Loose Graph Simulations

Alessio Mansutti
ENS Paris-Saclay
alessio.mansutti@lsv.fr

Marino Miculan
University of Udine
marino.miculan@uniud.it

Marco Peressotti
University of Southern Denmark
peressotti@imada.sdu.dk

Abstract

We introduce loose graph simulations (LGS), a new notion about labelled graphs which subsumes in an intuitive and natural way subgraph isomorphism (SGI), regular language pattern matching (RLPM) and graph simulation (GS). Being an unification of all these notions, LGS allows us to express directly also problems which are “mixed” instances of previous ones, and hence which would not fit easily in any of them.

After the definition and some examples, we show that the problem of finding loose graph simulations is NP-complete, we provide formal translation of SGI, RLPM, and GS into LGSs, and we give the representation of a problem which extends both SGI and RLPM.

1 Introduction

Graph pattern matching is the problem of finding patterns satisfying a specific property, inside a given graph. This problem arises naturally in many research fields: for instance, in computer science it is used in automatic system verification, network analysis and data mining [5, 15, 24, 27]; in computational biology it is applied to protein sequencing [23]; in cheminformatics it is used to study molecular systems and predict their evolution [1, 4]; in forensic science and social network analysis to profile users and their behaviours [8].

Given a so wide range of applications, many definitions of patterns have been proposed, each aiming to highlight different properties of a graph; for instance, these properties can be specified by another graph, by a formal language, by a logical predicate, etc. This situation has lead to different notions of graph pattern matching, such as subgraph isomorphism (SGI), regular language pattern matching (RLPM) and graph simulation (GS). Each of these notions has been studied in depth, yielding similar but different theories, algorithms and tools.

A drawback of this situation is that it is difficult to deal with matching problems which do not fit directly in any of these variants. In fact, most often we need to search for patterns that can be seen as a compositions of multiple notions of graph pattern matching. An example is when we have to find a pattern which has to satisfy multiple notions of graph pattern matching at once; due to the lack of proper tools, these notions can only be checked one by one with a worsening of the performances. Another example can be found in [8, 9], where the authors define new problems that extend RLPM, with applications in network analysis and graph database [12]. Moreover a mixed problem between RLPM and SGI is presented in [2].

This situation would benefit from a more general notion of graph pattern matching, able to subsume naturally the more specific ones find in literature. This general notion would be a

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common ground to study specific problems and their relationships, as well as to develop common
techniques for them. Moreover, a more general pattern matching notion would pave the way for
more general algorithms, which would deal more efficiently with “mixed” problems.

To this end, in this paper we propose a new notion about labelled graphs, called loose graph
simulation (LGS, Section 2). The semantics of its pattern queries allow us to check properties
different classical notions of pattern matching, at once and without cumbersome encodings.
LGS queries have a natural graphical representation that simplifies the understanding of their
semantic; moreover, they can be composed using a sound and complete algebra (Section 3).
Various notions of graph pattern matching can be naturally reduced to LGSs, as we will formally
prove in Sections 4 to 6; in particular, the encoding of subgraph isomorphism allows us to prove
that computing LGSs is a NP-complete problem. Moreover, “mixed” matching problems can
be easily represented as LGS queries; in fact, these problems can be obtained compositionally
from simpler ones by means of the query algebra, as we will show in Section 7 where we solve
a simplified version of the problem in [2]. Final conclusions and directions for further work (such
as a distributed algorithm for computing loose graph simulations) are in Section 8.

2 Hosts, Guests and Loose Graph Simulations

Graph simulations solutions to the problem of finding occurrences of certain labelled multigraphs
graphs into other. The former are called guests and the latter are called hosts. Loose graph
simulations are solutions to a similar but more general problem where guests are multigraphs
-equipped with additional information and capable of expressing several (even infinitely many)
multigraph guests at once.

Before we formalise LGSs, let us fix some auxiliary notions and notation.

Definition 2.1. A labelled directed multigraph is a triple \((\Sigma, V, E)\) consisting of a finite set of
symbols \(\Sigma\) (also called alphabet), a set \(V\) of nodes and a set \(E \subseteq V \times \Sigma \times V\) of edges. For an
edge \(e = (v, l, v')\) we write \(s(e)\), \(\sigma(e)\), and \(t(e)\) for its source node \(v\), label \(l\), and target node \(v'\),
respectively. For a vertex \(v\) we write \(\text{in}(v)\) and \(\text{out}(v)\) for the sets \(\{e \mid t(e) = v\}\) and \(\{e \mid s(e) = v\}\)
of its incoming and outgoing edges.

Hereafter, by host we mean a labelled directed multigraph.

Definition 2.2. A host is labelled directed multigraph.

In the sequel we adopt the convention of denoting hosts as \(H\) (and variations thereof) and
writing \((\Sigma_H, V_H, E_H)\) for the components of the host \(H\). For the sake of exposition, we will often
refer to labelled directed multigraphs just as graphs, when clear from the context.

Roughly speaking, a guest is a labelled directed multigraph whose:

- nodes are decorated with usage constraints telling whether they must appear in the host, if
  their occurrence should be unique, and if their occurrences can also be occurrences of other
  nodes or are exclusive;
  - edges are grouped into possible “choices of sets of ongoing edges” for any given source node
    to be considered by a simulation.

