Graph Abstraction and Abstract Graph Transformation

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Abstract Many important systems like concurrent heap-manipulating programs, communication networks, or distributed algorithms are hard to verify due to their inherent dynamics and unboundedness. Graphs are an intuitive representation of states of these systems, where transitions can be conveniently described by graph transformation rules.

We present a framework for the abstraction of graphs supporting abstract graph transformation. The abstraction method naturally generalises previous approaches to abstract graph transformation. The set of possible abstract graphs is finite. This has the pleasant consequence of generating a finite transition system for any start graph and any finite set of transformation rules. Moreover, abstraction preserves a simple logic for expressing properties on graph nodes. The precision of the abstraction can be adjusted according to properties expressed in this logic to be verified.

Contents

1 Introduction

Graphs constitute an important means of representation of the state of a system. Interesting qualities of a given state have natural graph-theoretic counterparts. Specially if the system in question is one that manipulates the memory "heap". Also, their inherent graphical representation makes them the "lingua franca" of software engineering, they are good to convey ideas back and forth between different communities such as formal verification and specification, software engineering and even end users. If we add the concept of graph transformation for modelling transitions between system states, we form a framework that will allow people to talk about both the states of a system and how it evolves in time.

This paper presents work carried out in the context of the GROOVE project that seeks to develop such a framework for software verification: states of a software system are represented by graphs and statements of a programming language are given the semantics of graph transformation rules. As an example, on Figure 1 is depicted a possible graph representation of a list. Adding a new element to the list consists in creating a new node labelled Cell with possibly associated Object-node, and inserting it in the desired place in the list. Removing an element from the list and many other list operations can also be seen as graph transformations.

1.1 Graph Transformations for System Analysis

A graph transformation rule $p : L \to R$ is given by its name p and a couple of graphs L, R, often called left-hand side and right-hand side, respectively. Performing a graph transformation on a graph G using the rule p can be seen as finding a subgraph of G that is isomorphic to L and replacing it with R. Systems and system behaviour can be modelled by graphs and graph transformations. Let G_0 be a graph representing an initial state of a system (*e.g.* the list on Figure 1) and let $\mathcal{P}$ be a set of transformation rules encoding all possible transitions of the system (*e.g.* operations on lists). It is possible to explore all possible accessible configurations and evolutions of the system given by G_0 and $\mathcal{P}$. This is done by applying all possible transformations from $\mathcal{P}$ to the start graph G_0 and repeating it iteratively to all graphs resulting from these transformations. This gives rise to a labelled transitions system whose states are graphs and whose transitions are applications of graph transformation rules. One can then verify properties, *e.g.* temporal properties, on the system using the transition system. The GROOVE tool [10] allows to construct (final portions of) such transition systems and verify temporal properties using CTL logic.

Problems do arise when approaching this task. One such problem is the possible infinite behaviour of a system which in most cases makes it impossible to study the whole behaviour of the system. Another problem is space: even for a finite state space, each state can be quite big to represent if one does it naively. A usual way to circumvent these two problems is abstraction. In Section 8 we will describe several related approaches that exist.

1.2 Contributions

In previous work some of the authors have proposed abstraction techniques in which graph nodes with similar incoming and outgoing edges [9] or similar direct neighbours [2] are summarised into a single one. Such abstract graphs have sometimes been called *shapes* [14,9] and we borrow here the same vocabulary. The number of possible such shapes is bounded. This, combined with a suitable notion of graph transformations for abstract graphs [11], guarantees a finite number of states of a transition system.

As a first contribution of the paper we introduce a family of *neighbourhood shapes* as a part of a general abstraction mechanism that subsumes previous works. For the abstraction, nodes are grouped

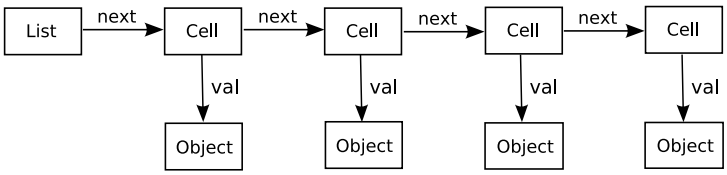


Figure 1. Graph representation of a list with four elements. Each Cell contains a pointer to the Object stored into it via a Val-edge, and possibly a pointer to the next cell via a Next-edge.

if they have similar neighbourhood up to some "radius" i, parameter of the abstraction. This allows us to have abstractions with different precisions. Additionally, the number of possible neighbourhood shapes is bounded. Moreover, we define graph transformations for our neighbourhood shapes, which allows to over-approximate system behaviour while keeping a finite state space.

Our second contribution is a logic that goes hand-in-hand with our abstraction method. That is, given a formula describing a property we are interested in, our abstraction method will guarantee that *a*) if the formula holds for the original graph, then it holds for the abstracted graph (we call this property preservation); and *b*) if the formula holds for the abstracted graph, then it holds for the original one too (we call this reflection).

Finally, all these ingredients can be combined for defining a fully automatic method which, given an initial graph, a set of graph transformation rules and a set of logic properties on the reachable graphs we are interested in, will construct a finite state abstract labelled transition system on which these properties can be verified.

The present paper is structured as follows. Section 2 introduces graphs and graph transformations. Section 3 introduces the general abstraction mechanism as well as so called neighbourhood shapes. In Section 4 are defined canonical shapes, which are a family of shapes including neighbourhood shapes that enjoy the good property of having a unique representation. Then in Sections 5 and 6 we define transformations on shapes and describe how it can be used for approximating system behaviour into finite labelled transition systems. In Section 7 we introduce a modal logic that is preserved and reflected by the neighbourhood shaping mechanism. Section 8 describes some related work. Finally, we conclude in Section 9.

2 Graphs and Graph Transformations

We are interested in finite graphs whose edges and nodes are labelled from a finite set of labels Lab. Formally, we do not associate labels with the nodes of the graph, we use instead special edges whose target is a particular object $\perp$ not in the set of nodes of the graph. This in particular allows to have nodes with multiple labels, which shows to be very useful for modelling with graphs. Moreover, we authorise multiple parallel edges, *ie* there can be several different edges having the same source and target nodes and the same label.

Definition 1 (graph). *A* graph G *is a tuple* $(N_G, E_G, \mathsf{src}_G, \mathsf{tgt}_G, \mathsf{lab}_G)$ *where*

- N_G *is a finite set of nodes,*
- E_G *is a finite set of edges disjoint from* N_G*,*
- $\mathsf{src}_G : E_G \to N_G$ *and* $\mathsf{tgt}_G : E_G \to N_G \cup \{\perp\}$ *with* $\perp \notin (N_G \cup E_G)$ *are mappings associating with each edge its source and target nodes, respectively, and*
- $\mathsf{lab}_G : E_G \to \mathsf{Lab}$ *is labelling map for the edges of the graph.* ◀

The mapping lab_G is extended on nodes to designate the set of labels of a node, *ie* $\mathsf{lab}_G(v) = \{\mathsf{a} \in \mathsf{Lab} \mid \exists e \in E_G : \mathsf{src}_G(e) = v, \mathsf{tgt}_G(e) = \bot, \mathsf{lab}_G(e) = \mathsf{a}\}$. [1] We will denote as $v\triangleright^{\mathsf{a}}_G$ and $v\triangleleft^{\mathsf{a}}_G$ the set of a-outgoing edges and a-incoming edges of the node v, respectively. That is, $v\triangleright^{\mathsf{a}}_G = \{e \in E_G \mid \mathsf{src}_G(e) = v, \mathsf{lab}_G(e) = \mathsf{a}\}$ and symmetrically for $v\triangleleft^{\mathsf{a}}_G$. For a set of nodes V, $V\triangleright^{\mathsf{a}}_G$ (resp. $V\triangleleft^{\mathsf{a}}_G$) is the extension of $\triangleright^{\mathsf{a}}_G$ (resp. $\triangleleft^{\mathsf{a}}_G$) on sets. Finally, for X, Y sets of nodes or nodes, we denote $X \bowtie^{\mathsf{a}}_G Y$ the set of edges labelled a and going from X to Y, *ie* $X \bowtie^{\mathsf{a}}_G Y = X \triangleright^{\mathsf{a}}_G \cap Y \triangleleft^{\mathsf{a}}_G$. When the graph G is clear from the context, we may omit the subscript G in N_G, E_G, src_G, tgt_G, lab_G, $\triangleright^{\mathsf{a}}_G$, $\triangleleft^{\mathsf{a}}_G$, and $\bowtie^{\mathsf{a}}_G$.

Definition 2 (graph morphism). *If G and H are graphs, a* graph morphism *$f : G \to H$ is a function from $N_G \cup E_G \cup \{\bot\}$ to $N_H \cup E_H \cup \{\bot\}$ such that*

- *f preserves $\bot$, ie $f(\bot) = \bot$, $f^{-1}(\bot) = \{\bot\}$,*
- *f maps nodes to nodes and edges to edges, ie $f(N_G) \subseteq N_H$, $f(E_G) \subseteq E_H$,*
- *f is compatible with source and target mappings, ie $\mathsf{src}_H \circ f = f \circ \mathsf{src}_G$, and $\mathsf{tgt}_H \circ f = f \circ \mathsf{tgt}_G$, and*
- *f preserves labels, $f \circ \mathsf{lab}_G = \mathsf{lab}_H$.* ◀

A morphism f is called *injective* (resp. *surjective*, resp. *bijective*) if it defines an injective (resp. surjective, resp. bijective) map. A bijective morphism is also called an *isomorphism*.

For the sake of clarity, in the sequel of the paper we ignore the node $\bot$ and simply talk about node labels. It is easy to see that all the proofs can be adapted to this formal definition using the $\bot$ node.

Background on Graph Transformations

Let's start with some notations for functions. For a set A, we denote id_A the identity function on A. For two functions f, g, we denote $f \cup g$ their union, that is, $f \cup g$ is the function whose domain is the union of the domains of f and g and whose co-domain is the union of the co-domains of f and g. The union of functions is defined only if for any x belonging both to the domains of f and g, f and g agree on their value for x.

Definition 3 (Production Rule). *A graph production rule P is a pair of graphs (L, R), called left-hand side and right-hand side respectively. A production rule can be viewed as the single graph $L \cup R$. In this case we distinguish the following sets :*

- *$N_P^{\text{del}} = N_L \setminus N_R$ and $E_P^{\text{new}} = E_L \setminus E_R$ are the elements to be deleted;*
- *$N_P^{\text{new}} = N_R \setminus N_L$ and $E_P^{\text{new}} = E_R \setminus E_L$ are the elements to be created;*
- *$N_P^{\text{use}} = N_R \cap N_L$ and $E_P^{\text{new}} = E_R \cap E_L$ are the elements that remain unchanged.*

The subscript P is omitted when clear from the context.

Definition 4 (Graph Transformation). *Let G be a graph and $P = (L, R)$ be a production rule such that G and P are disjoint. A* matching *m for P into G is an injective morphism $m : L \to G$ satisfying the so called dangling edges application condition : for any edge e of G, if $\mathsf{src}(e) \in m(N^{\text{del}})$ or $\mathsf{tgt}(e) \in m(N^{\text{del}})$, then $e \in m(E^{\text{del}})$.*

If m is a matching for P into G, then the transformation of G according to P and m *is the graph H defined as follows (with $m' : P \to G$ the morphism $m \cup id_{N^{\text{new}} \cup E^{\text{new}}}$):*

- *$N_H = (N_G \setminus m(N^{\text{del}})) \cup N^{\text{new}}$;*

[1] Note that $\mathsf{lab}_G(e)$ is a label for an edge e, and $\mathsf{lab}_G(v)$ is a set of labels for a node v.

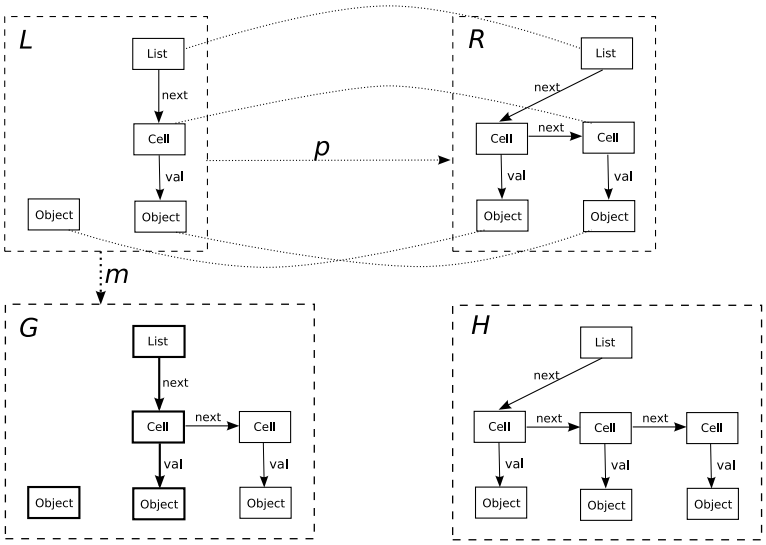


Figure 2. Example of a production rule $P = (L, R)$ and its application to a graph G via matching $m : L \to G$. The rule morphism p is indicated by the dotted lines. For the sake of readability, the matching $m : L \to G$ is indicated by highlighting its image $m(L)$ in G. The host graph G represents a list with two elements with some additional object in the environment. The application of the rule results in adding a new element at the head of the list.

- $E_H = (E_G \setminus m(E^{\text{del}})) \cup E^{\text{new}}$*;*
- $\mathsf{src}_H = \mathsf{src}_G \cup m' \circ \mathsf{src}_P$ *restricted to* E_H*;*
- $\mathsf{tgt}_H = \mathsf{tgt}_G \cup m' \circ \mathsf{tgt}_P$ *restricted to* E_H*;*
- $\mathsf{lab}_H = \mathsf{lab}_G \cup \mathsf{lab}_P$ *restricted to* E_H*.*

We write $G \xrightarrow{P,m} H$ *to designate that* m *is a matching for* P *in* G *and* H *is the graph resulting from the transformation.* ◀

The dangling edges application condition is standard in so called double push-out approach for graph transformation. It ensures that performing a transformation does not introduce dangling edges (edges without source or target node).

On Figure 2 is depicted a production rule aiming to add an element in head of a list, as well as an example application of this rule.

3 Graph Abstraction

It this section abstract graphs are called shapes. The name “shape” comes from work in shape analysis [14], where abstract graphs are used to represent pointer structures. Any node and any edge of a given shape may represent several nodes/edges of some *concrete* graph. We want it to carry information on the number of summarised nodes/edges. For defining interesting abstractions, it seems necessary for this multiplicity information to be approximate: think for instance about abstracting a list independently of its length. In Section 3.1 we introduce the notion of *multiplicity* for handling approximate information on cardinals of sets. Then, in Section 3.2 we define the shapes that we consider, as well as the abstraction mechanism called *shaping*. It is essentially a morphism from a graph to a shape that satisfies some conditions.

Shapes may be more or less abstract. In particular, a shape may be abstracted to another shape. This yields a sub-shape relation between shapes. We define sub-shaping in Section 3.3. In the same section, we also define isomorphism of shapes and show that isomorphic shapes represent the same sets of concrete graphs.

Finally, in Section 3.4 we define a particular family of shapes called *neighbourhood shapes*. Neighbourhood shapes represent numerous advantages that will be studied in the rest of the paper.

3.1 Multiplicities

A multiplicity is an approximation of the cardinal of a (finite) set. Intuitively, all sets having strictly more than μ elements, for some fixed natural μ, are considered having the same cardinal. This notion of multiplicity was also used in [9].

Definition 5 (multiplicity). *For any natural number $\mu > 0$, let $\mathbf{M}_\mu$ be the set $\{0, 1, 2, \ldots, \mu, \omega\}$ where ω is distinct from all natural numbers. The* multiplicity with precision μ *is the function associating with each finite set U the value $|U|_\mu$ in $\mathbf{M}_\mu$ defined by:*

$$|U|_\mu = \begin{cases} Card(U) & \text{if } Card(U) \leq \mu, \\ \omega & \text{otherwise.} \end{cases}$$

The value $|U|_\mu$ is called the μ-multiplicity *of U, or simply the multiplicity of U if μ is clear from the context. Elements of $\mathbf{M}_\mu$ are called multiplicities. We write $\mathbf{M}_\mu^+$ for the set $\mathbf{M}_\mu \setminus \{0\}$.* ◀

We extend the usual ordering $\geq$ over elements of $\mathbf{M}_\mu$ by defining $\omega \geq \lambda$ for any λ in $\mathbf{M}_\mu$. Sum can also be extended over multiplicities on the expected way: let I be a finite index set and the $(\lambda_i)_{i \in I}$ be elements of $\mathbf{M}_\mu$. Then $\sum_{i \in I}^{\mu} \lambda_i$, the μ-sum of the $(\lambda_i)_{i \in I}$, is $\left|\bigcup_{i \in I} A_i\right|_\mu$ where the $(A_i)_{i \in I}$ are pairwise disjoint sets such that $|A_i|_\mu = \lambda_i$ for any i in I.

