (a, c), (b, b), (b, c), (c, a), (c, b)\} = \emptyset. \]

Now, \( O((S_1, S_2)) = l(K_{V(S_2)}, V(S_1) \setminus N_G(S_2)) = l(K_{\{a,b,c\}, \{b\}}) = \{(a, b), (b, b), (c, c)\} \). Hence by condition (3') either \((b, N) \notin E \) or \((a, b) \notin E \). The latter is a contradiction, hence \((b, N) \notin E \). Consequently,
\[ E = \{(a, b), (b, a), (c, c), (a, N), (c, N)\} \]
is compatible for \((S_1, S_2)\), in fact, in this case, it is the unique \( E \) such that it is compatible for \((S_1, S_2)\) in \( G' \). Note that adding \((b, N)\) to \( E \) would indeed make it incompatible – the generated graph would then have edges from the vertex labelled \( b \) in \( S_1 \) to the two vertices labelled \( a \) in \( S_2 \). Also note that this \( E \) is not compatible for \((S_2, S_1)\) in \( G' \).

Using Lemma 12, the existence of an embedding relation \( E \) is elegantly characterized, as shown in the next lemma.

**Lemma 15.** Let \( S_1 \) and \( S_2 \) be touching graphs. There is a compatible \( E \subseteq L \times L \) for \((S_1, S_2)\) iff \( (I_{[S_1, S_2]} \cup I_{(S_1, S_2)}) \cap O_{[S_1, S_2]} = \emptyset, \pi_2(I_{[S_1, S_2]} \cap \pi_2(I_{(S_1, S_2)} \cap O_{(S_1, S_2)})) = \emptyset, \) and \( I_{(S_1, S_2)} \cap O_{(S_1, S_2)} = \emptyset \). Moreover, if this is the case, then \((I_{[S_1, S_2]} \cup I_{(S_1, S_2)}) \cap O_{(S_1, S_2)} = \emptyset \).

**Proof.** Assume first that that right-hand side holds. Then take \( E' = I_{[S_1, S_2]} \cup I_{(S_1, S_2)}, \) take \( F' = \pi_2(I_{[S_1, S_2]}), \) and let \( E = E' \cup \{(x, N) \mid x \in F'\} \). Now, conditions (1), (2), and (4) of Lemma 12 hold trivially. Finally to prove condition (3), we need to show that \( e \in O((S_1, S_2)) \cap E \) implies \((\pi_2(e), N) \notin E \). Let \( e \in O((S_1, S_2)) \cap E \). We have, by definition of \( E \), that \( e \in I_{[S_1, S_2]} \) or \( e \in I_{(S_1, S_2)} \). The latter is a contradiction of \( I_{(S_1, S_2)} \cap O_{(S_1, S_2)} = \emptyset \). The former implies, by the second equation of this lemma, that \( \pi_2(e) \notin \pi_2(I_{(S_1, S_2)}) = F' \). Consequently, \((\pi_2(e), N) \notin E \).

Now, we prove the other implication. If there is such compatible \( E \), then, by Lemma 12, \((I_{[S_1, S_2]} \cup I_{(S_1, S_2)}) \cap O_{[S_1, S_2]} = \emptyset \). Assume \( I_{(S_1, S_2)} \cap O_{(S_1, S_2)} \neq \emptyset \) and let \( e \in I_{(S_1, S_2)} \cap O_{(S_1, S_2)} \). Since \( e \in I_{(S_1, S_2)} \), we have, by condition (1) in Lemma 12, \( e \in E \), and we have by condition (2) \((\pi_2(e), N) \in E \). Now since \( e \in O_{(S_1, S_2)} \) we have a contradiction by condition (3). Finally, assume \( \pi_2(I_{[S_1, S_2]} \cap \pi_2(I_{(S_1, S_2)} \cap O_{(S_1, S_2)})) \neq \emptyset \) and let \( x \in \pi_2(I_{(S_1, S_2)} \cap O_{(S_1, S_2)}) \). Then, by condition (2), \((x, N) \in E \), and by condition (3), \((x, N) \notin E \) – a contradiction.