Definition 2.3. A guest \(G = (\Sigma, V, E, M, U, E, C)\) is a labelled directed multigraph \((\Sigma, V, E)\)
equipped with:

- three sets \(M, U, E \subseteq V\), called respectively must, unique and exclusive set.
We extend Their tensor product graph Definition 2.5. A of vertices can express the existence of multiple paths. Let \( v, v' \) denote with Definition 2.4. Let \( G = (\Sigma, V, E) \) be a labelled directed multigraph over a set of labels \( \Sigma \). We denote with \( P_G \) the set of all paths in \( G \). Formally
\[
P_G \triangleq \bigcup_{n \in \mathbb{N}^+} \{(e_0, \ldots, e_n) \in E^n \mid \forall i \in \{1, \ldots, n\} \ s(e_i) = t(e_{i-1})\}
\]
We extend source, label and target functions of Definition 2.1 as follows:
\[
s((e_0, \ldots, e_n)) \triangleq s(e_0) \quad s : P_G \to V
\]
\[
t((e_0, \ldots, e_n)) \triangleq t(e_n) \quad t : P_G \to V
\]
\[
\sigma((e_0, \ldots, e_n)) \triangleq \sigma(e_0) \cdots \sigma(e_n) \quad \sigma : P_G \to \Sigma^*
\]
Let \( v, v' \in V \). \( P_G(v, v') \) will denote the set of all paths starting from \( v \) and ending in \( v' \), i.e. \( P_G(v, v') \triangleq \{ \rho \in P_G \mid s(\rho) = v \land t(\rho) = v' \} \).

Note how paths are represented by sequences of edges, since in a multigraph setting a sequence of vertices can express the existence of multiple paths.

**Definition 2.6.** A loose graph simulation (LGS) of \( G \) in \( H \) is a subgraph \((\Sigma_G \cap \Sigma_H, V^{G \to H}, E^{G \to H})\) of \( G \times H \) s.t.:

**LS1** vertices of \( G \) in the must set occur in \( V^{G \to H} \), i.e.:
\[
\forall u \in \mathcal{M} \ \exists u' \in V_H : (u, u') \in V^{G \to H}
\]

**LS2** vertices in the unique set can be assigned to at most one vertex of \( H \):
\[
\forall u \in \mathcal{U} \ \forall u', v' \in V_H : (u, u') \in V^{G \to H} \land (u, v') \in V^{G \to H} \implies u' = v'
\]

**LS3** vertices in \( H \) in relation with a vertex of \( G \) in the exclusive set cannot be in relation with other vertices of \( G \), i.e.
\[
\forall u \in \mathcal{E} \ \forall v \in V_G \ \forall u' \in V_H : (u, u') \in V^{G \to H} \land (v, u') \in V^{G \to H} \implies u = v
\]

**LS4** \( H \) simulates \( G \) w.r.t. the choice function \( C \): for all \((u, u') \in V^{G \to H}\) there exists \( \gamma \in C(u) \) such that for all \((u, a, v) \in \gamma \) there exists \( v' \in V_H \) such that \((u, u'), a, (v, v') \in E^{G \to H}\). Moreover, for all \((u, u'), a, (v, v') \in E^{G \to H}\) there exists \( \gamma \in C(u) \) such that \((u, a, v) \in \gamma \) and for all \((u, b, w) \in \gamma \) there exists \( w' \in V_H \) such that \((u, u'), b, (w, w') \in E^{G \to H}\).
∃v ∈ M

∃v ∈ U

v ∈ E

∅ ∈ C(v)

{e_1, e_2, ..., e_n} ∈ C(v)

Figure 1: Description of the graphic notation for guest.

Figure 2: Description of the graphic notation for guest.

LS5 the simulation preserves the connectivity with respect to nodes marked as must: for each \((u, u') \in V^{G \rightarrow H}\) and \(v \in M\) if \(P_G(u, v) \neq \emptyset\) then there exists \(v' \in V_H\) such that \(P_{(\Sigma_G \odot \Sigma_H, V^{G \rightarrow H}, E^{G \rightarrow H})}((u, u'), (v, v')) \neq \emptyset\).

We write \(S^{G \rightarrow H}\) for the domain of all loose graph simulations over a guest \(G\) and a host \(H\).

As already mentioned at the end of Definition 2.3, the definition of LGS attributes a semantics for the must, unique, exclusive sets and the choice function. Regarding the unique set, the condition LS2 requires that every vertex of the guest in this set to be mapped by at most one element of the host. Similarly, condition LS3 requires the vertices of the host paired in the LGS with a node of the exclusive set to be only paired with that node. Condition LS4 defines the semantics of the choice function: given a pair of vertices \((u, u') \in V^{G \rightarrow H}\), it requires to select a set from \(C(u)\) and the host to simulate it. Lastly, conditions LS1 and LS4 defines the semantics of the must set: the first condition imposes that every vertex in this set must appear in the LGS, while the second condition requires that, for each \((u, u') \in V^{G \rightarrow H}\), each vertex in the must set reachable in the guest from \(u\) is also reachable in the LGS, with a path starting from \((u, u')\).