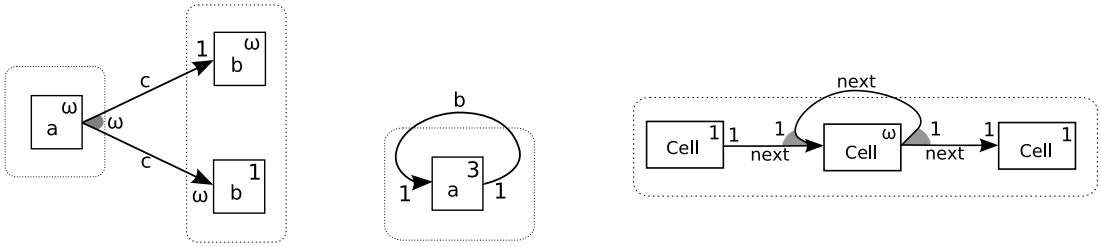
In the sequel of the paper, we consider two naturals ν, μ. Whenever their value is not specified, they may have any positive value. ν-multiplicity will be used for giving the multiplicity of sets of nodes, and μ-multiplicity for giving the multiplicity of sets of edges. In particular, these two numbers will be parameters of graph abstractions.

3.2 Shapes and Shaping

A shape is a graph together with a *node multiplicity function* that indicates, for each node of the shape, how many nodes it summarises. Moreover, the set of nodes is partitioned into groups. Edges with same source node, and ending into nodes in the same group (or, respectively, edges with the same target node, and starting in nodes in the same group) cannot be distinguished. Only the number of such edges is indicated with the help of the *edge multiplicity functions* of the shape.

We start by giving a flavour of what a shape is, in the following example.

Example 6 (Shape). On Figure 3 are depicted three shapes as well as values for μ and ν for these shapes. With each node of each shape is associated a multiplicity from $\mathbf{M}_\nu^+$, indicating the number of concrete graph nodes it represents; this is called the *node multiplicity*. The dotted rectangles are delimiting groups of nodes. By definition, this grouping can be arbitrary; in practise it would be defined by some common characteristic (*e.g.* nodes with same label, nodes with similar neighbourhood, etc). All edges have associated multiplicity information (from $\mathbf{M}_\mu$) in their end points. Sometimes, this multiplicity is shared by several edges, indicated by the grey arc relating them. These are the so-called



(a) $\mu = 1, \nu = 1$ (b) $\mu = 1, \nu = 3$ (c) $\mu = 1, \nu = 1$

Figure 3. Examples of shapes.

outgoing edges multiplicity, when associated to source of the edge, and *incoming edges multiplicity* when associated to the target. Edge multiplicity intuitively indicate how many of the depicted edges should be there in a concrete graph. One can notice that edges related in one of their end points all have their other end point in the same group of nodes, and all have the same label. Actually, this is the condition for relating edges. To be even more precise, according to the formal definition, edge multiplicities are associated with a triple composed of a node, a label and a group of nodes. This will be explained in Definition 7.

Let us now explain how one should interpret these example shapes.

(a). The shape on Figure 3(a) represents a set of bipartite concrete graphs in which a-nodes are connected to b-nodes by c-edges. Each of these graphs has at least two (here ω on nodes or edges stands for "two or more", as $\nu = 1$) a-nodes and at least three (ω plus one) b-nodes. Moreover, every a-node has at least two (*ie* ω) outgoing c-edges going to b-nodes. All b-nodes except one have only one incoming edge; the remaining b-node has at least two incoming edges. See Figure 4(a) for some example concrete graphs.

(b). The shape on Figure 3(b) represents a set of concrete graphs having three a-nodes connected to each-others and forming cycles of b-edges. See Figure 4(b) for some example concrete graphs.

(c). The shape on Figure 3(c) represents a set of list-like concrete graphs having Cell-nodes connected by next-edges. Each of these graphs has at least one acyclic connected component of length four or more with several (possibly zero) cyclic connected components of arbitrary length. See Figure 4(c) for some example concrete graphs. ◀

Before giving the formal definition of a shape, let us fix some notations. Let A be a set and $\sim \subseteq A \times A$ be an equivalence relation over A. For $x \in A$, we denote $[x]_\sim$ the equivalence class of x induced by $\sim$, *ie* $[x]_\sim = \{y \in A \mid y \sim x\}$. We denote $A/\sim$ the set of equivalence classes in A, *ie* $A/\sim = \{[x]_\sim \mid x \in A\}$. Moreover, if $\sim$ and $\sim'$ are two equivalence relations over A, we write $\sim \subseteq \sim'$ whenever for all $x, y \in A$, $x \sim y$ implies $x \sim' y$. Note that if $\sim \subseteq \sim'$, then any equivalence class for $\sim$ is included into the equivalence class for $\sim'$, that is, for all $x \in A$, $[x]_\sim \subseteq [x]_{\sim'}$. This means in particular that any equivalence class for $\sim'$ can be obtained as an union of equivalence classes for $\sim$.

Formally, a shape is defined as follows:

Definition 7 (shape). *A* shape S *is a structure* $(G_S, \simeq_S, \mathsf{mult}_{\mathrm{n},S}, \mathsf{mult}_{\mathrm{out},S}, \mathsf{mult}_{\mathrm{in},S})$ *where*

- $G_S = (N_S, E_S, \mathsf{src}_S, \mathsf{tgt}_S, \mathsf{lab}_S)$ *is a graph;*
- $\simeq_S \subseteq N_S \times N_S$ *is an equivalence relation on* N_S *called the grouping relation of* S*;*
- $\mathsf{mult}_{\mathrm{n},S} : N_S \to \mathbf{M}_\nu^+$ *is a nodes' multiplicity function;*
- $\mathsf{mult}_{\mathrm{out},S} : N_S \times \mathsf{Lab} \times N_S/{\simeq_S} \to \mathbf{M}_\mu$ *is an outgoing edges multiplicity function and*

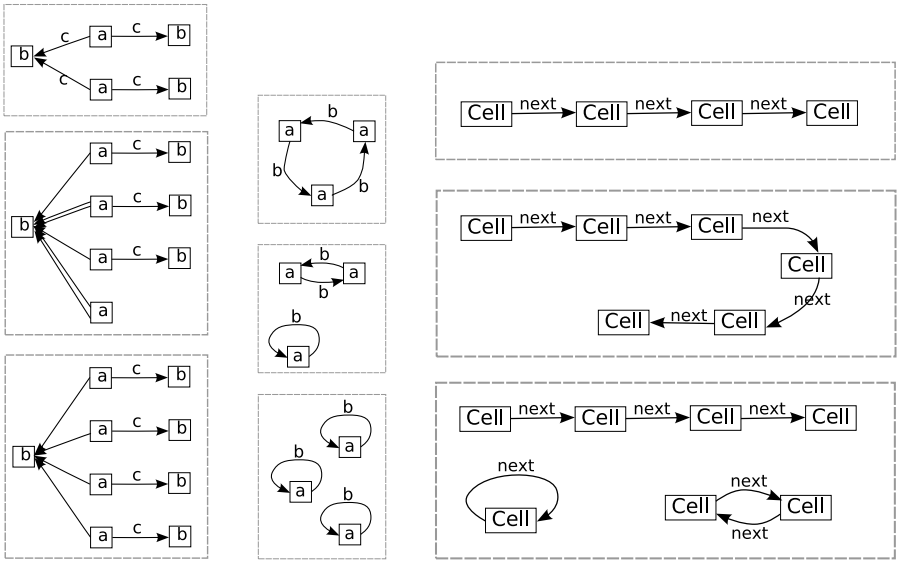


Figure 4. Example concrete graphs that can be abstracted to the shapes on Figure 3.

– $\mathsf{mult}_{\text{in},S} : N_S \times \mathsf{Lab} \times N_S/{\simeq_S} \to \mathbf{M}_\mu$ *is an incoming edges multiplicity function.*

Moreover, for any node $v \in N_S$*, any label* $\mathsf{a} \in \mathsf{Lab}$ *and any equivalence class of nodes* $C \in N_S/{\simeq_S}$*, we require that* $\mathsf{mult}_{\text{out},S}(v, \mathsf{a}, C) = 0$ *if, and only if,* $v \rhd\!\!\rhd^{\mathsf{a}}_{G_S} C = \varnothing$*, and* $\mathsf{mult}_{\text{in},S}(v, \mathsf{a}, C) = 0$ *if, and only if,* $C \rhd\!\!\rhd^{\mathsf{a}}_{G_S} v = \varnothing$*.* ◀

As already mentioned, a shape is a representation of a set of concrete graphs. In this sense, it is an abstract graph. The fact that some concrete graph is *abstracted* to a given shape is determined by the presence of so called *shaping morphism*, which is a morphism from the graph to the shape that complies to some additional constraints. We say then that the graph is a *concretisation* of the shape.

Definition 8 (shaping morphism, concretisation). *Let* G *be a graph and* S *be a shape. A* shaping morphism, or shaping, of G into S *is a graph morphism* $s : G \to G_S$ *such that the following conditions are met:*

– *for all* $w \in N_S$*,* $\mathsf{mult}_{\text{n},S}(w) = \left|s^{-1}(w)\right|_\nu$*;*
– *for all* $w \in N_S$*, for all* $\mathsf{a} \in \mathsf{Lab}$*, for all* $C \in N_S/{\simeq_S}$*, and for all* $v \in s^{-1}(w)$*,*

$$\mathsf{mult}_{\text{out},S}(w, \mathsf{a}, C) = \left|v \rhd\!\!\rhd^{\mathsf{a}}_{G}(s^{-1}(C))\right|_\mu$$

and

$$\mathsf{mult}_{\text{in},S}(w, \mathsf{a}, C) = \left|(s^{-1}(C)) \rhd\!\!\rhd^{\mathsf{a}}_{G} v\right|_\mu .$$

If G *is a graph and* S *is a shape such that there exists a shaping* $s : G \to S$*, then we say that* G *is a* concretisation *of* S*. The set of concretisations of a shape* S *is denoted* $Concr(S)$*.* ◀

Example 9. The list structure from Figure 1 is a concretisation for the shape shown in Figure 5. The corresponding shaping maps the List-node of the graph to the List-node of the shape, the right-most Cell-node and the right-most Object-node from the graph are mapped to the corresponding right-most nodes from the shape. The remaining Cell-nodes and Object-nodes from the graph are mapped to the left-hand side such nodes of the shape.

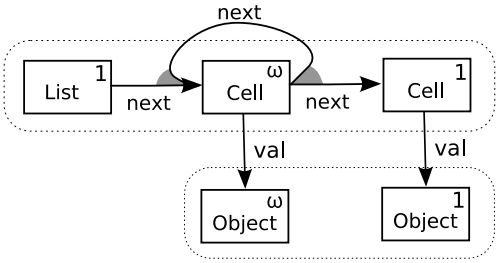


Figure 5. Example of a shape for a list. All edge multiplicities are equal to one and are omitted.

Note that a shaping is a surjective morphism; this follows from the requirement for the $\mathsf{mult}_{\mathrm{n},S}$ function together with the fact that $\mathsf{mult}_{\mathrm{n},S}$ maps to non null multiplicities, by definition of shapes. The requirements on outgoing (resp. incoming) edge multiplicities guarantee in particular that two different nodes v, v' from a graph G can be mapped to the same node w of a shape S only if v, v' have the same outgoing (resp. incoming) edges multiplicities with respect to a label and group of nodes.

Construction of Shapes In Definitions 7 and 8, a shape S is a graph-like structure defined independently on any of its concretisations. A graph G can be abstracted to a shape S if there exists a morphism from G to the graph part of S satisfying some conditions. In particular, these definitions do not give a hint how to construct shapes. In what follows, we present an alternative, constructive way of defining a shape by providing a graph and two equivalence relations on its nodes.

Let G be a graph and $\sim, \equiv \subseteq N_G \times N_G$ be two equivalence relations on the nodes of G satisfying the following conditions:

(C1) $\equiv \subseteq \sim$, that is, if $v \equiv v'$, then $v \sim v'$;

(C2) for any v, v' nodes of G, for any $\sim$-equivalence class of nodes $C \in N_G/\!\sim$ and for any label a, if $v \equiv v'$, then

$$\left|v \bowtie^{\mathsf{a}}_G C\right|_\mu = \left|v' \bowtie^{\mathsf{a}}_G C\right|_\mu$$

and

$$\left|C \bowtie^{\mathsf{a}}_G v\right|_\mu = \left|C \bowtie^{\mathsf{a}}_G v'\right|_\mu$$

Let the equivalence relation $\equiv$ be extended on edges of G in the following way: $e \equiv e'$ if $\mathsf{src}_G(e) \equiv \mathsf{src}_G(e')$, $\mathsf{tgt}_G(e) \equiv \mathsf{tgt}_G(e')$ and $\mathsf{lab}_G(e) = \mathsf{lab}_G(e')$.

Consider now the graph $S_G = (N_S, E_S, \mathsf{src}_S, \mathsf{tgt}_S, \mathsf{lab}_S)$ defined by:

- nodes of S_G are $\equiv$-equivalence classes of nodes of G, *ie* $N_S = N_G/\!\equiv$;
- edges of S are $\equiv$-equivalence classes of edges of G, *ie* $E_S = E_G/\!\equiv$;
- for any edge $[e]_\equiv$ in E_S, $\mathsf{src}_S([e]_\equiv) = [\mathsf{src}_G(e)]_\equiv$, $\mathsf{tgt}_S([e]_\equiv) = [\mathsf{tgt}_G(e)]_\equiv$ and $\mathsf{lab}_S([e]_\equiv) = \mathsf{lab}_G(e)$. Remark that, because of the definition of $\equiv$ on edges, the particular choice of e for $[e]_\equiv$ is not important.

Consider finally the mapping $s : N_G \cup E_G \to N_S \cup E_S$ defined by: $s(v) = [v]_\equiv$ and $s(e) = [e]_\equiv$ for any v in N_G and any e in E_G. The next lemma is not difficultly seen from the definitions, so we present it without proof.

Lemma 10. *1. The mapping s canonically extended to $\perp$ defines a surjective graph morphism from G into S_G; by abuse of notation we denote this morphism s as well.*

2. Let

– $\sim_S \subseteq N_S \times N_S$ *be the equivalence relation on nodes of* G_S *defined by* $[v]_{\equiv} \sim_S [v']_{\equiv}$ *if* $v \sim v'$ *for all* v, v' *nodes of* G*. Thanks to Condition (C1),* $\sim_S$ *is well defined;*
– $\mathsf{mult_n} : N_S \to \mathbf{M}_\nu^+$ *be the mapping defined by* $\mathsf{mult_n}(w) = \left|s^{-1}(w)\right|_\nu$ *for all* w *in* N_S*;*
– $\mathsf{mult_{out}}, \mathsf{mult_{in}} : N_S \times \mathsf{Lab} \times N_S/{\sim_S} \to \mathbf{M}_\mu$ *be the mappings defined by*

$$\mathsf{mult_{out}}([v]_{\equiv}, \mathsf{a}, C) = \left|v \rhd\!\!\rhd^{\mathsf{a}}_G C\right|_\mu \qquad \mathsf{mult_{in}}([v]_{\equiv}, \mathsf{a}, C) = \left|C \rhd\!\!\rhd^{\mathsf{a}}_G v\right|_\mu$$

for all $v \in N_G$*,* $\mathsf{a} \in \mathsf{Lab}$ *and* $C \in N_S/{\sim_S}$*. Thanks to Condition (C2),* $\mathsf{mult_{out}}$ *and* $\mathsf{mult_{in}}$ *are well-defied.*

Then $S = (G_S, \sim_S, \mathsf{mult_n}, \mathsf{mult_{out}}, \mathsf{mult_{in}})$ *is a shape and* s *is a shaping morphism.* □

It follows from this lemma that, given a graph G and two equivalence relations on the nodes of G satisfying Condition (C1) and Condition (C2), one can define a shape S such that there exists a shaping $s : G \to S$. Note that all shapes can not be defined this way, for two reasons.[2] First, shapes defined as in previous lemma necessarily have concretisations, and there exist shapes without concretisations. Second, shapes defined as in previous lemma can not have parallel edges (*ie* edges having same source, same target and same label), whereas shapes may have such parallel edges. Nevertheless, it is the case that any shape admitting concretisations and without parallel edges can be defined[3] by a graph G and two equivalence relations, as explained previously.