By Lemma 12, we have in this case \((I_{[S_1, S_2]} \cup I_{(S_1, S_2)}) \cap O_{(S_1, S_2)} = \emptyset \), since \( I_{[S_1, S_2]} \cup I_{(S_1, S_2)} \subseteq E \) and \( E \cap O_{(S_1, S_2)} = \emptyset \). \( \Box \)
Recall that \( I_{\langle S_1, S_2 \rangle} = I_{\langle (S_1, S_2) \rangle} \), hence the third equation of Lemma 15 may be rephrased more symmetrically as “\( I_{\langle (S_1, S_2) \rangle} \cap O_{\langle (S_1, S_2) \rangle} = \emptyset \)”.

Notice that the case \( N_G(V(S_1) \cup V(S_2)) = \emptyset \) (roughly) corresponds to the situation where the original graph \( F \) that generates \( G \) has a connected component \( N - N \).

In this case, by Lemma 15, there is a compatible \( E \subseteq L \times L \) for \( (S_1, S_2) \) iff \( I_{\langle (S_1, S_2) \rangle} \cap O_{\langle (S_1, S_2) \rangle} = \emptyset \) (since \( I_{\langle S_1, S_2 \rangle} = O_{\langle S_1, S_2 \rangle} = \emptyset \).

**Example 16.** We continue Example 14 (our running example). Recall that \( I_{\langle S_1, S_2 \rangle} \cup I_{\langle S_1, S_2 \rangle} = \{(a, b), (b, a), (c, e)\} \) and \( O_{\langle S_1, S_2 \rangle} = \{(b, b), (c, b)\} \) – hence they are disjoint. Also, \( \pi_2(I_{\langle S_1, S_2 \rangle}) = \{a, e\} \) and \( \pi_2(I_{\langle S_1, S_2 \rangle} \cap O_{\langle (S_1, S_2) \rangle}) = \pi_2(\{(a, b)\}) = \{b\} \), and therefore they are disjoint. Finally, \( I_{\langle S_1, S_2 \rangle} \cap O_{\langle (S_1, S_2) \rangle} = \emptyset \). Consequently, by Lemma 15, there is a compatible \( E \) for \( (S_1, S_2) \) – such an \( E \) is given in Example 14.

### 6 Set of touching graphs

Let \( S = \{S_i \mid i \in \{1, \ldots, n\}\} \) be a set of mutually isomorphic and disjoint subgraphs of \( G \). In this section we turn to the question of whether or not there is an \( E \subseteq L \times L \) and a linear ordering \( C = (S_1, S_2, \ldots, S_n) \) of \( S \) such that \( E \) is a compatible embedding relation for \( C \).

The following result is easily obtained from Lemma 5.

**Lemma 17.** Let \( G \) be a graph, \( E \subseteq L \times L \), and \( C = (S_1, \ldots, S_n) \) be a sequence of mutually disjoint induced subgraphs of \( G \) isomorphic to \( S \). Then \( E \) is compatible for \( C \) iff (1) \( I_{\langle S_1, \ldots, S_n \rangle} \subseteq E \subseteq L^2 \setminus (O_{\langle S_1, \ldots, S_n \rangle}) \) and (2) for each two touching \( S_i \) and \( S_j \) with \( i < j \), we have that the first three conditions of Lemma 12 hold w.r.t. \( E \) and \( (S_i, S_j) \).

Clearly, if \( S_i \) and \( S_{i+1} \) are non-touching, then \( E \) is compatible for \( (S_1, \ldots, S_i, S_{i+1}, \ldots, S_n) \) if \( E \) is compatible for \( (S_1, \ldots, S_{i+1}, S_i, \ldots, S_n) \). Thus, as we have already seen in Section 4, the case where \( S_1, S_2, \ldots, S_n \) are mutually non-touching is much less involved: \( E \) is compatible for each linear ordering of \( S \).