3 A graphical notation and an algebra for guests

Guests represent a specification used to check if a pattern appears inside a host. To simplify their usability and intuitiveness we provide a graphical notation and a algebra to represent and construct guests easily.

The semantics of the three sets \(M, U, E\) and the choice function \(C\) will be presented formally in the definition of loose graph simulations (Definition 2.6).

Alongside the definition of guest, we introduce its graphical notation, as shown in Figure 1. In this representation, a node belonging to the must, unique or exclusive set is decorated with the symbols \(\exists\), ! and \(\not\) respectively. To represent the choice function \(C\) of a vertex \(v\) we will decorate the edges of \(\text{out}(v)\) with a chord highlighting each edge of a set in \(C(v)\). Moreover, in the eventuality that \(\emptyset \in C(v)\) we will decorate the node \(v\) with a “corked edge” ( \(\not\)).
Example 3.1. Figure 3 shows a guest and its loose graph simulation over a host. In this example
\( \mathcal{M} = \{m\} \) and \( \mathcal{U} = \mathcal{E} = \emptyset \). Moreover, the choice function is linear, i.e. \( \mathcal{C} = \lambda x. \{\{e\} \mid e \in \text{out}(x)\} \cup \{\emptyset \mid \text{out}(x) = \emptyset\} \). LGSs of this guest represent paths \((e_0, e_1, \ldots, e_n)\) of arbitrary length in the host such that for all \( i \leq n \), \( \sigma(e_i) = a \) and \( \sigma(e_n) = b \). The guest is therefore similar to the regular language \( a^*b \) and a LGS identifies paths in the host labelled with words in this language.

We define an algebra for presenting all guests.

Definition 3.2. A guest with only one vertex and no edges is a unary guest. We will denote unary guests as \( \rho_{\alpha} \triangleq (\emptyset, \{p\}, \emptyset, \{p \mid \exists \in \mathcal{A}\}, \{p \mid ! \in \mathcal{A}\}, \{p \rightarrow \{\emptyset \mid \emptyset \in \mathcal{A}\}\}) \) where \( \mathcal{A} \subseteq \{\exists, !, \emptyset\} \). Let \( \alpha \) be a name, \( P \) and \( Q \) be two unary guests, respectively

\[
P = (\emptyset, \{p\}, \emptyset, \mathcal{M}_P, \mathcal{U}_P, \mathcal{E}_P, \{p \rightarrow c_P\}) \quad Q = (\emptyset, \{q\}, \emptyset, \mathcal{M}_Q, \mathcal{U}_Q, \mathcal{E}_Q, \{q \rightarrow c_Q\})
\]

The \textbf{arrow operator} from \( P \) to \( Q \) labelled with \( \alpha \) is defined as

\[
P \xrightarrow{\alpha} Q \triangleq (\{\alpha\}, \{p, q\}, \{(p, \alpha, q)\}, \mathcal{M}_P \cup \mathcal{M}_Q, \mathcal{U}_P \cup \mathcal{U}_Q, \mathcal{E}_P \cup \mathcal{E}_Q, \{c_P \cup \{(p, \alpha, q)\} \cup c_Q \text{ if } p = q \land x = p\
\{c_P \cup \{(p, \alpha, q)\} \text{ if } p \neq q \land x = p\
\{c_Q \text{ if } p \neq q \land x = q\})
\]

The empty guest, all unary guests and all guests constructed with only the arrow operator are called \textbf{elementary guests}.

For example, a node \( p \) with only a self loop labelled \( \alpha \) can be expressed with the term \( p \xrightarrow{\alpha} p \). Besides the elementary guests, the algebra is completed by introducing two binary operators used to combine guests.

Definition 3.2. Given \( G_1 = (\Sigma_1, V_1, E_1, \mathcal{M}_1, \mathcal{U}_1, \mathcal{E}_1, \mathcal{C}_1) \) and \( G_2 = (\Sigma_2, V_2, E_2, \mathcal{M}_2, \mathcal{U}_2, \mathcal{E}_2, \mathcal{C}_2) \) two guests, their \textbf{addition} is the graph

\[
G_1 \oplus G_2 \triangleq (\Sigma_1 \cup \Sigma_2, V_1 \cup V_2, E_1 \cup E_2, \mathcal{M}_1 \cup \mathcal{M}_2, \mathcal{U}_1 \cup \mathcal{U}_2, \mathcal{E}_1 \cup \mathcal{E}_2, \mathcal{C}_1 \cup \mathcal{C}_2)
\]

where the choice function \( \mathcal{C}_\oplus \) is defined as

\[
\mathcal{C}_\oplus \triangleq \lambda x. \begin{cases} 
\mathcal{C}_1(x) \cup \mathcal{C}_2(x) & \text{if } x \in V_1 \land x \in V_2 \\
\mathcal{C}_1(x) & \text{if } x \in V_1 \\
\mathcal{C}_2(x) & \text{if } x \in V_2
\end{cases}
\]
Furthermore we define the multiplication of $G_1$ and $G_2$ as

$$G_1 \otimes G_2 \triangleq (\Sigma_1 \cup \Sigma_2, V_1 \cup V_2, E_1 \cup E_2, M_1 \cup M_2, U_1 \cup U_2, E_1 \cup E_2, C^\otimes)$$

where the choice function $C^\otimes$ is defined as follows

$$C^\otimes \triangleq \lambda x. \begin{cases} C_1(x) & \text{if } x \in V_1 \\ C_2(x) & \text{if } x \in V_2 \end{cases}$$