For a graph G and equivalence relations $\sim$ and $\equiv$ satisfying Condition (C1) and Condition (C2), we define $shape(G, \sim, \equiv)$ as the shape described by Lemma 10 and we define $shaping(G, \sim, \equiv)$ as the corresponding shaping.

3.3 Abstraction Morphism and Isomorphism of Shapes

Just like graphs can be abstracted to shapes, shapes can be abstracted to (more abstract) shapes. In this section we describe this abstraction relation, defined by the presence of so called *abstraction morphism* between shapes. Then we show that this abstraction relation is composable. We also use abstraction morphisms to define the notion of *isomorphism* between shapes with the interesting property that isomorphic shapes have the same concretisations. As we will see, these properties of shapes allow to define a pre-order on shapes.

Definition 11 (Abstraction Morphism). *Let* S *and* T *be two shapes. An* abstraction morphism between *them is a graph morphism* $f : S \to T$ *that complies to the following axioms:*

1. $\forall v, v' \in N_S$*:* $v \simeq_S v'$ *implies* $f(v) \simeq_T f(v')$*;*
2. $\forall w \in N_T$*:* $\mathsf{mult_{n},}_T(w) = \left(\sum^{\nu}_{v \in f^{-1}(w)} \mathsf{mult_{n},}_S(v)\right)$*;*
3. $\forall w \in N_T$*,* $\forall \mathsf{a} \in \mathsf{Lab}$*,* $\forall C \in N_T/{\simeq_T}$*,* $\forall v \in f^{-1}(w)$*, it holds*

$$\mathsf{mult_{out},}_T(w, \mathsf{a}, C) = \sum^{\mu}_{D \in (f^{-1}(C))/{\simeq_S}} \mathsf{mult_{out},}_S(v, \mathsf{a}, D)$$

[2] Actually, there is a third reason which has to do with representation, and that is ignored here. The shapes defined as in Lemma 10 come with their representation: nodes are equivalence classes of nodes of some graph, edges are equivalence classes of edges of some graph, and so on. Thus, two isomorphic, but not equal, graphs would define two different shapes, although intuitively we would consider these two shapes as equivalent. This "equivalence" of shapes is called shape isomorphism and is defined in Section 3.3.

[3] Up to isomorphism; see also Footnote 2.

and

$$\mathsf{mult}_{\text{in},T}(w, \mathsf{a}, C) = \sum_{D \in (f^{-1}(C))/\simeq_S}^{\mu} \mathsf{mult}_{\text{in},S}(v, \mathsf{a}, D).$$

When such a morphism exists, we say that S is a subshape *of T, and we denote it as $S \sqsubseteq T$.* ◀

Note that the subshape relation falls to be an ordering relation because it is not antisymmetric. Let us now argue that the axioms in the previous definition are well defined. In the third axiom we are summing up the $\mathsf{mult}_{\text{out},S}(v, \mathsf{a}, D)$ and $\mathsf{mult}_{\text{in},S}(v, \mathsf{a}, D)$ for all $D \in (f^{-1}(C))/\simeq_S$. It is then necessary that all the triples (v, a, D) belong to the domain of $\mathsf{mult}_{\text{in},S}$, that is, it is necessary that any such D belongs to $N_S/\simeq_S$. This is indeed the case thanks to the first axiom. Let us now make a parallel between shaping and abstraction morphism. The second condition for abstraction morphism corresponds to the first condition for shaping, but we are summing up node multiplicities instead of simply counting nodes. The third condition on abstraction morphisms is very close to the second condition for shaping, but we are taking into account outgoing and incoming edge multiplicities instead of simply counting edges.

Proposition 12 (Abstraction Morphisms are Composable). *Let S, T and U be shapes, f be an abstraction morphism between S and T and g another such morphism between T and U. Then $g \circ f$ (the function composition of f and g) is an abstraction morphism between S and U.*

Proof. See Appendix A.

Let us also point out that a shaping and an abstraction morphism can also be composed, resulting into a shaping. The next proposition is presented without proof, but it is not difficultly seen to follow from Proposition 12 and the definition of shaping.

Proposition 13 (Shapings and Abstraction Morphisms). *Let G be a graph and S and T be shapes such that there exist a shaping $s : G \to S$ and an abstraction morphism $f : S \to T$. Then, $f \circ s : G \to T$ is a shaping.* □

Shapes that are the abstraction of one another will be called isomorphic:

Definition 14 (Isomorphism of Shapes). *Two shapes S and T are* isomorphic *if there exists an isomorphism $f : G_S \to G_T$ such that f and f^{-1} are abstraction morphisms. In this case, f is called an* abstraction isomorphism. ◀

It is easy to see from the definitions that if $f : S \to T$ is an abstraction isomorphism, then the grouping relation $\simeq_T$ is such that $f(v) \simeq_T f(w)$ if, and only if, $v \simeq_S w$, the node multiplicity function $\mathsf{mult}_{\text{n},T}$ is such that $\mathsf{mult}_{\text{n},T}(f(v)) = \mathsf{mult}_{\text{n},S}(v)$, and analogously for the edge multiplicity functions.

Lemma 15 (Isomorphism and Concretisations). *If two shapes S and T are isomorphic, then they have the same concretisations.*

Proof. Immediately follows from the definitions and Proposition 13. □

The inverse is not true. Consider for instance the two shapes S and T as follows: S has a single node of multiplicity two and no edges. T has two nodes, each of multiplicity one, and no edges. S and T both have a unique concretisation (up to graph isomorphism) which is the graph with two nodes and no edges, but S and T are clearly not isomorphic. Another example are shapes without concretisations, that may have very different underlying graphs, but all have the same concretisations.

Partial order relation over shapes Two shapes will be considered equivalent if they have the same concretisations; we denote this equivalence relation $=_{\text{concr}}$. That is, for all shapes S, T, $S =_{\text{concr}} T$ if, and only if, $Concr(S) = Concr(T)$.

Lemma 16 (Partial Order). *The subshape relation $\sqsubseteq$ defines a partial order between shapes with respect to the equivalence relation $=_{concr}$.*

Proof. $\sqsubseteq$ is clearly reflexive; it is antisymmetric, for the equivalence relation $=_{\text{concr}}$, by definition of isomorphism of shapes and by Lemma 15. Finally, $\sqsubseteq$ is transitive by Proposition 12.

It is also easy to see that the $\sqsubseteq$ relation is compatible with the subset relation on concretisations, in the sense that $S \sqsubseteq T$ implies that $Concr(S) \subseteq Concr(T)$. This is an immediate consequence of Proposition 12 and Proposition 13. This partial order could be a first step making the link between our abstraction mechanism and abstract interpretation (see, *e.g.*, [6]). However, it does not allow to define immediately a Galois connection between graphs and shapes, but between sets of graphs and sets of shapes, as the subshaping relation is in connection with the subset relation on graphs.

3.4 Neighbourhood Shapes

Neighbourhood shapes are a special family of shapes that represent several interesting properties established in the rest of the paper. For the moment, let us only point out the possibility to parametrise the precision of abstraction offered by neighbourhood shapes. Precision of (general) shapes, that we considered up to now, can already be parametrised by the two multiplicities μ and ν. In a neighbourhood shape, each (abstract) node represents concrete graph nodes that have similar neighbourhood, up to some "radius" i. This i is also a parameter of the precision of neighbourhood shapes.

Neighbourhood shaping (*ie* abstracting into a neighbourhood shape) is always defined for graphs. That is, for any values of the parameters μ, ν and i, and for any graph G, there exists a neighbourhood shape with the corresponding precision that is a shape for G. This does not hold for shapes with abstraction morphisms: some shapes can be abstracted to a neighbourhood shape with a given precision, for other shapes it is not possible.

Hereafter, we define neighbourhood shaping for graphs and for shapes, describing the conditions for existence of the latter. For both, we first define the so-called *neighbourhood equivalence* over nodes and edges of a graph (resp. shape) on which the neighbourhood shaping is based.

Neighbourhood Shape for a Graph We start by defining a family of equivalence relations over the nodes of a graph that relate nodes having similar neighbourhoods, up to some "radius" i.

Definition 17 (Neighbourhood Equivalence). *Let G be a graph. For each natural i, the i* neighbourhood equivalence *relation $\equiv_i$ between nodes of G is recursively defined as:*

- $v \equiv_0 v'$ *if* $\mathsf{lab}_G(v) = \mathsf{lab}_G(v')$*;*
- $v \equiv_{i+1} v'$ *if* $v \equiv_i v'$*, and* $|v \bowtie^{\mathsf{a}} C|_\mu = |v' \bowtie^{\mathsf{a}} C|_\mu$*, and* $|C \bowtie^{\mathsf{a}} v|_\mu = |C \bowtie^{\mathsf{a}} v'|_\mu$ *for all label* a *in* Lab *and for all set of nodes* $C \in N / \equiv_i$*.*

The i-neigborhood equivalence relation is extended to edges of G by $e \equiv_i e'$ if $\mathsf{lab}(e) = \mathsf{lab}(e')$ and $\mathsf{src}(e) \equiv_i \mathsf{src}(e')$ and either (i) e, e' are binary edges and $\mathsf{tgt}(e) \equiv_i \mathsf{tgt}(e')$ or (ii) e, e' are edges with target $\bot$. ◀

We can now define the family of neighbourhood shapings. Two nodes are mapped to the same shape node if they are neighbourhood equivalent up to some radius. The grouping relation is also given by neighbourhood equivalence, but using a smaller radius.

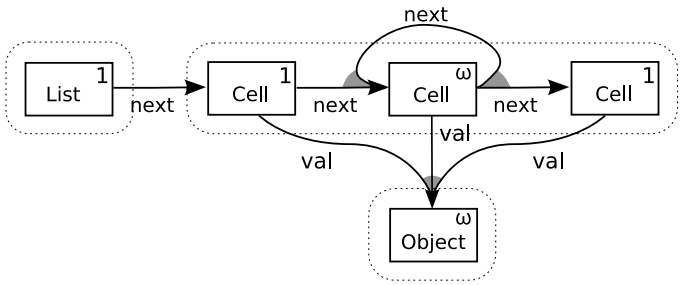


Figure 6. Level one neighbourhood shape of a list. All edge multiplicities are equal to one and are omitted.

Definition 18 (Neighbourhood Shape of a Graph, Neighbourhood Shaping of a Graph). *For any* $i \geq 1$*, the* level i neighbourhood shape of G *is* $shape(G, \equiv_{i-1}, \equiv_i)$ *and the* level i neighbourhood shaping of G *is* $shaping(G, \equiv_{i-1}, \equiv_i)$. ◀

In Figure 6 and Figure 7 are depicted respectively the level one and the level two neighbourhood shapes of the list from Figure 1, for $\mu = 1$ and $\nu = 1$. Defining the corresponding shaping morphisms is left to the reader.

The neighbourhood shape of a graph can not be dissociated from the graph because of its representation: nodes and edges of the shape are sets of nodes and sets of edges of the graph. This situation is not very convenient, we would like to be able to talk about neighbourhood shapes of graphs to designate their properties and not some particular representation, that is, to designate their isomorphism class. Thus, we overload the terms neighbourhood shape and neighbourhood shaping in the following way. In the sequel, we will use *the neighbourhood shape of the graph* G to designate the isomorphism class of the actual neighbourhood shape of G in the sense of Definition 18, and we will use *the neighbourhood shaping of the graph* G for shapings $s : G \to S$ such that $s = f \circ s'$, where $s' : G \to S'$ is the actual neighbourhood shape of G and $f : S' \to S$ is a shape isomorphism.

Neighbourhood Shape for a Shape

Definition 19 (Neighbourhood Equivalence for Shapes). *Let* $S = (G, \simeq, \mathsf{mult_n}, \mathsf{mult_{out}}, \mathsf{mult_{in}})$ *be a shape. For any* $i \geq 0$*, the binary relation* $\sim_i$ *over nodes of* S *is defined by:*

- $w \sim_0 w'$ *if* $\mathsf{lab}(v) = \mathsf{lab}(v')$*;*
- $w \sim_{i+1} w'$ *if* $w \sim_i w'$*,* $\simeq \subseteq \sim_i$ *and for all* $C \in N_S/\sim_i$*, and for all labels* a*,*

$$\sum_{K \in N_S/\simeq \mid K \subseteq C}^{\mu} \mathsf{mult_{out}}(w, \mathsf{a}, K) = \sum_{K \in N_S/\simeq \mid K \subseteq C}^{\mu} \mathsf{mult_{out}}(w', \mathsf{a}, K)$$

and analogously for incoming edges multiplicity function.

The relation $\sim_i$ *is extended to edges of* S *by:* $e \sim_i e'$ *if* $\mathsf{src}(e) \sim_i \mathsf{src}(e')$*,* $\mathsf{tgt}(e) \sim_i \mathsf{tgt}(e')$ *and* $\mathsf{lab}(e) = \mathsf{lab}(e')$. ◀

The requirement $\simeq \subseteq \sim_i$ intuitively says that the grouping relation should be "finer" in the sense of grouping less nodes, than the $\sim_i$ relation that we are trying to define. Note that this requirement $\simeq \subseteq \sim_i$ is necessary, as it ensures that any $K \in N_S/\simeq$ is a subset of some $C \in N_S/\sim_i$. If

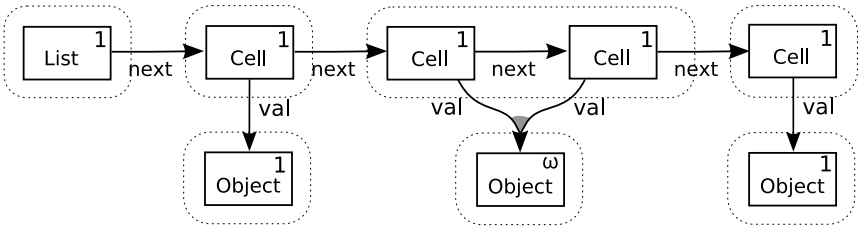


Figure 7. Level two neighbourhood shape of a list with four cells. All edge multiplicities are equal to one and are omitted.

this requirement is not fulfilled, then the sums in the definition above are not defined. In this case, the relations $\sim_j$ for any $j > i$ are empty. The following Example 20 illustrates the impossibility of defining a neighbourhood shaping relation when this requirement is not fulfilled.

Example 20. Consider the shape depicted on Figure 8, and let us try to compute $\sim_1$, the level one neighbourhood relation on the nodes of the shape. We have $[\text{v1}]_{\sim_0} = [\text{v2}]_{\sim_0} = \{\text{v1}, \text{v2}\}$ and $[\text{v3}]_{\sim_0} = [\text{v4}]_{\sim_0} = \{\text{v3}, \text{v4}\}$. Clearly, $\simeq \not\subseteq \sim_0$. For testing whether v3 $\sim_1$ v4, we need to know whether the number of outgoing c-edges from v3 to nodes in $\{\text{v1}, \text{v2}\}$ is the same as for v3. But this information is not given by the shape, as we only know that v3 has ω outgoing c-edges that may go either to the group $\{\text{v1}, \text{v2}\}$ or to the group $\{\text{v3}, \text{v4}\}$.

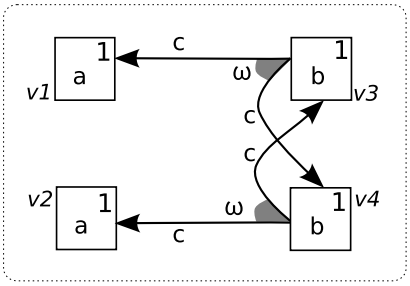


Figure 8. A shape with $\mu = 1$ and $\nu = 1$. All omitted edge multiplicities are equal to one. v1 . . . v4 are node identities.