For touching graphs, the situation is different as the conditions in Lemma 12 are not symmetric: e.g. \( I_{\langle S_i, S_j \rangle} \) and \( I_{\langle S_j, S_i \rangle} \) generally differ. Hence, we must choose a linear ordering in a “compatible” way. First, we focus on the question whether or not there exists an \( E \) compatible for a given linear ordering \( C \) of \( S \). We characterize the existence by generalizing Lemma 15 for the case where more than two graphs can touch each other. To this aim consider the following graph that represents whether or not subgraphs \( S_i \) and \( S_j \) in \( S \) touch.

**Definition 18.** Let \( G \) be a graph and \( S = \{S_i \mid i \in \{1, \ldots, n\}\} \) be a set of induced subgraphs of \( G \). The **touching graph** of \( G \) w.r.t. \( S \), is the (undirected) graph \( \langle S, \{\langle S_i, S_j \rangle \mid S_i \text{ and } S_j \text{ touch} \} \rangle \).

We now give the edges of a touching graph an orientation such that the obtained graph, called directed touching graph, is acyclic.
Definition 19. Let $T$ be the touching graph of $G$ w.r.t. $S$. Then the directed touching graph of $G$ w.r.t. to an ordering $(S_1, S_2, \ldots, S_n)$ of $S$ is the directed graph $D = (V(D), E(D))$ where, $V(D) = V(T)$ and $(S_i, S_j) \in E(D)$ iff \( \{ S_i, S_j \} \in E(T) \) and $i < j$.

For $e = (S_i, S_j) \in E(D)$ we write $O_e = O_{(S_i, S_j)}$ and $O_{(e)} = O_{((S_i, S_j))}$ (and similarly for the insets $I_e$ and $I_{(e)}$).

We now obtain the main result – it generalizes Lemma 15.

Theorem 20. Let $G$ be a graph and $C = (S_1, \ldots, S_n)$ be a sequence of induced subgraphs of $G$ and let $D$ be the directed touching graph of $G$ w.r.t. $C$. There is a compatible $E \subseteq L \times L$ for $C$ iff

\[
\begin{align*}
(I_{[S_1, \ldots, S_n]} \cup (\cup_{e \in E(D)} I_e)) \cap O_{(S_1, \ldots, S_n)} &= \emptyset, \quad (1) \\
\pi_2(\cup_{e \in E(D)} I_e) \cap \pi_2(I_{[S_1, \ldots, S_n]} \cap (\cup_{e \in E(D)} O_{(e)})) &= \emptyset, \text{ and} \quad (2) \\
(\cup_{e \in E(D)} I_e) \cap (\cup_{e \in E(D)} O_{(e)}) &= \emptyset. \quad (3)
\end{align*}
\]

Moreover, if this is the case, then \( (I_{[S_1, \ldots, S_n]} \cup (\cup_{e \in E(D)} I_e)) \cap (\cup_{e \in E(D)} O_{e}) = \emptyset. \)

Proof. This proof will be in the same spirit as the proof of Lemma 15.

Assume first that that right-hand side holds. Then take $E' = I_{[S_1, \ldots, S_n]} \cup (\cup_{e \in E(D)} I_e)$, and take $F' = \pi_2(\cup_{e \in E(D)} I_e)$, Now, let $E = E' \cup \{ (x, N) \mid x \in F' \}$. By Lemma 17 it suffices to show that for each two touching $S_i$ and $S_j$ with $i < j$, the first three conditions of Lemma 12 hold w.r.t. $E$ and $r = (S_i, S_j)$. Now, conditions (1), (2), and (4) of Lemma 12 hold trivially. Finally to prove condition (3), we need to show that $e \in O_{(r)} \cap E$ implies $(\pi_2(e), N) \notin E$. Let $e \in O_{(r)} \cap E$. We have, by definition of $E$, that $e \in I_{[S_{s_1}, S_{s_2}]}$ or $e \in I_{[S_{s_3}, S_{s_4}]}$ for some $k_1, \ldots, k_4$. The latter is a contradiction of $I_{[S_{s_3}, S_{s_4}]} \cap O_{(r)} = \emptyset$. The former implies by the second equation of this theorem that $\pi_2(e) \notin \pi_2(\cup_{e \in E(D)} I_e) = F'$. Consequently, $(\pi_2(e), N) \notin E$.