Notice how addition and multiplication operators differs only by the definition of the choice function for vertices of both $G_1$ and $G_2$. In the case of addition, the resulting choice function is the union of the two choice function $C_1$ and $C_2$, whereas for the multiplication, given a vertex $v \in V_1 \cap V_2$, every set of $C^\otimes(v)$ is the union of a set in $C_1(v)$ and one in $C_2(v)$. Moreover, the set of all guests with addition or multiplication is a commutative monoid, these two operations are idempotent and the multiplication is distributive over the addition.

As we will see in the next section, this algebra can be used to represent cleanly loose graph simulations’ guests and can be used as a tool to build hybrid queries w.r.t. this notions. Furthermore, a notion of normal form can be easily defined for the syntactical terms of this algebra.

**Definition 3.3.** A guest syntactical term is considered in normal form if and only if is an addition of one or more subterm, where each subterm is a multiplication of elementary guests.

**Example 3.2.** The term $q(\exists, q) \oplus (p(\exists) \otimes p \rightarrow b) \rightarrow q$ is in normal form and represent the guest

$$(\{a, b\}, \{p, q\}, \{(p, a), (p, b, q)\}, \{p, q\}, \emptyset, \emptyset, \{p \mapsto \{(p, a, p), (p, b, q)\}, q \mapsto \{\emptyset\}\})$$

also shown in Figure 2.

**Theorem 3.1.** Every guest $G = (\Sigma, V, E, M, U, E, C)$ can be expressed in normal form by the term

$$\bigoplus_{v \in V} C(v) \cup \bigoplus_{e \in T} s(e) \xrightarrow{\sigma(e)} t(e)$$

**Proof.** The thesis follows from by straightforward definition unfolding.

In order to simplify the exposition, we end the definition of the guests’ theory by introducing their renaming. Let $V$ and $E$ be respectively a set of vertices and a set of edges. We define their renaming as follows:

$$V[p/q] = \begin{cases} V & \text{if } p \notin V \\ (V \setminus \{p\}) \cup \{q\} & \text{otherwise} \end{cases}$$

$$E[p/q] = \begin{cases} (u, a, v) & \text{if } (u', a, v') \in E \\ (u' \neq p \Rightarrow u = u') \wedge (u' \neq p \Rightarrow v = v') & \text{if } (u' \neq p \Rightarrow v = v') \wedge (v' \neq p \Rightarrow v = q) \end{cases}$$

Let $G = (\Sigma, V, E, M, U, E, C)$ be a guest. We define the renaming of $p \in V$ w.r.t. a fresh name $q \notin V$ as follows:

$$G[p/q] = (\Sigma, V[p/q], E[p/q], M[p/q], U[p/q], E[p/q], C[p,q])$$

where

$$C[p,q] = \lambda x. \begin{cases} \{S[p/q] \mid S \in C(x)\} & \text{if } x \neq p \wedge x \neq q \\ \{S[p/q] \mid S \in C(p)\} & \text{if } x = q \end{cases}$$
4 The LGS problem is NP-complete

In this section we analyse the complexity of computing loose graph simulations by studying their emptiness problem. Without loss of generality, we will now consider only guests and hosts with the same alphabet $\Sigma$. In the following, let $G = (\Sigma_G, V_G, E_G, M, U, E, C)$ and $H = (\Sigma_H, V_H, E_H)$ be respectively a guest and a host.

**Definition 4.1.** The emptiness problem for loose graph simulations by

**Proposition 4.1.** Computing loose graph simulations, as well as their emptiness problem, is in $NP$.

**Proof.** Let $S = (\Sigma, V^{G \rightarrow H}, E^{G \rightarrow H})$ be a subgraph of $G \times H$. We will now prove that there exists a polynomial algorithm w.r.t. the size of $G$ and $H$ that checks whenever $S$ satisfies all the conditions of Definition 2.6. The satisfiability checking of Condition LS1 is in $O(M \times V^{G \rightarrow H})$ since it is sufficient for every vertex in the must set $M$ to check whenever a vertex of the host paired with it exists. For similar reasons, conditions LS2 and LS3 can also be checked in polynomial time. Moreover, to check condition LS4 it is sufficient to check, for each $(u, v) \in V^{G \rightarrow H}$, whenever there exists $\gamma \in C(v)$ s.t. $\gamma \subseteq \pi_1 \circ \text{out}((u, v))$ and if for all $u' \in \pi_1 \circ \text{out}((u, v))$ there exists $\gamma \in C(v)$ s.t. $u' \in \gamma \subseteq \pi_1 \circ \text{out}((u, v))$. This can be done by a naive algorithm in $O(V_h \times E_G \times (V_Q \times E_H + C \times E_Q^2))$. Lastly, checking whenever $S$ satisfies Condition LS5 requires the evaluation of the reachability relation of $G$ and $S$ and therefore can be computed in $O(V_G^2 \times V_H^2)$ using the Floyd-Warshall Algorithm [11]. Since every condition can be checked in polynomial time we can conclude that the problem of computing loose graph simulations is in $NP$. \qed

4.1 NP-hardness: Subgraph Isomorphisms via LGSs

We will now show the NP-hardness of the emptiness problem for loose graph simulations by reducing the emptiness problem for subgraph isomorphism to it. The subgraph isomorphism problem requires to check whenever a subgraph of a graph (host) and isomorphic to a second graph (query) exists. Application of this problem can be found in network analysis [15], bioinformatics and chemoinformatics [1, 4].