Lemma 21. *Let S be a shape and $i \geq 1$. If the relation $\sim_i$ over the nodes of S is not empty, then $\sim_i$ is an equivalence relation.*

Proof. By definition of $\sim_i$, $\sim_i$ is empty if and only if $\simeq \not\subseteq \sim_{i-1}$. Now, if $\simeq \subseteq \sim_{i-1}$, then it is easy to see that $\sim_i$ is symmetric, reflexive and transitive. □

Definition 22 (Neighbourhood Shape of a Shape, Neighbourhood Shaping of a Shape). *Let S be a shape and $i \geq 1$. If the relation $\sim_i$ over the nodes of S is not empty, let T be the shape defined by:*

- *nodes are T are $[v]_{\sim_i}$ for v node of N_S;*
- *edges of T are $[e]_{\sim_i}$ for e edge of E_S;*

– *for any edge* $e' = [e]_{\sim_i}$ *in* E_T *(for* $s \in E_S$*),* $\mathsf{src}_T(e') = [\mathsf{src}_S(e)]_{\sim_i}$, $\mathsf{tgt}_T(e') = [\mathsf{tgt}_S(e)]_{\sim_i}$ *and* $\mathsf{lab}_T(e') = \mathsf{lab}_S(e)$*. By definition of* $\sim_i$ *these are well defined;*
– $\simeq_T = \sim_{i-1}$*;*
– *for any* $w \in N_T$*,*

$$\mathsf{mult}_{\mathrm{n},T}(w) = \sum_{v \in N_S \mid [v]_{\sim_i} = w}^{\nu} \mathsf{mult}_{\mathrm{n},S}(v)$$

;
– *for any* $w \in N_T$*, any label* a *and any* $C \in N_T/\simeq_T$*,*

$$\mathsf{mult}_{\mathrm{out},T}(w, \mathsf{a}, C) = \sum_{K \in N_S/\simeq \mid K \subseteq C}^{\mu} \mathsf{mult}_{\mathrm{out}}(w, \mathsf{a}, K)$$

and similarly for incoming edges multiplicities.

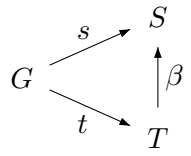
Then T *is called the* level i neighbourhood shape of S. ◀

Note that the edge multiplicity functions are well defined by definition of $\sim_i$.

We terminate the section by two properties of neighbourhood shapes and neighbourhood shapings that well be used in Section 6.

Lemma 23 (Composition of neighbourhood shapings). *Let* G *be a graph,* S, T *be shapes,* $s : G \to S$*,* $t : G \to T$ *be shaping morphisms, and* $\beta : T \to S$ *be an abstraction morphism such that* $s = \beta \circ t$*. Then for all* i *the following hold.*

1. *If* s *is the level* i *neighbourhood shaping of* G*, then* β *is the level* i *neighbourhood shaping of* T*.*
2. *If* β *is the level* i *neighbourhood shaping of* T*, then* s *the level* i *neighbourhood shaping of* G*.*



Proof. See Appendix B

Lemma 24 (Common concretisation implies isomorphism). *If two neighbourhood shapes have a common concretisation, then they are isomorphic.*

Proof. The proof of the lemma uses the canonical representation of neighbourhood shapes, defined in Section 4. Thus, we give it in Appendix C.

4 Canonical Shapes

Canonical shapes are a special class of shapes that includes neighbourhood shapes. More precisely, it is composed of neighbourhood shapes, and of shapes that do not admit concretisations. Canonical shapes have so called "canonical" representation which is a representation of isomorphism classes of such shapes. This in particular allows to define a normalised representation of (isomorphism classes of) neighbourhood shapes. Moreover, for each shaping precision (*ie* values for μ, ν and the neighbourhood radius i), the number of canonical shapes is finite. Additionally, it is decidable whether a shape is (isomorphic to a) canonical shape, and in this case its canonical representation can be computed. All these properties make canonical shapes a good over-approximation of the set of neighbourhood shapes.

4.1 Canonical Names

In this section, we introduce the notion of a *canonical name*. Each equivalence class with respect to a neighbourhood equivalence is uniquely identified by such a name. For example, each equivalence class with respect to $\equiv_0$ contains only nodes having the same labels and is identified by this set of labels. It becomes the canonical name of this equivalence class. Each equivalence relation $\equiv_i$ comes with a set NCan^i of canonical names. As we will see, a neighbourhood shape can be viewed as a graph whose nodes and edges are canonical names. The notion of a canonical name occurs frequently in literature, for example in [15].

Definition 25 (Canonical Name). *The set of* level i node canonical names, NCan^i*, is defined inductively for* $i \geq 0$*:*

$$\begin{aligned}\mathsf{NCan}^0 &= 2^{\mathsf{Lab}}\\ \mathsf{NCan}^{i+1} &= \mathsf{NCan}^i \times (\mathsf{NCan}^i \times \mathsf{Lab} \to \mathbf{M}_\mu) \times (\mathsf{NCan}^i \times \mathsf{Lab} \to \mathbf{M}_\mu).\end{aligned}$$

The set ECan^i *of* level i edge canonical names *is* $\mathsf{ECan}^i = \mathsf{NCan}^i \times \mathsf{Lab} \times \mathsf{NCan}^i$.

Let G be a graph. The mapping name^i_G *maps nodes and edges of G to their level i canonical name as follows. For v node of G,* $\mathsf{name}^0_G(v) = \mathsf{lab}_G(v)$*, and* $\mathsf{name}^{i+1}_G(v) = (\mathsf{name}^i_G(v), \mathit{out}, \mathit{in})$ *where for each canonical name C in* NCan^i *and for each label* a *in* Lab *(N_C stands for the set of nodes v' such that* $\mathsf{name}^i_G(v') = C$*),*

$$\mathit{out}(C, \mathsf{a}) = |v \rhd\!\!\rhd^{\mathsf{a}}_G N_C|_\mu \qquad\qquad \mathit{in}(C, \mathsf{a}) = |N_C \rhd\!\!\rhd^{\mathsf{a}}_G v|_\mu .$$

For e edge of G, $\mathsf{name}^i_G(e) = (\mathsf{name}^i_G(\mathsf{src}(e)), \mathsf{lab}(e), \mathsf{name}^i_G(\mathsf{tgt}(e)))$. ◀

Example 26. Consider the level zero node canonical name $C_0 = \{\mathsf{c}, \mathsf{d}\}$ and the level one node canonical name $C_1 = (\{\mathsf{a}\}, \mathbf{0}, \mathit{in})$, where $\mathbf{0}$ indicates the constant function associating 0 to all elements of its domain, and $\mathit{in}(C_0, \mathsf{b}) = 1$, and $\mathit{in}(C', x) = 0$ for all $C' \neq C_0$ and all $x \neq \mathsf{a}$. C_0 is the class of nodes labelled c and d. C_1 is the class of nodes labelled a that have one incoming b-edge from a node labelled c and d and *no more* adjacent nodes. ◀

Note that the number of level i canonical names is exponentially growing in i. However, for any i, this number is bounded in terms of the number of atomic propositions and μ

Note 27. For any $i \geq 0$, the sets of level i node canonical names and edge canonical names are finite. ◀

The number of different canonical names is growing super-exponentially in i, that is, $|\mathsf{NCan}^i| \geq {}^i m = \underbrace{m^{m^{\cdots^m}}}_{i}$, where $m = \mu + 2$. We are convinced that in practical cases the number of used different canonical names would not reach this upper bound.

4.2 Canonical Representation of Neighbourhood Shapes

There is a quite clear relation between canonical names and the neighbourhood equivalence relation: two nodes (resp. edges) in a graph are i-neigborhood equivalent if, and only if, they have the same level i canonical names. Next lemma easily follows from the definitions, thus we present it without proof.

Lemma 28. *For any $i \geq 0$, any graph G, any two nodes v, v' of G and any two edges e, e' of G, $v \equiv_i v'$ if, and only if, $\mathsf{name}^i_G(v) = \mathsf{name}^i_G(v')$, and $e \equiv_i e'$ if, and only if, $\mathsf{name}^i_G(e) = \mathsf{name}^i_G(e')$.* □

In what follows we will show that this correspondence gives rise to a canonical representation of neighbourhood shapes. We will first introduce the actual representation, and then show that it is canonical, in the sense of unique (up to shape isomorphism).

Let G be a graph. Consider the triple $\mathcal{C}_G = (\mathsf{name}^i(N_G), \mathsf{name}^i(E_G), \mathsf{mult})$, where $\mathsf{name}^i(N_G)$ and $\mathsf{name}^i(E_G)$ are the sets of node and edge level i canonical names of the graph G, respectively, and $\mathsf{mult} : \mathsf{name}^i(N_G) \to \mathbf{M}^+_\nu$ is the function defined by $\mathsf{mult}(C) = \left|\{v \in N_G \mid \mathsf{name}^i_G(v) = C\}\right|_\nu$ for all $C \in \mathsf{name}^i(N_G)$. We will show that $\mathcal{C}_G$ is a canonical representation of the isomorphism class of the level i neighbourhood shape of G. This will provide us with a representation of neighbourhood shapes that is independent on the graphs they were computed from.

Lemma 29 (Canonical Representation). *Let G, H be graphs, and let $i \geq 1$. The level i neighbourhood shapes of G and H are isomorphic if, and only if, $\mathcal{C}_G$ and $\mathcal{C}_H$ are equal.*

By $\mathcal{C}_G$ and $\mathcal{C}_H$ are equal, we mean component-wise equality, that is, equality of the sets of node and edge canonical names and equality of the node multiplicity functions that define them.

Proof. The proof is given in Appendix D. It uses results that will be introduced later, namely relationship between the neighbourhood shaping and the modal logic defined in Section 7.

Thus, by Lemma 29 we know that any isomorphism class of level i neighbourhood shapes has a canonical representation of the form $(\mathcal{N}, \mathcal{E}, \mathsf{mult})$, where $\mathcal{N} \subseteq \mathsf{NCan}^i$, $\mathcal{E} \subseteq \mathsf{ECan}^i$, and $\mathsf{mult} : \mathcal{N} \to \nu$. Then the question arises what is the relationship between triples from $(\mathcal{N}, \mathcal{E}, \mathsf{mult})$ and neighbourhood shapes. This is studied in the next section.

4.3 Canonical Shapes

We denote $\mathcal{CS}^i_*$ the set of triples $\wp(\mathsf{NCan}^i) \times \wp(\mathsf{ECan}^i) \times (\mathsf{NCan}^i \rightharpoonup \mathbf{M}^+_\nu)$ such that for any $(\mathcal{N}, \mathcal{E}, \mathsf{mult}) \in \mathcal{CS}^i_*$, $dom(\mathsf{mult}) = \mathcal{N}$. We will see that some elements of $\mathcal{CS}^i_*$ define shapes. It is decidable to know for a given $\mathcal{C} \in \mathcal{CS}^i_*$ whether it defines a shape. Moreover, some elements of $\mathcal{CS}^i_*$ define neighbourhood shapes, but we think that it is not decidable to know whether an element of $\mathcal{CS}^i_*$ defines a neighbourhood shape. However, we give a syntactic definition of a subset of $\mathcal{CS}^i_*$ which contains all neighbourhood shapes.

From Canonical Names to Shapes Let $(\mathcal{N}, \mathcal{E}, \mathsf{mult}) \in \mathcal{CS}^i_*$, and consider the structure $S = ((\mathcal{N}, \mathcal{E}, \mathsf{src}, \mathsf{tgt}, \mathsf{lab}), \simeq, \mathsf{mult}_\mathsf{n}, \mathsf{mult}_\mathsf{out}, \mathsf{mult}_\mathsf{in})$, where $\mathsf{src}, \mathsf{tgt} : \mathcal{E} \to \mathsf{NCan}^i$, $\mathsf{lab} : \mathcal{E} \to \mathsf{Lab}$, $\simeq$ is an equivalence relation in $\mathcal{N}$, $\mathsf{mult}_\mathsf{n} : \mathcal{N} \to \mathbf{M}^+_\nu$, and $\mathsf{mult}_\mathsf{out}, \mathsf{mult}_\mathsf{in} : \mathcal{N} \times Lab \times \mathcal{N}/{\simeq} \to \mathbf{M}_\mu$ defined by:

- for any $e = (C, \mathsf{a}, C')$ in $\mathcal{E}$, $\mathsf{src}_S(e) = C$, $\mathsf{tgt}_S(e) = C'$ and $\mathsf{lab}_S(e) = \mathsf{a}$;
- $\simeq$ is the smallest equivalence relation such that $C \simeq C'$ if C and C' have the same first component. Remind that C and C' are level i node canonical names and their first component is a level $i-1$ canonical name;
- $\mathsf{mult}_\mathsf{n} = \mathsf{mult}$;
- for all $C \in N_S$, $\mathsf{a} \in \mathsf{Lab}$, and $K \in \mathsf{NCan}^{i-1}$, $\mathsf{mult}_\mathsf{out}(C, \mathsf{a}, K) = \mathit{out}_C(K, \mathsf{a})$, where out_C is the function second component of C (remind that C is a level i canonical name and $\mathit{out}_C : \mathsf{NCan}^{i-1} \times \mathsf{Lab} \to \mu$);

– for all $C \in N_S$, $\mathsf{a} \in \mathsf{Lab}$, and $K \in \mathsf{NCan}^{i-1}$, $\mathsf{mult}_{\text{out}}(C, \mathsf{a}, K) = \mathit{in}_C(K, \mathsf{a})$, where in_C is the function third component of C.

The following lemma identifies the conditions on $(\mathcal{N}, \mathcal{E}, \mathsf{mult})$ under which S is a shape.

Lemma 30. *If*

1. $\mathcal{E} \subseteq \mathcal{N} \times \mathsf{Lab} \times \mathcal{N}$*, and*
2. *for all* $C \in \mathcal{N}$*, all* K *in* NCan^{i-1} *and all label* a*,* $\mathit{out}_C(K, \mathsf{a}) = 0$ *if, and only if,* $\{(C, \mathsf{a}, C') \in \mathcal{E} \mid \pi_1(C') = K\} = \varnothing$ *(where* $\pi_1(C')$ *denotes the first component of* C'*), and similarly for* in_C*.*

then S *is a shape.*

Proof. The first condition ensures that $(\mathcal{N}, \mathcal{E}, \mathsf{src}, \mathsf{tgt}, \mathsf{lab})$ is a graph, and the second condition ensures that the edge multiplicity functions of S are consistent with its graph structure, *ie* edge multiplicity is positive if, and only if, there are indeed edges to which it corresponds. □

For $\mathcal{C} \in \mathcal{CS}^i_*$ satisfying the condition from Lemma 30, we denote $S_{\mathcal{C}}$ the corresponding shape.

We have now a characterisation of elements of $\mathcal{CS}^i_*$ that define shapes. In what follows we will give some characteristics of elements of $\mathcal{CS}^i_*$ that represent neighbourhood shapes.

Definition 31 (Canonical shape). *A* level i canonical shape *is a shape of the form* $S_{\mathcal{C}}$*, for* $\mathcal{C} \in \mathcal{CS}^i_*$*, and such that* $S_{\mathcal{C}}$ *is (isomorphic to) its own level* i *neighbourhood shape.*

We denote $\mathcal{CS}^i$ the set of level i canonical shapes. Canonical shapes will be usually represented as elements of $\mathcal{CS}^i_*$, *ie* triples composed of a set of node canonical names, a set of edge canonical names, and a multiplicity function. This is called their *canonical representation*.

Lemma 32 (Relationship between Neighbourhood Shapes and Canonical Shapes). *The following two are equivalent, for all level* i *canonical shape* $\mathcal{C}$*:*

1. *The shape* $S_{\mathcal{C}}$ *is isomorphic to the neighbourhood shape of some graph* G*.*
2. *The shape* $S_{\mathcal{C}}$ *admits concretisations.*

Proof. The implication $1 \Rightarrow 2$ is immediate from the definitions. For the implications $2 \Rightarrow 1$, let $\beta : S_{\mathcal{C}} \to S_{\mathcal{C}}$ be the level i neighbourhood shaping of $S_{\mathcal{C}}$. By hypothesis, we know that there exists a graph G and a shaping $s : G \to S_S$. Then, by Proposition 13 we know that $\beta \circ s$ is a shaping, and by Lemma 23 we deduce that $\beta \circ s$ is the level i neighbourhood shaping of G.

That is, shapes that can be obtained by neighbourhood shaping are exactly canonical shapes that admit concretisations, up to isomorphism. In the following, we will be interested at the set $\mathcal{CS}^i$ as a superset of the set of level i neighbourhood shapes.

We do not know whether it is decidable to check if a canonical shape is a neighbourhood shape. Note that according to Lemma 32 it falls to decide whether a canonical shape admits concretisations.

Conjecture 33. It is not decidable whether a shape admits concretisations.

Even if this conjecture is confirmed, it still does not answer the previous question of decidability whether a canonical shape admits concretisations. Our intuition is that the conjecture also holds for canonical shapes.

Remark 34 (On Isomorphism of Canonical Shapes). We do not know whether two canonical shapes can be isomorphic without having the same node and edge sets. However, if it could happen, let's say $\mathcal{C}$ and $\mathcal{C}'$ are isomorphic but do not have the same node and edge sets, then necessarily $\mathcal{C}$ and $\mathcal{C}'$ are not neighbourhood shapes (*ie* do not have concretisations). Indeed, by Lemma 15, two shapes are isomorphic if, and only if, they have the same concretisations and, by definition, the canonical representation of a neighbourhood shape is unique for its entire isomorphism class.