Now, we prove the other implication. Assume that there is a compatible $E \subseteq L \times L$ for $C$. Then by Lemma 17, (1) $I_{[S_1, \ldots, S_n]} \subseteq E \subseteq L^2 \backslash O_{(S_1, \ldots, S_n)}$ and (2) for each two touching $S_i$ and $S_j$ with $i < j$, we have that the first three conditions of Lemma 12 hold w.r.t. $E$ and $(S_i, S_j)$. Hence, by Lemma 12, $(I_{[S_1, \ldots, S_n]} \cup (\cup_{e \in E(D)} I_e)) \cap O_{[S_1, \ldots, S_n]} = \emptyset$. Assume now that $I_{f_1} \cap O_{(f_2)} \neq \emptyset$ for some $f_1, f_2 \in E(D)$, and let $e \in I_{f_1} \cap O_{(f_2)}$. Since $e \in I_{f_1}$, we have, by condition (1) in Lemma 12, $e \in E$, and we have by condition (2) $(\pi_2(e), N) \notin E$. Now since $e \in O_{(f_2)}$ we have a contradiction by condition (3). Finally, assume $\pi_2(I_{f_1}) \cap \pi_2(I_{[S_1, \ldots, S_n]} \cap O_{(f_2)}) \neq \emptyset$ and let $x \in \pi_2(I_{f_1}) \cap \pi_2(I_{[S_1, \ldots, S_n]} \cap O_{(f_2)})$. Then, by condition (2), $(x, N) \in E$, and by condition (3), $(x, N) \notin E$ – a contradiction.

Finally, by Lemma 15, if this is the case, then $(I_{[S_1, \ldots, S_n]} \cup (\cup_{e \in E(D)} I_e)) \cap (\cup_{e \in E(D)} O_{e}) = \emptyset$. □
7 Determining compatible sequences of subgraphs

In this section we turn to the question of efficiently determining, given a set
$S = \{S_i \mid i \in \{1, \ldots, n\}\}$ of disjoint subgraphs, an ordering of $C$ of $S$ (if it exists)
such that there is a compatible $E \subseteq L \times L$ for $C$.

We proceed as follows. First, assuming such ordering $C$ exists, by Theorem 20,
the following equality

$$
(I_{[S_1, \ldots, S_n]} \cup (\cup_{e \in E(D)} I_e)) \cap (O_{[S_1, \ldots, S_n]} \cup (\cup_{e \in E(D)} O_e)) = \emptyset
$$

holds, where $D$ is the directed touching graph w.r.t. $C$. We consider this equality
instead of $(I_{[S_1, \ldots, S_n]} \cup (\cup_{e \in E(D)} I_e)) \cap O_{[S_1, \ldots, S_n]} = \emptyset$
for computational efficiency reasons, as we will see below.