**Definition 4.2.** Let $H = (\Sigma, V_H, E_H)$ and $Q = (\Sigma, V_Q, E_Q)$ be two labelled directed multigraphs called respectively host and query. There exists a subgraph of $H$ isomorphic to $Q$ whenever there exists a pair of injections $\phi_{SG} : V_Q \hookrightarrow V_H$ and $\eta_{SG} : E_Q \hookrightarrow E_H$ s.t. for each edge $e \in E_Q$

$$\sigma(e) = \sigma \circ \eta_{SG}(e) \quad s(e) = s \circ \eta_{SG}(e) \quad t(e) = t \circ \eta_{SG}(e)$$

The subgraph isomorphism problem, as well as the emptiness problem associated to it, is shown to be NP-complete by Cook [6]. Its complexity and its importance makes it one of the most studied problem and multiple algorithmic solution where derived for it[4, 7, 26]. We will now show that the emptiness problem for subgraph isomorphism can be solved using LGSs.

**Proposition 4.2.** Let $H = (\Sigma, V_H, E_H)$ and $Q = (\Sigma, V_Q, E_Q)$ be respectively a host and a query for subgraph isomorphism. Moreover, let

$$G = \bigoplus_{v \in V_Q} v \| [\exists i \cup \{\emptyset \} \circ \text{out}(v) = \emptyset] \bigoplus \bigotimes_{e \in E_Q} s(e) \xrightarrow{\sigma(e)} t(e)$$

There exists a subgraph of $H$ isomorphic to $Q$ if and only if there exists a loose graph simulation of $G$ in $H$, i.e. $S^{G \rightarrow H} \neq \emptyset$. 7
Proof. From the definition of $G$, its must, unique and exclusive sets, as well as its choice function, are respectively $M = U = E = V_Q$ and $C = \lambda x.\{\text{out}(x)\}$; therefore, according to conditions LS1, LS2 and LS3, every loose graph simulation $(\Sigma, V^{G\rightarrow H}, E^{G\rightarrow H}) \in S^{G\rightarrow H}$ must be such that $V^{G\rightarrow H}$ and $E^{G\rightarrow H}$ corresponds to two injective functions. Moreover, condition LS4 together with the definition of $C$ implies that every edge of $G$ must appear in $E^{G\rightarrow H}$, i.e. for all $(u, a, v) \in G$ there exists $u', v' \in H$ such that $((u, u'), a, (v, v')) \in E^{G\rightarrow H}$. Lastly, LGS are subgraphs of $G \times H$. We can therefore conclude that Definition 2.6 and Definition 4.2 are equivalent. Lastly, the space required by $Q$ and $G$ have the same order of magnitude, i.e. they both are in $O(V_H + E_H)$. 

Remark 4.1. In the above proof, it should be noted that if $C = \lambda v.\{\text{out}(v)\}$ then condition LS4, coupled with the fact that loose graph simulations are subgraphs of the product $G \times H$, implies LS5.

Note how the translation from subgraph isomorphism’s queries to guest for LGSs defined in Proposition 4.2 is structure-preserving. Indeed, an example of this can be seen in Figure 4. This property is important since it makes defining LGSs’ guests to solve the subgraph isomorphism problem as intuitive as the respective queries for it. This is also the case for other notions commonly used in the graphs’ pattern matching community. Moreover, since the translated guest will be as intuitive as the original query, this property strengthens the idea of using guests and LGSs to represent and compute hybrid queries w.r.t. these notions.

From Proposition 4.1 and Proposition 4.2 follows that:

**Theorem 4.3.** The emptiness problem for LGSs is NP-complete.

5 Graph Simulations are Loose Graph Simulations

Graph simulations are relations between graphs used extensively by social networks companies to perform user analysis [8]. They also can be applied to bioinformatics and urban planning [10]. The graph simulation problem requires to check whenever a portion of a graph (host) simulates another graph (query).

**Definition 5.1.** Let $H = (\Sigma, V_H, E_H)$ and $Q = (\Sigma, V_Q, E_Q)$ be two graphs called host and query, respectively. There exists a graph simulation of $Q$ in $H$ if and only if there is a relation $\mathcal{R} \subseteq V_Q \times V_H$ such that:

- for each node $u \in V_Q$ there exists a node $v \in V_H$ such that $(u, v) \in \mathcal{R}$;

![Figure 4: A possible query for subgraph isomorphism (on the left) and its translation to a guest for LGSs (on the right).](image-url)
• for each pair \((u, v) \in \mathcal{R}\) and for each edge \(e \in \text{out}(u)\) there exists an edge \(e' \in \text{out}(v)\) such that \(\sigma(e) = \sigma(e')\) and \((t(e), t(e')) \in \mathcal{R}\).