5 Shape Transformations

In this section we define transformations of shapes. We also establish how transformations of shapes are related to transformations of their concretisations. Finally, we discuss on properties of transformations of neighbourhood shapes.

5.1 Transformations of Shapes

Definition 35 (pre-matching). *Let L be a graph and S be a shape. A* pre-matching *p of L into S is a graph morphism $p : L \to G_S$ such that:*

1. *for all node w in $p(L)$, $\mathsf{mult}_{\mathrm{n},w} \geq \left|p^{-1}(w)\right|_\nu$,*
2. *for all edge e in $p(L)$ with source node w, target node w' and label a, it holds $\mathsf{mult}_{\mathrm{out},S}(w, \mathsf{a}, [w']_{\simeq_S}) \geq \left|p^{-1}(e)\right|_\nu$ and $\mathsf{mult}_{\mathrm{in},S}(w', \mathsf{a}, [w]_{\simeq_S}) \geq \left|p^{-1}(e)\right|_\nu$.*

A pre-matching p is called concrete *if p is an injective morphism and additionally satisfies the following properties :*

3. *for all node v in $p(N_L)$, $\mathsf{mult}_{\mathrm{n},S}(v) = 1$;*
4. *for all node v in $p(N_L)$, the equivalence class $[v]_{\simeq_S}$ is the singleton set $\{v\}$.*
5. *for all nodes v, w in $p(N_L)$ and for all label a, $\mathsf{mult}_{\mathrm{out}}(v, \mathsf{a}, \{w\}) = \left|v \bowtie\!\!\rhd^{\mathsf{a}}_{G_S} w\right|_\mu = \mathsf{mult}_{\mathrm{in}}(v, \mathsf{a}, \{w\})$.*

As shown in the next lemma, the existence of a concrete pre-matching $p : L \to S$ guarantees the existence of a matching $m : L \to G$ for some graphs G concretisations of S. A concrete pre-matching p is a pre-matching whose image can be considered as a concrete "subgraph" of the shape. That is, nodes in the image of p are concrete nodes, *ie* with multiplicity one. Let us explain in more detail what the conditions on edges and edge multiplicities are meant for. First, Condition 2 guarantees that the actual number of edges can indeed exist in some concretisation, so that an injective morphism from L into this concretisation can be constructed. Injectiveness of p guarantees that there are at least as many edges present from v to w in G_S as there are edges from $p^{-1}(v)$ to $p^{-1}(w)$ in L (this for all label a). Finally, Condition 5 guarantees that the actual number of edges present from v to w in G_S is the same that what is required by edge multiplicities. This of course is underspecified if $\mathsf{mult}_{\mathrm{out}}(v, \mathsf{a}, \{w\}) = \omega$, in which case any number of edges greater or equal to $\mu+1$ is correct as soon as this number is greater or equal to $(p^{-1}(v)) \bowtie\!\!\rhd^{\mathsf{a}}_L (p^{-1}(w))$ so that it guarantees injectiveness. This underspecified number of edges plays a role in the definition of a concrete shape transformation.

Lemma 36. *If $c : L \to S$ is a concrete pre-matching from the graph L to the shape S, then for any graph G concretisation of S with* injective *shaping $s : G \to S$, there exists an injective morphism $m : L \to G$ such that $c = s \circ m$.*

Proof. Let G be a concretisation of S with corresponding injective shaping $s : G \to S$. Remark first that for any $x \in N_L \cup E_L$ node or edge of L, $s^{-1}(c(x))$ is a singleton set. This fact is easily shown using that c is a concrete pre-matching and that s is a shaping. Consider now the mapping $m : N_L \cup E_L \to N_G \cup E_G$ defined by $m(x) = y$ where y is the unique element of $s^{-1}(c(x))$. Thus, $c = s \circ m$. The fact that m is a morphism follows from the fact that s and c are morphisms, and injectiveness of m follows from injectiveness of c and injectiveness of s. □

Definition 37 (concrete shape transformation). *Let $P = (L, R)$ be a transformation rule and S be a disjoint shape, and let c be a concrete pre-matching from L into S satisfying the following dangling edges condition: for all edge e of S, if $\mathsf{src}(e) \in c(N^{\text{del}})$ or $\mathsf{tgt}(e) \in c(N^{\text{del}})$, then $e \in c(E^{\text{del}})$. Then the transformation of S according to P and c is the shape T defined by:*

- *the graph part of T, is the graph G_T such that $G_S \xrightarrow{P,c} G_T$;*
- *the grouping relation $\simeq_T$ is defined by*
  - *for all $v \in N_S \cap N_T$, $[v]_{\simeq_T} = [v]_{\simeq_S}$;*
  - *for all $v \in N^{\text{new}}$, $[v]_{\simeq_T} = \{v\}$;*
- *the node-multiplicity function of T is given by: for all $v \in N_T$,*

$$\mathsf{mult}_{\text{n},T}(v) = \begin{cases} \mathsf{mult}_{\text{n},S}(v) & \text{if } v \in N_S \cap N_T \\ 1 & \text{if } v \in N^{\text{new}}; \end{cases}$$

- *the outgoing edges multiplicity function of T is given by: let $N_{concr} = c(N^{\text{use}}) \cup N^{\text{new}}$ and $N_{abstr} = N_T \setminus c(N^{\text{use}})$; thus N_{concr} and N_{abstr} are disjoint, $N_T = N_{concr} \cup N_{abstr}$ and $N_S \cap N_T = N_{abstr} \cup c(N^{\text{use}})$. Then, for all $v \in N_T$, $\mathsf{a} \in \mathsf{Lab}$, $C \in N_T/\simeq_T$,*

$$\mathsf{mult}_{\text{out},T}(v, \mathsf{a}, C) = \begin{cases} \left| v \rhd\!\!\rhd^{\mathsf{a}}_{G_T} C \right|_{\mu} & \text{if } v \in N_{concr} \text{ and } C \subseteq N_{concr}, \\ \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, C) & \text{if } v \in N_{abstr} \text{ and } C \subseteq N_{abstr}, \\ \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, C) & \text{if } v \in N_{abstr} \text{ and } C \subseteq c(N^{\text{use}}) \text{ or } v \in c(N^{\text{use}}) \text{ and } C \subseteq N_{abstr}, \\ 0 & \text{otherwise;} \end{cases}$$

- *the incoming edges multiplicity function of T is given by: for all $v \in N_T$, $\mathsf{a} \in \mathsf{Lab}$, $C \in N_T/\simeq_T$,*

$$\mathsf{mult}_{\text{in},T}(v, \mathsf{a}, C) = \begin{cases} \left| C \rhd\!\!\rhd^{\mathsf{a}}_{G_T} v \right|_{\mu} & \text{if } v \in N_{concr} \text{ and } C \subseteq N_{concr}, \\ \mathsf{mult}_{\text{in},S}(v, \mathsf{a}, C) & \text{if } v \in N_{abstr} \text{ and } C \subseteq N_{abstr}, \\ \mathsf{mult}_{\text{in},S}(v, \mathsf{a}, C) & \text{if } v \in N_{abstr} \text{ and } C \subseteq c(N^{\text{use}}) \text{ or } v \in c(N^{\text{use}}) \text{ and } C \subseteq N_{abstr}, \\ 0 & \text{otherwise.} \end{cases}$$

We write then $S \xrightarrow{P,c} T$. ◀

In Definition 37 we make some explicit assumptions on the sets C used in the definitions of the edge multiplicity functions of T. Let us show that these assumptions hold and thus T is well defined.

The first assumption is that for all $C \in N_T/\simeq_T$ we have $C =\subseteq N_{\text{concr}}$ or $C \subseteq N_{\text{abstr}}$, or $C \subseteq c(N^{\text{use}})$. Let us show that for all v node of T, $[v]_{\simeq_T}$ is a subset of one of the sets N_{abstr}, N^{new} or $c(N^{\text{use}})$. It is sufficient as, by definition, $N_{\text{concr}} = N^{\text{new}} \cup c(N^{\text{use}})$. If $v \in c(N^{\text{use}})$, by hypothesis c being a concrete pre-shaping, we know that $[v]_{\simeq_S} = \{v\}$, and by definition of $\simeq_T$, $[v]_{\simeq_T} = [v]_{\simeq_S}$. If $v \in N^{\text{new}}$, then, by definition of $\simeq_T$ we know that $[v]_{\simeq_T} = \{v\}$. Finally, if $v \in N_{\text{abstr}}$, by definition

of $\simeq_T$ we have $[v]_{\simeq_T} = [v]_{\simeq_S} \subseteq N_S$. Moreover, as stated previously, we know that $v \not\simeq_S w$ for all $w \in c(N^{\text{new}})$, thus $[v]_{\simeq_T} \subseteq N_S \cap c(N^{\text{new}}) = N_{\text{abstr}}$.

The second assumption we make is that whenever $C \subseteq N_{\text{abstr}}$ or $C \subseteq c(N^{\text{use}})$, C is also a set in $N_S / \simeq_S$ (as it is used as argument of the edge multiplicity functions of S). It is the case because of the definition of $\simeq_T$, and reminding that $N_S \cap N_T = N_{\text{abstr}} \cup c(N^{\text{use}})$.

Another point to be clarified in Definition 37 is the definition of the value of $\mathsf{mult}_{\text{out},T}(v, a, C)$ when $v \in N_{\text{concr}}$ and $C = \{w\} \subseteq N_{\text{concr}}$ (the same for incoming edges multiplicity). This value is defined as the number of edges actually present in the shape (up to μ), and not as some computation involving edge multiplicity functions of S, as one may expect. This in particular means that the shape T is not uniquely defined, and depends on the representation of the graph part of S. However, this non determinism is intended, and guarantees correctness of concrete shape transformation with respect to the corresponding graph transformations when deletion of edges is involved. Consider nodes v, w in $c(N^{\text{use}})$ and label a with $\mathsf{mult}_{\text{out},S}(v, \mathsf{a}, \{w\}) = \mathsf{mult}_{\text{in},S}(v, \mathsf{a}, \{w\}) = \omega$, and suppose that the rule P specifies the deletion of k a-labelled edges between these nodes. Then T has $\omega - k$ a-labelled edges from v to w, and of course this is not uniquely specified, as there may be several multiplicities $\lambda \in \mathbf{M}_\mu$ such that $\lambda + k = \omega$.

Definition 38 (Abstract Shape Transformation). *Let $P = (L, R)$ be a transformation rule, S be a shape and $f : L \to S$ be a pre-matching. We say that S* abstractly transforms into *T* according to *P* and *c, and we write $S \overset{(P,f)}{\rightsquigarrow} T$, whenever there exists a shape S', an abstraction morphism $\beta : S' \to S$ and a concrete pre-matching $c : L \to S'$ such that $f = \beta \circ c$, and there exists an abstraction morphism $\beta' : T' \to T$, where T' is the shape such that $S' \overset{(P,c)}{\longrightarrow} T'$.*

5.2 Properties of Shape Transformations

We consider a fixed natural $i \geq 1$. When we talk about neighbourhood shape and neighbourhood shaping, we mean level i neighbourhood shape and level i neighbourhood shaping.

Theorem 39 (A concrete transformation is captured by some abstract one). *Let $P = (L, R)$ be a transformation rule, G, H be graphs and $m : L \to G$ be a matching such that $G \overset{(P,m)}{\longrightarrow} H$. For any shape S and shaping $s : G \to S$ such that $s \circ m$ is a concrete pre-matching, there exists a shaping morphism $t : H \to T$, where T is the shape such that $S \overset{(P,s\circ m)}{\longrightarrow} T$.*

Proof. Consider the morphism $t : H \to T$ defined by $t(x) = s(x)$ for all x node or edge of G, and $t(x) = x$ for all x in $N^{\text{new}} \cup E^{\text{new}}$. (It is immediate to see from the definitions of graph transformation and concrete shape transformation that t is indeed a morphism). We show that t is a shaping morphism. As in the definition of a concrete shape transformation, we distinguish the sets of nodes N_{concr} and N_{abstr} in T, and let H' be the full[4] sub-graph of H with nodes $N_G \setminus m(L)$. By definition, t coincides with s on H' and t maps nodes of H' to nodes in N_{abstr} and edges of H' to edges whose two ends are in N_{abstr}. Also, H' is a full sub-graph of G. Thus, the multiplicity functions of T satisfy the requirements of a shaping when their domain is restricted to N_{abstr}. For the node multiplicity function for nodes $w \in N_{\text{concr}}$, we know by definition $\mathsf{mult}_{\text{n},T}(w) = \mathsf{mult}_{\text{n},S}(w) = 1$ and that $t^{-1}(w)$ is a singleton set. For the edge multiplicity function $\mathsf{mult}_{\text{out},T}(w, \mathsf{a}, C)$ (we consider only $\mathsf{mult}_{\text{out},T}$, by symmetry the same holds for $\mathsf{mult}_{\text{in},T}$), we distinguish two cases: (i) w and C are not both in N_{concr}, and (ii) w and C are both in N_{concr}. For (i), once again pre-images of w and C coincide for t and s, and also

[4] By full sub-graph we mean a sub-graph defined by a subset of the nodes and *a*ll connecting edges.

the value of $\mathsf{mult}_{\text{out},T}$ and $\mathsf{mult}_{\text{out},S}$. For (ii), remind that C is a singleton set, $\mathsf{mult}_{\text{out},T}(w, \mathsf{a}, C)$ is the actual number of edges in the graph G_T (up to μ), and by definition t is an isomorphism in this concrete part. □

Theorem 40 (A concrete transformation is captured by canonical abstract transformation). *Let $P = (L, R)$ be a transformation rule, G, H be graphs and $m : L \to G$ be a matching such that $G \overset{(P,m)}{\longrightarrow} H$. Let S be the neighbourhood shape of G with corresponding shaping morphism $s : G \to S$, and let T be the neighbourhood shape of H with corresponding neighbourhood shaping $t : H \to T$. Then $S \overset{(P,f)}{\rightsquigarrow} T$ for some pre-matching f.*

Proof. By definition of abstract shape transformation, we need to show that there exist a pre-matching $f : L \to S$, a shape S', an abstraction morphism $\beta : S' \to S$, and a concrete pre-matching $c : L \to S'$ such that $f = \beta \circ c$, and there exists an abstraction morphism $\beta' : T' \to T$, where T' is the shape such that $S' \overset{(P,c)}{\longrightarrow} T'$. Take S' the trivial shape of G, T' the trivial shape of H, $\beta = s$, $\beta' = t$, $c = m$ and $f = s \circ m$. Then the required conditions are satisfied by hypothesis. □

Theorem 41 (Concrete shape transformation vs. graph transformation). *Let $P = (L, R)$ be a production rule, S be a shape and $c : L \to S$ be a concrete pre-matching satisfying the dangling edge condition. For any graph G concretisation of S with shaping $s : G \to S$, there exists a matching $m : L \to G$ such that $c = s \circ m$ and if H is the graph such that $G \overset{P,m}{\longrightarrow} H$, then there exists a shaping $t : H \to T$, where T is the shape obtained by $S \overset{P,c}{\longrightarrow} T$.*

Proof. The injective morphism $m : L \to G$ exists due to Lemma 36. We can define $m(v) = s^{-1} \circ c(v)$, because s is injective on the image of c. (As a proof assume $v_1, v_2 \in N_G$ s.t. $s(v_1) = s(v_2)$ for some $v \in V_L$ with $c(v) = s(v_1)$. By definition of a shape, we obtain $\mathsf{mult}_{\text{n},S}(s(v_1)) = 1$ and thus $\left|s^{-1}(v_1)\right| = 1$ and $v_1 = v_2$.)

Let H be such that $G \overset{P,m}{\longrightarrow} H$. Define the mapping $t : H \to T$ defined by

$$t(v) = \begin{cases} v & \text{if } v \in N^{\text{new}} \\ s(v) & \textit{otherwise} \end{cases}$$

and analogously on E_H. Mapping t is well-defined, because, by the definition of transformation, $N_H = (N_G \setminus m(N^{\text{del}})) \cup N^{\text{new}}$, and s is defined on N_G. We need to show, that t is a shaping, that is:

1. t is a morphism from H to T
2. for all $v \in N_T$ holds $\mathsf{mult}_{\text{n},T}(v) = \left|t^{-1}(v)\right|_\nu$
3. for all $w \in N_T$, for all $\mathsf{a} \in \mathsf{Lab}$, for all $C \in N_T/{\simeq_T}$, and for all $v \in t^{-1}(w)$,

$$\mathsf{mult}_{\text{out},T}(w, \mathsf{a}, C) = \left|v \rhd\!\!\rhd^{\mathsf{a}}_H (t^{-1}(C))\right|_\mu$$

and analogously for incoming edges multiplicities.

ad 1. First, we show that $t(N_H) \subseteq N_T$. Assume $t(v) = v' \in t(N_H)$. There are two cases. If $v' \in N^{\text{new}}$, then $v' = v \in N^{\text{new}} \subseteq N_T$. Otherwise, $v' = s(v)$ for $v \in N_G \setminus s^{-1}(c(N^{\text{del}}))$ $(\star)$. Assume $v' \notin N_T$ but $v' \in s(N_G)$. As v' is not new, it must be the case, due to the definition of $N_T = (N_S \setminus c(N^{\text{del}}) \cup N^{\text{new}})$, that $v' \in c(N^{\text{del}})$. Hence, $v \in s^{-1}(c(N^{\text{del}}))$ contradicting $(\star)$. The case for edges is similar.