Note that, because of distributivity $(A \cup B) \cap C = (A \cap C) \cup (B \cap C)$,
Equation (4) is equal to

$$
\left( \bigcup_{e, f \in E(D)} (I_e \cap O_f) \right) \cup \left( \bigcup_{e \in E(D)} ((I_{[S_1, \ldots, S_n]} \cap O_e) \cup (I_e \cap O_{[S_1, \ldots, S_n]}) \right)

\cup (I_{[S_1, \ldots, S_n]} \cap O_{[S_1, \ldots, S_n]}).
$$

Now, for touching graphs $S_1$ and $S_2$, we define $e = (S_1, S_2)$ admissible
w.r.t. $S$ if $(I_{[S_1, \ldots, S_n]} \cap O_e) \cup (I_e \cap O_{[S_1, \ldots, S_n]}) = \emptyset$. Or equivalently,

$$
I_{[S_1, \ldots, S_n]} \cap O_e = \emptyset \text{ and } I_e \cap O_{[S_1, \ldots, S_n]} = \emptyset.
$$

Now, to determine the existence of an ordering of $C$ of $S$ and a $E \subseteq L \times L$
such that $E$ is compatible for $C$, we first check whether or not $I_{[S_1, \ldots, S_n]} \cap O_{[S_1, \ldots, S_n]} = \emptyset$.
If this does not hold, there is no such $C$ (and $E$). Otherwise, we construct the
admissible touching graph.

**Definition 21.** Let $T$ be the touching graph of $G$ w.r.t. $S$. Then the
admissible touching graph of $G$ w.r.t. $S$ is the directed graph
$D = (V(D), E(D))$ where, $V(D) = V(T)$ and, for $e = (S, S')$ with $S, S' \in V(D)$, $e \in E(D)$ iff $e$ is admissible.

Now, since we consider Equation (4), this graph will be considerably smaller
than the corresponding graph for the original equation. This may correspond to
a substantial speedup as we subsequently check conditions between edges of this
graph.

Recall that $O_f \subseteq O(f)$, and hence $I_e \cap O(f) = \emptyset$ implies $I_e \cap O_f = \emptyset$. Thus we
need to check for each topological ordering $C$ of the admissible touching graph
whether or not

$$
\bigcup_{e, f \in E(D)} (I_e \cap O(f)) = \emptyset, \text{ and } \bigcup_{e, f \in E(D)} (\pi_2(I_e) \cap \pi_2(I_{[S_1, \ldots, S_n]} \cap O(f))) = \emptyset
$$

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where \( D \) is the directed touching graph w.r.t. \( C \). If there is such a \( C \), then there is an \( E \) compatible for \( C \). Otherwise, there is no linear ordering \( C \) and embedding relation \( E \) where \( E \) is compatible for \( C \).

8 Discussion

In this paper we considered the problem of graph grammar inference for the case where one is given a disjoint set \( S \) of isomorphic subgraphs to be generated by a single rule \( r = N \to S/E \), where the embedding relation \( E \) is allowed to contain tuples containing \( N \). In this way we generalize results in [1]. This result is to be seen as a further step towards a systematic account of NLC graph grammar inference.

Formally, we characterized, given a \( S = \{ S_i \mid i \in \{1, \ldots, n\} \} \), the existence of an ordering \( C \) of \( S \) and a \( E \subseteq L \times L \) such that \( E \) is compatible for \( C \). Moreover, if such a \( C \) exists, then it is shown to be a topological ordering of a suitable graph that identifies admissible pairs of touching subgraphs. The efficiency of the proposed algorithm depends significantly on the cardinality of \( S \) – for small \( S \) the algorithm seems feasible, however this has yet to be verified in practice.

Finding a graph \( S \), such that the set \( S \) of subgraphs of \( G \) isomorphic to \( S \) is (1) “compressible”, i.e. there is a compatible embedding relation for suitable ordering of \( S \), and (2) optimal (either in cardinality, or in some other measure) remains to be investigated.

Also, it is natural to consider the case where for rule \( r = N \to S/E \), \( N \) is allowed to be a label on a nodes of \( S \) instead of \( N \) contained in (tuples of) \( E \). This would have the consequence that an infinite number of graphs can be generated by \( r \), and, moreover, multiple copies of \( S \) can overlap – loosening the restriction of disjointness considered here.

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