Checking whenever a graph simulation exists between two graphs can be done in polynomial time [3, 13]. We will now show how to reduce the emptiness problem for graph simulations to the emptiness problem for LGSs.

**Proposition 5.1.** Let \(H = (\Sigma, V_H, E_H)\) and \(Q = (\Sigma, V_Q, E_Q)\) be respectively a host and a query for graph simulation. Moreover, let

\[
G = \bigoplus_{v \in V_Q} \{\exists\}_{v \text{ out}(v) = \emptyset} \bigoplus \bigotimes_{e \in E_Q} s(e) \xrightarrow{\sigma(e)} t(e)
\]

There exists a graph simulation of \(Q\) in \(H\) if and only if there exists a LGS of \(G\) in \(H\), i.e., \(\mathcal{S}^{G \rightarrow H} \neq \emptyset\).

**Proof.** From the definition of \(G\), its must, unique and exclusive sets, as well as its choice function, are respectively \(\mathcal{M} = V_Q, \mathcal{U} = \mathcal{E} = \emptyset\) and \(\mathcal{C} = \lambda x.\{\text{out}(x)\}\). Similarly to Proposition 4.2, it is quite trivial to show that the space required by \(G\) is polynomial w.r.t. the size of \(Q\) and, under the auxiliary conditions fixed by the definition of \(G\), Definitions 2.6 and 5.1 are equivalent. \(\mathcal{M} = V_Q\) implies the equivalence between LS1 and the first condition of Definition 5.1, whereas the choice function of \(G\) implies the equivalence between LS4 and the second condition of Definition 5.1. Lastly, \(\mathcal{U} = \mathcal{E} = \emptyset\) makes conditions LS2 and LS3 always true.

**Example 5.1.** Figure 5 shows a query for graph simulations and the equivalent guest for loose graph simulations. As already seen in Section 4.1, the translation preserve the structure of the graph.

### 6 Regular languages pattern matching

Regular languages defines finite sequences of characters (called words or strings) from a finite alphabet \(\Sigma\) [14]. Although widely used in text pattern matching, they are also used in graph pattern matching [2, 20]. In this section we will restrict ourselves to \(\epsilon\)-free regular languages, i.e. regular languages without the empty word \(\epsilon\) [28]. This restriction is quite common in the pattern matching setting, since the empty word is matched by any text or graph and therefore it doesn’t represent a meaningful pattern.

**Definition 6.1.** Let \(\Sigma\) be an alphabet. \(\emptyset\) is a \(\epsilon\)-free regular language. For each \(a \in \Sigma\), \(\{a\}\) is a \(\epsilon\)-free regular language. If \(A\) and \(B\) are \(\epsilon\)-free regular language, so are the following:

\[
A \cdot B \triangleq \{vw \mid v \in P \land w \in Q\} \quad A \mid B \triangleq A \cup B \quad A^+ \triangleq \bigcup_{n \in \mathbb{N}} A^{n+1}.
\]
In [28] it is shown that every regular language without the empty letter \( \epsilon \) can be expressed with the operations defined for \( \epsilon \)-free regular languages. We will now introduce the pattern matching problem for non-empty \( \epsilon \)-free regular languages. In the following let \( H = (\Sigma, V_H, E_H) \) and \( \mathcal{L} \) be respectively a host and a \( \epsilon \)-free regular language such that \( \mathcal{L} \neq \emptyset \).

**Definition 6.2.** The Emptiness problem for Regular Language Pattern Matching (RLPM) consist in checking whenever there exists a path \( \rho \in \mathbb{P}_H \) s.t. \( \sigma(\rho) \in \mathcal{L} \).

To solve this problem using LGSs we will use the equivalence between regular languages and non-deterministic finite automata [25].

**Definition 6.3.** An NFA is a 5-tuple, \( N = (\Sigma, Q, \Delta, q_0, F) \) consisting of

- an alphabet \( \Sigma \);
- a finite set of states \( Q \);
- a transition function \( \Delta : Q \times \Sigma \rightarrow \mathcal{P}(Q) \);
- an initial state \( q_0 \in Q \);
- a set of accepting (or final) states \( F \subseteq Q \).

Let \( w = a_0, a_1, \ldots, a_n \in \Sigma^* \). The NFA \( N \) accepts \( w \) if there is a sequence of states \( r_0, r_1, \ldots, r_{n+1} \) in \( Q \) s.t. \( r_0 = q_0, r_{i+1} \in \Delta(r_i, a_i) \) for \( i = 0, \ldots, n \), and \( r_{n+1} \in F \).

**Remark 6.1.** Any non-empty regular language without \( \epsilon \) can be translated to a non-deterministic finite automaton where the initial state does not have any incoming edges and the only final state does not have any outgoing edges. This can be shown, starting from the Thompson’s construction [25], by adding a new initial state and a new final state that mimic the old initial and final state w.r.t. the set of states that where already in the construction.