As a next step, we will prove that $t(\mathsf{src}_H(e)) = \mathsf{src}_T(t(e))$ for an arbitrary edge $e \in E_H$. First, assume $\mathsf{src}_H(e) \in N^{\text{new}}$ implying $e \in E^{\text{new}}$. We compute

$$\begin{aligned} t(\mathsf{src}_H(e)) &= \mathsf{src}_H(e) && \text{(Def. of } t\text{)} \\ &= \mathsf{src}_R(e) && \text{(Def. transformation and } \mathsf{src}_R(e) \text{ is new)} \\ &= \mathsf{src}_T(e) && \text{(Def. shape transformation)} \\ &= \mathsf{src}_T(t(e)) && \text{(Def. of } t\text{)} \end{aligned}$$

In the second case, we have $\mathsf{src}_H(e) \notin N^{\text{new}}$, that is $t(\mathsf{src}_H(e)) = s(\mathsf{src}_H(e))$ yielding another two cases depending on whether or not $e \in E^{\text{new}}$. If e is not new, we have

$$\begin{aligned} s(\mathsf{src}_H(e) &= s(\mathsf{src}_G(e)) \\ &= \mathsf{src}_S(s(e)) && (s \text{ morphism}) \\ &= \mathsf{src}_T(s(e)) && \text{(Def. transformation)} \\ &= \mathsf{src}_T(t(e)) && \text{(Def. of } t\text{)} \end{aligned}$$

If e is new, we have instead

$$\begin{aligned} s(\mathsf{src}_H(e)) &= s(\mathsf{src}_G(e)) \\ &= \mathsf{src}_S(s(e)) \\ &= \mathsf{src}_T(s(e)) \\ &= \mathsf{src}_T(t(e)) \end{aligned}$$

The cases for edges, target and label mapping are similar.

ad 2. Let $v \in N_T$ be arbitrary. If $v \in N^{\text{new}}$, then there is only $\{v\} = t^{-1}(v)$ and $\mathsf{mult}_{\text{n},T}(v) = 1$ by definition of abstract transformations. Assume $v \notin N^{\text{new}}$. As s is a shaping, we know that $\left|s^{-1}(v)\right|_\nu = \mathsf{mult}_{\text{n},S}v = \mathsf{mult}_{\text{n},T}v$, and it suffices to show $s^{-1}(v) = t^{-1}(v)$, which is straightforward by definition of t.

ad 3. This result follows immediately from the definition of $\simeq_T$. By definition of $\mathsf{mult}_{\text{out},T}$, we can either employ the fact that s is a shaping or, in case of new edges, none of them are equivalent to either themselves or anything existing before, so all new multiplicities are in fact 1 as defined. This reasoning holds both for source and target multiplicities. □

Corollary 42 (Transformation of canonical shapes). *Let $P = (L, R)$ be a transformation rule, S, T be canonical shapes and $f : L \to S$ be a pre-matching such that $S \overset{(P,f)}{\rightsquigarrow} T$. Let S', T' be the shapes, $c : L \to S'$ the concrete pre-matching and $\beta : S' \to S$ and $\beta' : T' \to T$ the abstraction morphisms that witness $S \overset{(P,f)}{\rightsquigarrow} T$. Then for any concretisation G of S' with shaping morphism $s : G \to S'$, there exist a matching $m : L \to G$ and a graph H such that $G \overset{(P,m)}{\longrightarrow} H$ and T is (isomorphic to) the neighbourhood shape of H.*

Proof. The matching m exists by Theorem 41. By the same theorem, we know that there exists a shaping $t : H \to T'$. Thus, $\beta' \circ t$ is a shaping from H to T. We can conclude then that T is a neighbourhood shaping (as it has H as concretisation). By Lemma 24, $\beta' \circ t$ is the neighbourhood shaping of H. □

5.3 Using Shape Transformations

We saw in the previous section several properties of concrete graph transformations with respect to shape transformations and shaping. In this section we informally describe how these results can be used for over-approximating a concrete labelled transition system by an abstract one.

Consider a graph production system $\mathbf{P} = (G_0, \mathcal{P})$, where G_0 is the start graph and $\mathcal{P}$ is a set of graph productions. As briefly described in the introduction, this production system gives rise to a labelled transition system (LTS for short) $\mathcal{S}$ which states are graphs, with start state G_0, and which transitions are applications of graph transformation rules. That is, any state G of the LTS is a graph that can be derived from G_0 by a final number of applications of graph productions starting from G_0. If the rule $P = (L, R)$ is applicable in the graph G with matching $m : L \to G$ yielding the graph H, then H is a state in the LTS and there exists a transition from G to H labelled by (P, m). A *path starting in the state* G_1 in the LTS $\mathcal{S}$ is a sequence of graph transformation rules $P_1, \ldots, P_k$ such that there exists sequence of graphs $G_1, \ldots, G_k$ and a sequence of matchings $m_i : L_i \to G_i$ for all $i \in 1..k-1$ such that for all $i \in 1..k-1$, $G_i \overset{P_i, m_i}{\longrightarrow} G_{i+1}$.

Consider now some fixed positive naturals i, μ, ν defining a precision of a neighbourhood shaping. Define the LTS $\mathcal{S}'$ whose states are canonical shapes and whose transitions are abstract shape transformations with:

- states of $\mathcal{S}'$ are the neighbourhood shapes of states of $\mathcal{S}$, in their canonical representation and initial state is S_0, the neighbourhood shape of G_0;
- transitions of $\mathcal{S}'$ are the transitions $S \overset{P,f}{\rightsquigarrow} T$ such that there exists a transition $G \overset{P,m}{\longrightarrow} H$ in $\mathcal{T}$, where $s : G \to S$ and $t : H \to T$ are the neighbourhood shapings of G and H, respectively, and $f = s \circ m$.

By Theorem 40 we know that transitions in the LTS $\mathcal{S}'$ indeed correspond to abstract graph transformations. Note also that the LTS $\mathcal{S}'$ is finite, as there are only a finite number of canonical shapes for fixed i, μ and ν. Additionally, every path in $\mathcal{S}$ starting in the state G is also a path in $\mathcal{S}'$ starting in the neighbourhood shape of G. Remark that the inverse does not hold, as every state of $\mathcal{S}'$ may be the neighbourhood shape of several different states in $\mathcal{S}$. Therefore, $\mathcal{S}'$ is a finite over-approximation of $\mathcal{S}$ with respect to paths and can be used for verifying *e.g.* temporal properties on $\mathcal{S}$.

Unfortunately, the LTS $\mathcal{S}'$ can not be constructed without constructing $\mathcal{S}$, which may be infinite. However, we can construct an LTS, denote it $\mathcal{S}''$, that a computable and still finite over-approximation of $\mathcal{S}'$. The idea is to start from the canonical shape S_0 and construct iteratively all possible abstract transformations. For a fixed state S, the construction of its outgoing transitions in $\mathcal{S}''$ can be done in three steps:

Materialisation: in order to enumerate and construct all possible abstract transformations of a canonical shape S, we first have to find and construct witnesses for these transformations (according to Definition 38), *ie* find all rules $P = (L, R)$ and all pre-matchings $f : L \to S$ such that there exist a shape S' less abstract than S with abstraction morphism $\beta : S' \to S$ and a concrete pre-matching $c : L \to S'$ with $f = \beta \circ c$. Such shapes S' are called *materialisations* of S. Constructing the materialisations is described in Section 6.1 and Section 6.2;

Transformation: once we have computed all possible materialisations of the shape S w.r.t. the graph production system $\mathcal{S}$, we can perform the actual transformations as concrete shape transformations;

Normalisation: applying a concrete shape transformation on some materialisation of the canonical shape S does not necessarily result in a canonical shape. That is, the resulting graph cannot be a

state of $\mathcal{S}''$. The result of the transformation has to be abstracted to a neighbourhood shape. This is called *normalisation* and is described in Section 6.3.

6 Materialisation and Normalisation

We define in this section the set of materialisations of a canonical shape S w.r.t. some pre-matching of a transformation rule. This set of materialisations is finite. In Section 6.2 we briefly describe an algorithm that allows to construct the set of materialisations and give some examples.

6.1 Definition of the Set of Materialisations

Let us first give a formal definition of what we call a materialisation. In the sequel we consider fixed naturals i, μ, ν defining a precision of a neighbourhood shaping.

Definition 43 (materialisation). *Given a level i canonical shape S and a graph production $P = (L, R)$ with pre-matching $f : L \to S$, a* materialisation *of S according to f is a shape S' such that*

- *S is more abstract than S', i.e. there exists an abstraction $\beta : S' \to S$;*
- *there exists a concrete pre-matching $c : L \to S'$ such that $f = \beta \circ c$;*
- *let T' is the shape result of the transformation of S' with P, c. Then the level i neighbourhood shaping of T' exists.*

For any canonical shape S, graph production $P = (L, R)$ and pre-matching $f : L \to S$, we want to construct the set of materialisations $\mathcal{M}(S, P, f)$ that covers all possible transformations of some concretisation of S. That is, for all graph G concretisation of S, there exists a shape S' in $\mathcal{M}(S, P, f)$ such that S' is a shaping for G. This set is defined as follows (the first two points coincide with the definition of a materialisation).

Definition 44 (The set of materialisations $\mathcal{M}(S, P, f)$). *For a given level i canonical shape S and a graph production $P = (L, R)$ with pre-matching $f : L \to S$, the set $\mathcal{M}(S, P, f)$ is composed of the shapes S' that satisfy the following (up to shape isomorphism)*

- *S is more abstract than S', i.e. there exists an abstraction $\beta : S' \to S$;*
- *there exists a concrete pre-matching $c : L \to S'$ such that $f = \beta \circ c$;*
- *let S'' be the shape obtained from S' as follows: to every node v in $c(L)$ of S' is given an additional, fresh label l_v. Then the shape S'' is a canonical shape.*

Elements of the set $\mathcal{M}(S, P, f)$ are indeed materialisations. The point on which we have to argue is that after transformation, a shape S' in $\mathcal{M}(S, P, f)$ admits a level i neighbourhood shape.

Lemma 45. *Let S' in $\mathcal{M}(S, P, f)$. Then the shape T' result of the transformation of S' by c and P admits a level i neighbourhood shape.*

Proof. (Sketch) Let S'' be the shape that witnesses the fact that S' is a materialisation of S; that is, S'' is the same as S' except that it has fresh labels on the nodes in $c(L)$. Consider also the rule $P'' = (L'', R'')$ obtained from P by adding fresh labels to all nodes in a way that $c : L'' \to S''$ is a concrete matching. That is, fresh labels for L'' and $c(L)$ in S'' coincide. Then the rule P'' can be applied to S'' with matching c, thus obtaining the graph T''. It is not difficult to see that the shape T' is T'' from which the fresh labels have been removed. Then one can show that:

1. if T'' admits a level i neighbourhood shaping, then does also T'. It is shown in a more general way for a shape T' obtained from a shape T'' be removing some unique labels. The proof of this result is quite technical and is given in Appendix F;
2. for all $j \leq i$, $\sim_j$ is defined in T'' and moreover for all node $v \in T'' \cap S''$, $[v]_{\sim_j}$ in S'' is included into $[v]_{\sim_j}$ in T'' whenever this former exists (*ie* whenever $v \notin N^{\text{new}}$).

These two allow to conclude that T' admits a level i neighbourhood shaping. In what follows we sketch a proof for the latter statement. Let us first point out that if $\sim_j$ is defined on T'', then $[v]_{\sim_j} = \{v\}$ in T'' and in S'' for all node v in $c(L'') \cup N^{\text{new}}$ because v has a unique label, and also $[v]_{\simeq_{T''}} = \{v\}$ by definition. Thus, we only have to bother about nodes v not in $c(L'') \cup N^{\text{new}}$. Moreover, as by definition the grouping relations of S'' and T'' coincide on all nodes in $N_{S''}$, the fact that $\sim_j$ is defined is not a problem as long as $[v]_{\sim_{j-1}}$ in S'' is included into $[v]_{\sim_{j-1}}$ in T''. So let us simply suppose that $\sim_j$ is defined and argue that if $v \sim_j v'$ in S'', then $v \sim_j v'$ in T''. Remark that the unique labels in $c(L'')$ influence the equivalence classes for $\sim_j$ of the nodes that are in the j-neighbourhood of $c(L'')$. In other words, if $v \sim_j v'$ in S'', then either v and v' are both far away from $c(L'')$, or are both at the same distance from all nodes in $c(L'')$. In the first case, it is clear that they are also far away from the nodes $c(L'') \cup N^{\text{new}}$ in T'' so they remain $\sim_j$-equivalent in T''. In the second case, intuitively v and v' are connected exactly in the same way to all the nodes $c(L'')$, this is because of the uniqueness of labels of these latter. Now if *e.g.* v is in the j-neighbourhood of some of the newly added nodes from N^{new}, and thus "influenced" by this new node for its $\sim_j$ equivalence class, then v' is influenced in exactly the same way because nodes in N^{new} are only connected to nodes in $c(L'')$, and because of uniqueness of labels. □

Remark that the set $\mathcal{M}(S, P, f)$ is finite. Indeed, it is a set of canonical shapes over the initial set of labels augmented with the fresh labels l_v, for v in $c(L)$, and the number of different such canonical shapes is finite.

Lemma 46 (Completeness of the Set of Materialisations). *Let S be a neighbourhood shape. For all G concretisation of S with corresponding shaping $s : G \to S$, for all transformation rule $P = (L, R)$, and for all matching $m : L \to G$, there exist a pre-matching $f : L \to S$ and a shape S' in $\mathcal{M}(S, P, f)$ such that $f = s \circ m$ and H abstracts to T', where H and T' are the graph and the shape such that $G \xrightarrow{P,m} H$ and $S' \xrightarrow{P,f} T'$.*

Proof. It is immediate to see that if $m : L \to G$ is a matching, then there exists a pre-matching $f : L \to S$ such that $f = s \circ m$. This holds for all shaping $s : G \to S$, and not only for a neighbourhood shaping. Consider now the set $\mathcal{M}'(S, P, f)$ being the set of all shapes S' defined by the first two conditions for $\mathcal{M}(S, P, f)$. That is, $\mathcal{M}'(S, P, f)$ is a possibly infinite over-set of $\mathcal{M}(S, P, f)$. In particular, any graph G concretisation of S is in $\mathcal{M}'(S, P, f)$ as its trivial shape. In other words, $\mathcal{M}'(S, P, f)$ is complete in the sense of the lemma. It is then enough to show that for all shape G in $\mathcal{M}'(S, P, f)$, there exists a shape S' in $\mathcal{M}(S, P, f)$ such that S' is more abstract than G. This falls to show that the third condition in the definition of $\mathcal{M}(S, P, f)$ does not remove too much graphs and shapes from the set $\mathcal{M}'(S, P, f)$. This is indeed the case because this third condition ensures that materialisations are not too abstract neither too concrete, but correspond to the level of abstraction of a neighbourhood shaping. □

Proposition 47 (Minimality of the Set of Materialisations). *For all G concretisation of S with shaping $s : G \to S$, and all matching $m : L \to P$ such that $f = s \circ m$, there exists a unique shape S' in $\mathcal{M}(S, P, f)$ such that G can be shaped to S' with shaping $s : G \to S'$, and such that $c = s \circ m$, where $c : L \to S'$ is the concrete pre-matching extracted from f.*

Proof. Let S_1 and S_2 be two shapes in $\mathcal{M}(S, P, f)$ which both satisfy the conditions of the proposition, with shapings $s_1 : G \to S_1$ and $s_2 : G \to S_2$, and with concrete pre-matchings $c_1 : L \to S_1$ and $c_2 : L \to S_2$. Consider now the canonical shapes S_1' and S_2' that witness the fact that S_1 and S_2 are materialisations (according to the third condition in the definition of $\mathcal{M}(S, P, f)$.) Consider also the graph G' obtained from G by adding the fresh label l_v to the node $m(v)$, this for all v node of L. Then it is easy to see that $s_1 : G' \to S_1'$ and $s_2 : G' \to S_2'$ are shapings. Moreover, as S_1 and S_2 are canonical shapes, then necessarily s_1 and s_2 are canonical shapings. As each graph has a unique neighbourhood shape, necessarily S_1' and S_2' are the same canonical shape. By definition of S_1' and S_2' it immediately follows that S_1 and S_2 are the same shape, as by definition elements of $\mathcal{M}(S, P, f)$ are unique up to isomorphism. □

6.2 Effective Construction of $\mathcal{M}$

In order to effectively construct an abstract labelled transition system, one needs to be able to effectively construct the set of materialisations $\mathcal{M}(S, P, f)$ for all canonical shape S and a pre-matching $f : L \to S$ for the rule $P = (L, R)$. We give here a sketch of an algorithm for constructing the set of materialisations.