**Proposition 6.1.** Let \( N = (Q, \Sigma, \Delta, q_0, \{f\}) \) be a NFA where the initial state does not have any incoming edges and the only final state does not have any outgoing edges. Let \( H = (\Sigma, V_H, E_H) \) be a host. Let

\[
G = q_0 \{\exists \} \oplus f \{\exists, \emptyset\} \oplus \bigoplus_{q \in Q} q \xrightarrow{a} \Delta(q, a)
\]

There exists a path \( \rho \in \mathbb{P}_H \) in \( H \) s.t. \( \sigma(\rho) \) is accepted by \( N \) if and only if there exists a loose graph simulation of \( G \) in \( H \), i.e. \( S^{G \rightarrow H} \neq \emptyset \).

**Proof.** (\( \Rightarrow \)) If there exists \( (e_0, \ldots, e_n) \in \mathbb{P}_H \) s.t. \( \sigma(\rho) \) is accepted by \( N \) then from the definition of acceptance condition of NFAs there must exists a sequence

\[
(p_0, s(e_0)) \xrightarrow{\sigma(e_0)} (p_1, s(e_1)) \xrightarrow{\sigma(e_1)} \cdots \xrightarrow{\sigma(e_{n-1})} (p_n, s(e_n)) \xrightarrow{\sigma(e_n)} (p_{n+1}, t(e_n))
\]

such that \( p_0 = q_0 \) and \( p_{n+1} = f \); for all \( i \in \{1, \ldots, n\} \) \( t(e_{i-1}) = s(e_i) \); for all \( i \in \{0, \ldots, n\} \) \( p_{i+1} \in \Delta(p_i) \). It is easy to show that the graph \( S \) represented by this sequence is a loose graph simulation in \( S^{G \rightarrow H} \). Since \( G \) is constructed from \( N \) by preserving the transition relation \( \Delta \), \( S \) is a subgraph of \( G \times H \). Conditions LS1, LS2, LS3 trivially holds since \( p_0 = q_0, p_n = f \) and \( U = E = \emptyset \). From the definition of \( \mathcal{C} \), we have that for all \( i \in \{0, \ldots, n\} \) \( \{(p_i, \sigma(e_i), p_{i+1})\} \in \mathcal{C}(p_i) \) and therefore Condition LS4 holds. Condition LS5 is also verified since the path obtained by projecting the graph to its first component is a path from \( q_0 \) to \( f \). Lastly, the space required by \( G \) is polynomial w.r.t. the size of \( N \).
Example 6.2. Figure 6 shows the result of the translation of a NFA (left) accepting the regular language $\{ab\}^+$. As already seen in the previous section, the resulting guest (right) preserves the structure of the NFA.

7 Subgraph isomorphism with regular path expressions

Many approaches found in literature define hybrid notions of similarities between graphs w.r.t. more known ones such as graph simulations, subgraph isomorphism and RLPM [2, 9]. In this section we will see how to use LGSs to solve this type of problems by studying a problem similar to the one in [2]. In this problem, called Subgraph isomorphism with regular languages (RL-SGI), queries are graphs where each edge is decorated with a regular language.

Definition 7.1. A graph $G$ decorated with regular languages is a tuple $(\Sigma, V, E, \mathcal{L})$ consisting of an alphabet $\Sigma$, a set $V$ of nodes, a set $E \subseteq V \times V$ of edges and a labelling function $\mathcal{L} : E \rightarrow \text{RE}_\Sigma$ decorating each edge with a non-empty $\epsilon$-free regular language over $\Sigma$. We will denote with $s(e)$ and $t(e)$ respectively the first and second projection of an edge $e \in E$, i.e. its source and target.

Definition 7.2. Let $H = (\Sigma, V_H, E_H)$ be an host and let $Q = (\Sigma, V_Q, E_Q, \mathcal{L})$ be a graph decorated with regular languages. There exists an subgraph of $H$ isomorphic to a partial unfolding of $Q$ w.r.t. $\mathcal{L}$ if and only if there exists a couple of injections $\phi : V_Q \hookrightarrow V_H$ and $\eta : E_Q \hookrightarrow \mathcal{P}_H$ s.t. for each $e \in E_Q$

$$\phi \circ s(e) = s \circ \eta(e) \quad \phi \circ t(e) = t \circ \eta(e) \quad \sigma \circ \eta(e) \in \mathcal{L}(e)$$

Moreover, sources and targets of edges inside paths of $\eta(E_Q)$ cannot appear in $\phi(V_Q)$ with the exception of the source and target of each path, i.e.

$$\forall (e_0, \ldots, e_n) \in \eta(E_Q) \forall i \in \{1, \ldots, n\} \ s(e_i) \notin \phi(V_Q)$$

RL-SGI can be seen as an hybrid notion between subgraph isomorphism and RLPM. We will now show how to solve this problem with loose graph simulations by defining a proper translation from its queries to guests.
Proposition 7.1. Let $Q = (\Sigma, V_Q, E_Q, \mathcal{L})$ be a query for RL-SGI. Let

$$G = \bigoplus_{v \in V_Q} v[\exists!i] \oplus \bigotimes_{e \in E_Q} G_e[q_e/s(e)][f_e/t(e)]$$

s.t. $G_e$ is the translation of the automaton $N_e = (\Sigma, V_e, \delta_e, q_e, \{f_e\})$ for $\mathcal{L}(e)$, as per Proposition 6.1 and where $q_e$ and $f_e$ are merged whenever $s(e) = t(e)$. For each host $H = (\Sigma, V_H, E_H)$ there exists a RL-SGI of $H$ w.r.t. $Q$ iff $S^{G \rightarrow H} \neq \emptyset$.

Proof. We refer to Figures 7 to 9 as a graphic aid for the proof, where the first picture represents a query for RL-SGI. Similar to Proposition 6.1, we will first translate $Q$ to a specific guest $G$ and then show that we can use $G$ to check whenever there exists a RL-SGI w.r.t. an host $H$ and $Q$. For each edge $e \in E_Q$ of the query $Q$ we build the non-deterministic automaton $N_e = (\Sigma, V_e, \delta_e, q_e, \{f_e\})$ accepting the language $\mathcal{L}(e)$. As seen in Section 6, every non empty $\epsilon$-free regular language can be expressed with a LGSs’ guest. Therefore, the results in Proposition 6.1, we can translate every NFA $N_e$ to a guest $G_e$ using the same set of vertices of the NFA. For each $e \in E_Q$, if $e$ is a self-loop, i.e. $s(e) = t(e)$, we then remove the vertex $f_e$ from $G_e$ and update from $f_e$ to $q_e$ the target of all edges with target $f_e$. Referring to the algebra in Section 3, lets now consider the guest

$$G = \bigoplus_{v \in V_Q} v[\exists!i] \oplus \bigotimes_{e \in E_Q} G_e[q_e/s(e)][f_e/t(e)]$$

i.e. the union of all guests constructed from the edges of $Q$ and the set of vertices of $Q$ decorated with must, unique and exclusive attributes. We will now prove that the guest $G$ can be used to check whenever there exists a RL-SGI w.r.t. an host $H$ and $Q$. From the definition of $G$, the two following properties holds:

- $V_Q$ is a subset of the vertices of $G$ and $M = U = E = V_Q$;
- let $C$ the choice function of $G$ and let $v \in V_Q$. Each set $\gamma \in \mathcal{C}(v)$ contains exactly one edge for every $e \in \text{out}(v)$ of $Q$, that correspond to the first transition on the automaton $N_e$.

Similarly to the proof of Proposition 4.2, Conditions LS1, LS2, LS3 together with the first property ensures that each LGS over $G$ correspond to an injection w.r.t the vertices of $V_Q$. Moreover, following the results in Proposition 6.1, Conditions LS4 and LS5 and the second property ensures that every LGS over $G$ will contains, for each $e \in E_Q$ a path correspondent to a word in $\mathcal{L}(e)$, starting and ending with two vertices in $V_Q \times V_H$, whereas all other vertices of the path are in $(V_G \setminus V_Q) \times V_H$, where $V_G$ is the set of all vertices of $G$. It follows that $G$ can be used to verify the existence of a RL-SGI for $Q$, w.r.t. a host $H$, by checking whenever $S^{G \rightarrow H} \neq \emptyset$. \qed
Figure 7: Example of RE-SGISO query.

Figure 8: Simple guests required to encode the query in Figure 7. Vertices with the same name are highlighted by dashed edges between them.

Figure 9: A guest obtained via multiplication and addition operator from the guest in Figure 8 and equivalent to the RE-SGISO query in Figure 7.
8 Conclusions and future work

In this paper we have introduced loose graph simulations, a relation between graphs that can be used to check structural properties of labelled multigraphs. Loose graph simulations’ guests can be represented using a simple graphical notation, but also compositionally, by means of an algebra which is sound and complete. We have shown formally that computing LGSs is a NP-complete problem, where the NP-hardness is obtained via a trivial reduction of subgraph isomorphism to them. Moreover, we have shown that many other classical notions of graph pattern matching are naturally subsumed by LGSs. Loose graph simulations can therefore be seen as a simple common ground between multiple well-known notions of graph pattern matching and they can be used to define new hybrid fragments of these notions and develop common techniques for them.

An algorithm for computing LGSs in a decentralised fashion and inspired to the “distributed amalgamation” strategy is introduced in [16]. Roughly speaking, the host graph is distributed over process; each process has a partial view of the host which uses to compute partial solutions to exchange with its peers. Distributed amalgamation guarantees all solutions are eventually found. The same strategy is at the hearth of distributed algorithms for solving related problems such as bigraphical embeddings [17, 19]. In particular, the algorithm presented in loc. cit. is the cornerstone enabling the distributed execution of bigraphical rewriting systems [21, 22] on which rely the methodology for designing and prototyping multi-agent systems introduced in [18].

This similarity and the ability of LGS guests to subsume several graphs suggests to investigate rewriting systems where redex occurrences are defined in terms of LGSs.

Another topic for further investigation is how to systematically minimise guests or combine sets of guests into single instances, while preserving the semantics of LGSs. A result in this direction would have a positive practical impact on applications based on LGSs.

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