Intuitively, a materialisation is composed of an abstract part and a materialised part. The abstract part is the initial shape S or sub-graphs of it. The materialised part is composed of a concrete copy of $f(L)$ and its neighbourhood of radius i, where i is the level of neighbourhood shaping. The main idea of the algorithm is to "extract" a concrete copy of $f(L)$ from S, remap the matching f into this concrete part yielding a concrete pre-matching c, and then modify the obtained structure until it becomes a correct materialisation. Remind that the structure is a materialisation if one can attach fresh names to the nodes in $c(L)$ and obtain a neighbourhood shape. This intuitively means that in radius i from the concrete part $c(L)$, two nodes of any concrete graph may be grouped together only if they are connected in exactly the same way to all nodes from $c(L)$ (up to edge multiplicities).

The algorithm starts from the shape S and iteratively constructs structures that are a kind of pre-materialisations and refines these until they become correct materialisations. This is done by iterating over the following steps:

extract and connect for the first iteration, "extract" a concrete copy of $f(L)$ from the shape, remap f into this concrete copy yielding a concrete pre-matching $c(L)$ and associate fresh labels to the nodes in $c(L)$. This copy becomes the materialised part that will be widened by adding new nodes to it during the next iterations. For the second and next iterations, "pull" along the edges that connect the materialised part and the abstract part for extracting new nodes. One has to extract one node for any possible configuration with respect to the connection with $c(L)$. The new nodes become part of the materialised part. Any of these extractions is accompanied by connecting all newly extracted nodes with the abstract part in all possible ways and updating node end edge multiplicities;

update grouping relation the grouping relation is updated so that any node that is at distance less than $i - 1$ from the concrete part $c(L)$ becomes alone in its equivalence class for the grouping relation. This is necessary because the fresh labels in $c(L)$ influence the $\sim_{i-1}$ equivalence relation for these nodes, which should be equal to the grouping relation (in a neighbourhood shape);

choose nodes and edges as in the first step adds new nodes and edges, and the second step acts on the grouping relation by splitting groups, edges that previously had all their start (or end) points in the same group may not be grouped anymore, but still they have associated common edge multiplicity. The algorithm splits these multiplicity functions in all possible ways so that edges in

the materialised part have correct edges multiplicities. This is not done for edges in the abstract part (as it is not always possible).

6.3 Normalisation

Applying a shape transformation to a materialisation shape does not yield a canonical shape. The role of the normalisation is to perform the neighbourhood shaping of such shapes. Let S' be a materialisation in $\mathcal{M}(S, P, f)$, and T' be the graph resulting of the concrete shape transformation $S' \xrightarrow{(P,c)} T'$, where c is the concrete pre-matching corresponding to f. By definition, we know that T' admits a level i neighbourhood shape, denote it T.

6.4 Back to the Construction of the Abstract Labelled Transition System

Now all the ingredients for constructing an abstract labelled transition system $\mathcal{S}''$ (ALTS) are there. Consider the neighbourhood shape S_0 and set of production rules $\mathcal{P}$. Initially, S_0 is the unique state of the ALTS, and there are no transitions. For any state S in the ALTS, and for any production rule $P = (L, R)$, we compute all pre-matchings $f : L \to S$. For all pre-matching f, the set of materialisations $\mathcal{M}(S, P, f)$ is computed. For all materialisations S' in $\mathcal{M}(S, P, f)$, the actual concrete shape transformation is performed $S' \xrightarrow{(P,c)} T'$, where c is the concrete pre-matching $c : L \to S'$ deduced from f. Finally, the neighbourhood shape T of T' is computed. If T is not a state of the ALTS, then it is added as a state. Then a transition from S to T with label P, f is added to the ALTS.

Note that the ALTS is non deterministic (a state may have several outgoing transitions with the same label), whereas a concrete LTS is always deterministic. This is because the one state can have several materialisations for a fixed rule and a fixed pre-matching. In the concrete case, a rule with a matching uniquely define an application of a graph transformation and its result.

The ALTS $\mathcal{S}''$ constructed this way is an over-approximation of all (concrete) LTS $\mathcal{S}$ with start graph G_0 and set of rules $\mathbf{P}$, for all graphs G_0 which neighbourhood shape is S_0, in the following sense:

> For any path $G_1 \xrightarrow{P_1,m_1} G_2 \xrightarrow{P_2,m_2} \cdots \xrightarrow{P_{n-1},m_{n-1}} G_n$ in $\mathcal{S}$, where the G_i are states of $\mathcal{S}$, the $P_i = (L_i, R_i)$ are transformation rules and for all $i \in 1..n-1$, $m_i : L_i \to G_i$ are matchings, there exists a unique path $S_1 \xrightarrow{P_1,f_1} S_2 \xrightarrow{P_2,f_2} \cdots \xrightarrow{P_{n-1},m_{n-1}} S_n$ in $\mathcal{S}''$, where for all i, S_i is the neighbourhood shape of G_i with corresponding shaping $s_i : G_i \to S_i$, and $f_i = s_i \circ m_i$.

To show that this property indeed holds, we need to show what follows.

1. For all concrete transition $G \xrightarrow{P,m} H$, there exists an abstract transition $S \overset{P,f}{\rightsquigarrow} T$, where S and T are the neighbourhood shapes of G and H, respectively, and $f = s \circ m$ for $s : G \to S$ the neighbourhood shaping of G. This is ensured by Theorem 40.
2. This abstract transition is indeed computed and added as a transition of $\mathcal{S}''$. That is, show that a witness for this abstract transformation exists in the set $\mathcal{M}(S, P, f)$. This is ensured by the completeness of the set of materialisations (Lemma 46) and by the composition of neighbourhood shapings for graphs and shapes (Lemma 23). By completeness of the set of materialisations we know that there exists a shape S' in $\mathcal{M}(S, P, f)$ that abstraction for G, and that can be transformed to simulate the actual transformation of G; let the shape resulting from the transformation be T'. By composition of neighbourhood shapings, we know that the normalisation of T' yields is the neighbourhood shape of H.
3. Uniqueness of the path $S_1 \xrightarrow{P_1,f_1} S_2 \xrightarrow{P_2,f_2} \cdots \xrightarrow{P_{n-1},m_{n-1}} S_n$ is ensured by uniqueness of neighbourhood shapes.

7 A Modal Logic for Graphs and Shapes

In this section we define a modal logic with forward and backward modalities and counting that can be interpreted on graphs and on shapes. We show that this logic is preserved and reflected by shaping and abstraction morphisms.

Before giving a formal definition of syntax and semantics of this logic, let us give a flavour of it by some examples.

Example 48. Consider the graph depicted on Figure 1, representing a list structure. Here are some properties that one could want to express for similar list structures:

1. any cell has an associated value that is some object, *ie* any Cell-node has an outgoing val-edge leading to an Object-node. This can be expressed by the following formula:

$$\mathsf{Cell} \rightarrow \rangle\mathsf{val}\rangle^{1} \cdot \mathsf{Object}.$$

   The $\rangle\mathsf{val}\rangle^{1}$ operator is a forward existential modality, indicating the existence of an outgoing val edge. With the modality is associated a multiplicity, here 1, which is interpreted as "at least one" outgoing val-edge;
2. analogously, any object is the value associated to some cell, *ie* any Object-node has an incoming val-edge coming from a Cell-node. This is expressed by the formula

$$\mathsf{Object} \rightarrow \langle\mathsf{val}\langle^{1} \cdot \mathsf{Cell}.$$

   Here, $\langle\mathsf{val}\langle^{1}$ is a backward modality and indicates the existence of at least one incoming val-edge;
3. we can go further and express that objects are not shared between different list cells, *ie* every Object-node has exactly one incoming val-edge coming from a Cell-node:

$$\mathsf{Object} \rightarrow (\ \langle\mathsf{val}\langle^{1} \cdot \mathsf{Cell} \wedge \neg\langle\mathsf{val}\langle^{2} \cdot \mathsf{Cell}\ ).$$

   Here, $\neg$ is the negation operator and $\wedge$ is conjunction. ◀

7.1 Syntax of the Logic

Consider a finite set of atomic propositions $\mathcal{P}$. A $\mathcal{L}(\mathcal{P})$ logic formula ϕ is defined by the following syntax:

$$\phi ::= \mathtt{tt} \mid \mathsf{p} \mid \neg\phi \mid \phi \vee \phi \mid \phi \wedge \phi \mid \rangle\mathsf{a}\rangle^{\lambda} \cdot \phi \mid \langle\mathsf{a}\langle^{\lambda} \cdot \phi$$

where a is a label in Lab, $\mathsf{p} \in \mathcal{P}$ and λ is an element of $\mathbf{M}_{\mu}$; $\mathtt{tt}$ stands for the true formula, $\rangle\mathsf{a}\rangle^{\lambda} \cdot \phi$ and $\langle\mathsf{a}\langle^{\lambda} \cdot \phi$ are forward and backward existential modalities, respectively, and $\neg$, $\vee$ and $\wedge$ are the usual logical operators. [5]

In Example 48, we have used labels as atomic propositions, *ie* the formulae in this example are $\mathcal{L}(\mathsf{Lab})$ formulae.

The *nesting depth* $d(\phi)$ of a logic formula ϕ measures the maximal number of nested modalities. It is defined recursively on the structure of ϕ as : $d(\mathsf{p}) = d(\mathtt{tt}) = 0$, $d(\rangle\mathsf{a}\rangle^{\lambda} \cdot \phi) = d(\langle\mathsf{a}\langle^{\lambda} \cdot \phi) = 1 + d(\phi)$, $d(\neg\phi) = d(\phi)$, $d(\phi \vee \phi') = d(\phi \wedge \phi') = max(d(\phi), d(\phi'))$ for any a in Lab. We denote $\mathcal{L}_i(\mathcal{P})$ the set of logic formulae with nesting depth at most i.

[5] We explicitly add here the redundant operators $\mathtt{tt}$ and $\wedge$ because in the latter we will be interested in the logic without negation, which in this case can simply be defined as a syntactical fragment.

7.2 Satisfaction on Graphs and Shapes

Logic formulae are interpreted in graph nodes. Let G be a graph and $\gamma : N_G \to 2^{\mathcal{P}}$ be a valuation function that associates a set of atomic propositions with any node of G. For a graph G, a node v in N_G, a valuation γ, and a formula ϕ, the *satisfaction relation* $G, v, \gamma \models \phi$ is defined recursively on the structure of ϕ by:

- $G, v, \gamma \models \mathsf{tt}$;
- $G, v, \gamma \models \mathsf{p}$ if $\mathsf{p} \in \gamma(v)$;
- $G, v, \gamma \models \neg\phi$ if $G, n, \gamma \not\models \phi$;
- $G, v, \gamma \models \phi \vee \phi'$ if $G, v, \gamma \models \phi$ or $G, v, \gamma \models \phi'$;
- $G, v, \gamma \models \phi \wedge \phi'$ if $G, v, \gamma \models \phi$ and $G, v, \gamma \models \phi'$;
- $G, v, \gamma \models \rangle\mathsf{a}\langle^{\lambda}\cdot\phi$ if $|\{e \in v\triangleright^{\mathsf{a}} \mid G, \mathsf{tgt}(e), \gamma \models \phi\}|_{\mu} \geq \lambda$;
- $G, v, \gamma \models \langle\mathsf{a}\langle^{\lambda}\cdot\phi$ if $|\{e \in v\triangleleft^{\mathsf{a}} \mid G, \mathsf{src}(e), \gamma \models \phi\}|_{\mu} \geq \lambda$.

If $G, v, \gamma \models \phi$, we say that ϕ *holds in node* v. We sometimes omit γ if it is clear from the context. Intuitively, a formula of the form $\rangle\mathsf{a}\langle^{\lambda}\cdot\phi$ holds in a node v if the –μ-bounded– number of a-labelled edges (e) connecting it to some node v' ($\mathsf{src}_G(e) = v$ and $\mathsf{tgt}_G(e) = v'$) in which ϕ holds is at least λ. Analogously, $\langle\mathsf{a}\langle^{\lambda}\cdot\phi$ holds in v if the number of a-labelled edges connecting some such v' to v is at least λ.

Back to Example 48 with the definition of satisfaction of the logic in mind, one can notice that in this example the valuation γ is not specified. As we pointed out, the formulae in this example are in $\mathcal{L}(\mathcal{P})$. A natural valuation for this logic is the one that associates to each node the set of its labels; *ie* $\gamma(v) = \mathsf{lab}_G(v)$ for all v in N_G, and for all graph G.

The satisfaction relation is defined for a shape almost in the same manner as it is defined for a graph. The differences are in the way it is defined for a modality formula:

- $S, v, \gamma \models \rangle\mathsf{a}\langle^{\lambda}\cdot\phi$ if $\lambda \leq \sum_{C\in X}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, C)$ where

$$X = \{C \in N_S/{\simeq_S} \mid \forall w \in C.\ S, w, \gamma \models \phi\}\,;$$

- $S, v, \gamma \models \langle\mathsf{a}\langle^{\lambda}\cdot\phi$ if $\lambda \leq \sum_{C\in X}^{\mu} \mathsf{mult}_{\text{in},S}(v, \mathsf{a}, C)$ where:

$$X = \{C \in N_S/{\simeq_S} \mid \forall w \in C.\ S, w, \gamma \models \phi\}\,.$$

In the case of shapes, formulae are interpreted a bit differently. We no longer count individual a-labelled edges going out of (resp. coming into) a node, but instead sum-up the outgoing (resp. incoming) edge multiplicities associated to that node and to a group of nodes C such that all nodes in C satisfy the formula ϕ.

Example 49. Back to our list example, the formula $\mathsf{Cell} \to \langle\mathsf{Next}\langle^{1}\cdot(\mathsf{List} \vee \mathsf{Cell})$ holds all nodes of the shape on Figure 5.

7.3 Preservation by Abstraction Morphism

Let $s : G \to S$ be a shaping morphism from the graph G to the shape S. We say that s *preserves* a property p if whenever p holds in the node v of S, it also holds in the node $s(v)$ of S. Inversely, we say that s *reflects* p if whenever p holds in the node $\alpha(v)$ of S, it also holds in the node v of G. One can also talk about preservation and reflection by an abstraction morphism $\alpha : S \to T$.

Preservation and reflection are very important characterisations. If an abstraction preserves a set of properties, these properties can be verified on the abstract level. If an abstraction reflects a set of properties, then any characterisation of a shape graph also holds for its concretisations. If both preservation and reflection hold, verifying a property on a graph is equivalent to verifying it on the abstract level.

As we will see in the next section, the neighbourhood shaping preserves and reflects all properties defined by logic formulae of the corresponding depth. We start in this section by a more general result about preservation and reflection by abstraction morphism, identifying the necessary conditions for it to hold.

In Definition 50 we define what we mean by preservation and reflection of a property, in the most general case. In Proposition 51 we announce the result for preservation and reflection for abstraction morphisms, and in Proposition 53 the one for general shapings.

Definition 50. *Let $\mathcal{P}$ be a set of atomic propositions, S, T be shapes, $\gamma_S : N_S \to 2^{\mathcal{P}}$ and $\gamma_T : N_T \to 2^{\mathcal{P}}$ be valuations, and let $\mathcal{R}$ be a set of properties such that the satisfaction relations $S, v, \gamma_S \models p$ and $T, w, \gamma_T \models p$ are defined for any nodes $v \in N_S$, $w \in N_T$ and for any property $p \in \mathcal{R}$. We say that α* preserves *$\mathcal{R}$ under γ_S, γ_T if for any $p \in \mathcal{R}$ and for any $v \in N_S$ we have $S, v, \gamma_S \models p$ implies $T, \alpha(v), \gamma_T \models p$. We say that α* reflects *$\mathcal{R}$ under γ_S, γ_T if for any $p \in \mathcal{R}$ and for any $v \in N_T$ we have $T, v, \gamma_T \models p$ implies $S, w, \gamma_S \models p$ for any $w \in \alpha^{-1}(v)$.*

In the following we show how, under some conditions on the relationship between α, $\simeq_T$ and γ_T, the satisfaction of logic formulae of depth one is preserved and/or reflected by α. For a shape T and a valuation $\gamma : N_T \to 2^{\mathcal{P}}$ we say that $\simeq_T$ *is compatible with* γ if for any two nodes v, w of T, if $v \simeq_T w$, then $\gamma(v) = \gamma(w)$. The negation free fragment of $\mathcal{L}_1(\mathcal{P})$ is the set of $\mathcal{L}_1(\mathcal{P})$ formulae that do not use the negation operator ($\neg$).

Proposition 51 (Preservation and Reflection). *Let $\mathcal{P}$ be a set of atomic propositions, S, T be shapes, $\gamma_S : N_S \to 2^{\mathcal{P}}$ and $\gamma_T : N_T \to 2^{\mathcal{P}}$ be valuation functions such that $\simeq_T$ is compatible with γ_T, and let $\alpha : S \to T$ be an abstraction morphism.*

(preservation) *If α preserves $\mathcal{P}$ under γ_S, γ_T, then α preserves the negation free fragment of $\mathcal{L}_1(\mathcal{P})$ under γ_S, γ_T.*

(reflection) *If α reflects $\mathcal{P}$ under γ_S, γ_T, then α reflects the negation free fragment of $\mathcal{L}_1(\mathcal{P})$ under γ_S, γ_T.*

(preservation and reflection) [6] *If α preserves and reflects $\mathcal{P}$ under γ_S, γ_T, then α preserves and reflects $\mathcal{L}_1(\mathcal{P})$ (possibly with negation) under γ_S, γ_T.*

Proof. See appendix E.

This preservation and reflection result can easily be extended on shaping (*ie* for S being a graph and α a shaping morphism in the previous proposition). One can define preservation and reflection on the same way for shaping as for abstraction morphisms, as well as the notion of a grouping relation compatible with a shaping. We only enunciate the result without explicitly giving the definitions.

[6] Preservation for formulae with negation may seem contradictory with the Morphism Preservation Theorem for finite structures [13]. This theorem states that a first-order formula is preserved by morphism if, and only if, it is equivalent to an existential positive formula. Some modal logic formulae cannot be expressed in first-order logic without negation (*e.g.* $\neg\langle\mathsf{a}\rangle^{\lambda}\cdot\mathtt{tt}$.) However, in our case, shapes contain information on interpretation of such negated formulae, by means of the multiplicity functions, which explains this apparent contradiction.

Proposition 52. *Let $\mathcal{P}$ be a set of atomic propositions, G be a graph, S be a shape and $s : G \to S$ be a shaping compatible with $\mathcal{P}$.*

(preservation) *If s preserves $\mathcal{P}$, then s preserves any negation-free $\mathcal{M}(\mathcal{P})$ formula ϕ.*
(reflection) *If s reflects $\mathcal{P}$, then s reflects any negation-free $\mathcal{M}(\mathcal{P})$ formula ϕ.*
(preservation and reflection) *If s preserves and reflects $\mathcal{P}$, then s preserves and reflects any $\mathcal{M}(\mathcal{P})$ formula ϕ.*

Proof. It is easy to show for the trivial shaping t_G. Then the result follows from composition of abstraction morphisms and the Proposition 51.

7.4 Preservation and Reflection for Neighbourhood Shaping

The neighbourhood shaping enjoys the good properties of preservation and reflection of $\mathcal{L}(\mathsf{Lab})$ formulae with the appropriate depth.

Proposition 53 (Preservation and Reflection). *Let G be a graph and S be a shape obtained by the level i neighbourhood shaping of G, for some $i \geq 1$, with corresponding shaping $s : G \to S$. Then s preserves and reflects $\mathcal{L}_i(\mathsf{Lab})$.*

Proof. (Sketch) The proof goes by induction on i, using Proposition 51 and the fact that $\mathcal{L}_{i+1}(\mathsf{Lab})$ is equivalent to $\mathcal{L}_1(\mathcal{R})$ where $\mathcal{R}$ is the a set properties defined by $\mathcal{L}_i(\mathsf{Lab})$.

Thus, for any property ϕ of $\mathcal{L}(\mathsf{Lab})$ to be verified on a graph G, one can use the level i neighbourhood shape of G for verifying ϕ, where i is the nesting depth of the formula ϕ. This means that the neighbourhood shaping provides a graph abstraction mechanism that is parametrised by the properties we want to verify, and that guarantees preservation and reflection of these properties.

Example 54. Denote G the graph on Figure 1 and S its level one neighbourhood shape (Figure 6), and let $s : G \to S$ be the corresponding neighbourhood shaping. Let ϕ be the formula of nesting depth two $\langle\mathsf{Next}\rangle^1 \cdot \langle\mathsf{Next}\rangle^1 \cdot \mathtt{tt}$ (which intuitively expresses that there is a Next-path of length two starting from the node). We have that $S, w_3 \models \phi$, but $G, v_4 \not\models \phi$, and $s(v_4) = w_3$. That is, ϕ is not reflected by s. Consider now T the level two neighbourhood shape of G, depicted on Figure 7; the corresponding shaping $t : G \to T$ is not difficult to define. One can easily check that the formula ϕ is reflected by t. ◀

7.5 Relationship between the Logic and Neighbourhood Shaping

The modal logic that we presented in this section is tightly related to the neighbourhood equivalence relation and canonical names. We already stated in Lemma 28 that two nodes of a graph are neighbourhood equivalent if, and only if, they have the same canonical name. Here we enlarge this characterisation by the logic: two nodes are i-neighbourhood equivalent if, and only if, they satisfy the same logic formulae of depth i.

Lemma 55. *Two nodes v, v' of a graph G are i-neigborhood equivalent if, and only if, the same $\mathcal{L}_i(\mathsf{Lab})$ formulae hold in v and in v'.*

Proof. See appendix G

The following relationship between canonical names and logic formulae is also easy to see: to any canonical name corresponds a logic formula that holds exactly in the nodes having this name.

Lemma 56. *For any $i \geq 1$ and any level i node canonical name C, there exists an $\mathcal{L}_i(\mathsf{Lab})$ formula ϕ_C such that for any graph G and any node v of G, $\mathsf{name}^i(G)(v) = C$ if, and only if, $G, v \models \phi_C$.*

Proof. (Idea) The formula ϕ_C can be effectively constructed by induction on i.

8 Related Work

Abstract Graph Transformations In [9] one of the authors defined a notion of abstract graphs in which abstract graph nodes may summarise an unbounded number of concrete graph nodes. These abstractions are only used for deterministic simple graphs. With the abstract graph are associated constraints on the multiplicities of incoming and outgoing edges for the nodes in a concrete instance. In the same paper are also introduced canonical abstract graphs whose size is bounded and that roughly corresponds to the level one neighbourhood abstraction in the present work. In [11] these canonical abstract graphs are used for transformations.

In [2] are introduced the so called Partner Graph Grammars, suitable formalism for dynamic communication systems. They come with an abstraction mechanism on graphs and an adequate notion of abstract graph transformations. Preservation and reflection are shown for first-order logic without equality and an interesting subclass of abstraction morphisms. Moreover, a CTL-based logic on labelled transition systems is showed to be invariant under abstraction.

Shape Analysis and 3-Valued Logic The work of Sagiv *et al.* on shape analysis (see [14,15] for overviews) has resulted in different abstraction mechanisms allowing to finitely abstract structures of unbounded size. In [15] is presented an abstraction framework that can be parametrised by the properties to be preserved; the framework is implemented in the TVLA tool [8,16]. In this work, the authors use logical structures to represent memory states of programs; abstract structures are 3-valued logical structures. Properties on these structures are defined using first-order logic with transitive closure (FO+TC). Dynamics of systems are encoded by updating the sets of predicates associated to the (abstract or concrete) structure. As graphs are logical structures and our modal logic can be encoded into first-order logic, the abstraction mechanism proposed in [15] is more general than the ours. Concerning preservation of logical properties, Sagiv *et al.*'s "embedding theorem" states that any information extracted from an abstract structure via a FO+TC formula ϕ is a conservative approximation of the information extracted from the concrete structure via ϕ. In this sense, our preservation and reflection result is more general than the embedding theorem, but holds for a modal logic and abstraction mechanism that are weaker than FO+TC and abstraction using abstraction predicates. We believe that the benefits of our approach come from the possibility of full automation. A set of graph transformation rules that is given as concrete semantics can be used as is for the abstract semantics. Moreover, we guarantee to preserve the precision defined by depth i logic formulae, where i is the level of abstraction. In TVLA, it may be necessary to define "by-hand" some update-predicates in order to guarantee the required precision. Apart complexity issues, our framework should be easy to integrate into a graph transformation tool such as GROOVE [7].

Abstract Regular Model Checking In regular model checking (see *e.g.* [5,1]), states of programs are represented as words or trees on finite alphabets, and dynamics are modelled as word or tree transduction. Initial states of a system are represented by a regular (word or tree) automaton Init, and bad configurations by a regular automaton Bad. Checking whether a bad configuration is reached consists in testing whether the set $\tau^*(Lang(\mathsf{Init})) \cap Lang(\mathsf{Bad})$ is empty, where τ is the transduction, and τ^* designates a repetition of this transduction. In general the problem is not decidable, as $\tau^*(Lang(\mathsf{Init}))$

may not be computable in a finite number of steps. Abstract regular (word or tree) model checking [4,3] proposes a method for over-approximating the set of reachable states $\tau^*(Lang(\mathsf{Init}))$ by a set of the form $Lang(\tau^*_\alpha(\mathsf{Init}))$, where α is an appropriate abstraction function for automatons, and τ_α is intuitively the (tree or word) transducer τ lifted to automatons. That is, τ_α allows to apply transformations on sets of trees or words, and a parallel may be made with transformation of abstract graphs which actually aims to over-approximate transformations of the set of their concretisations.

Logic Based Approaches Not so closely related but still relevant are several methods for modelling program states – or the memory heap – by relational structures, and operations by instructions modifying these relational structures; these can be qualified as logic-based approaches. For example, in [17] is introduced a fragment of first-order logic with transitive closure for expressing properties on linked data structures, represented as graphs. The logic allows to specify pre-conditions and post-conditions, and to verify loop invariants. Program operations are directly expressed in the logic. We can also site separation logic (see [12] for an introduction) which has been a very active field of research for the last few years.

9 Conclusion and Further Directions

We presented a general mechanism for graph abstraction. We also defined graph transformations for abstract graphs that allows to approximate behaviour of systems defined as graphs and graph transformations. As the number of possible different abstract graphs is finite, this approximation is finite. The construction of an abstract labelled transition system can be fully automatised. Our abstraction mechanism can be parametrised in several ways, thus obtaining different levels of precision. In particular, this can be parametrised in order to preserve and reflect properties on graphs expressed in a modal logic that we also present in this paper. That is, the abstraction will guarantee that a (finite) set of properties hold in a graph if, and only if, they hold in its abstraction, and this also holds for all abstract graphs obtained by graph transformations starting from some initial start graph. This gives a parametrisable and fully automatised framework for verifying properties on systems described by graphs and graph transformations.

Our abstraction mechanism presents however some drawbacks which cause poor efficiency. This is related in the precision of the abstraction.

Precision Our abstraction mechanism is not very precise, in the sense that concretisations of the same abstract graph may be very different in their shape and structure (see for example the list-like shape on Figure 3(c) and its concretisations on Figure 4(c)). Obviously, abstraction always leads to loss of precision. However, one could hope that the abstraction method is precise enough for interesting examples such as list and list manipulations.

Complexity The insufficient precision is closely related to performance issues. Performing graph transformations on abstract graphs requires the so called materialisation step, which consists in locally concretising the abstract graph in order to extract a copy of the left-hand side of the graph transformation rule on which the actual transformation can be performed. In our abstraction mechanism, the materialisation part may lead to a very large number of materialisations. Each of this materialisations potentially results into a different application of the transformation rule, and a different result graph. This affects the performance of our algorithm, as we have to explore many different abstract transformations, and lots of them may never occur into a concrete labelled transition system. Moreover, as

we do not have a procedure for deciding whether an abstract graph admits concretisations (see Conjecture 33), the abstract labelled transition system may contain states that do not correspond to any concrete graph.

In order to improve our mechanism for abstract transformations, we need to improve the precision of the abstraction. This could be done in several ways.

One possible direction to be explored is restricting the graphs on which we apply the method. For instance, deterministic graphs have shown to be a good model for software systems and the memory heap and in our method we can expect that this restriction would decrease the number of possible abstract graphs.

Another improvement would be to increase the precision of the abstraction mechanism. However, one has to be careful with adapting the abstraction mechanism especially if the result of preservation of logic formulae is to be kept. The difficulty comes from the fact that whatever properties one decides to preserve (and make them parameters of the abstraction mechanism), these properties should be possible to update on abstract graphs after a graph transformation. We have several examples of such properties that give an interesting improvement of the precision, but can not be updated after transformation. Cyclicity and connectivity are such examples. That is, if a cyclicity or connectivity property is associated to some node or a set of nodes, then after performing an abstract graph transformation we cannot tell whether it still holds. However, the information on existence of cycles of small size may be integrated with using for instance hybrid logic.

A third possibility is to restrict the graph transformations that we allow. This is related to our second direction on improving precision. Actually, the abstract transformation mechanism and the abstraction mechanism are closely related, in the sense that properties used for abstraction should be possible to update, or at least conservatively update, after the graph transformation.

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A Proof of Proposition 12

Proposition 12 *Let S, T and U be shapes, f be an abstraction morphism between S and T and g another such morphism between T and U. Then $g \circ f$ (the function composition of f and g) is an abstraction morphism between S and U.*

Proof. The first two axioms of Definition 11 are not difficultly seen to be met for $g \circ f$. For the third one, we only consider the property on the outgoing edges multiplicity function; the one for incoming edges multiplicity follows by symmetry.

Consider a node w in N_U, a label a and a class of group-equivalent nodes $C \in N_U/\simeq_U$. Let also $v' \in N_T$ be a node such that $f(v) = v'$ and $g(v') = w$. Then, by g being an abstraction morphism, we know that

$$\mathsf{mult}_{\text{out},U}(w, \mathsf{a}, C) = \sum_{D' \in (g^{-1}(C))/\simeq_T}^{\mu} \mathsf{mult}_{\text{out},T}(v', \mathsf{a}, D').$$

On the other hand, by f being an abstraction morphism and by definition of v', the right-hand side of this equality can be developed giving the following

$$\mathsf{mult}_{\text{out},U}(w, \mathsf{a}, C) = \sum_{D' \in (g^{-1}(C))/\simeq_T}^{\mu} \sum_{D \in (f^{-1}(D'))/\simeq_S}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, D).$$

Now, given that any D' in the inner sum is mapped to one and only one D (this is a basic consequence of f being a – total – function), we can combine the two sums into one:

$$\mathsf{mult}_{\text{out},U}(w, \mathsf{a}, C) = \sum_{D \in (f^{-1}(g^{-1}(C)))/\simeq_S}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, C),$$

which asserts that $g \circ f$ is an abstraction morphism between S and U. □

B Proof of Lemma 23

Lemma 23 *Let G be a graph, S, T be a shapes, $s : G \to S$, $t : G \to T$ be shaping morphisms, and $\beta : T \to S$ be an abstraction morphism such that $s = \beta \circ t$.*

1. *If s is the neighbourhood shaping of G, then β is the neighbourhood shaping of T.*
2. *If β is the neighbourhood shaping of T, then s the neighbourhood shaping of G.*

For Statement 1, the proof goes as follows (see also Figure 9):

– We first show that the neighbourhood shaping of T exists, let it be the morphism $\beta' : T \to T'$,
– We then define that there exists a morphism $f : T' \to S$ which is an abstraction isomorphism and such that $\beta = f \circ \beta'$.

For Statement 2, we show that there exists a morphism $f : S' \to S$ such that $s = f \circ s'$, where $s' : G \to S'$ is the neighbourhood shaping of the graph G. See also Figure 10.
In the following we consider a fixed i for the level of neighbourhood shaping.

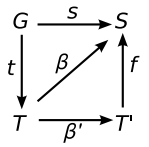


Figure 9. Proof of Statement 1

B.1 Proof of the Statement 1

The Neighbourhood Shaping of T exists For showing that the neighbourhood shaping of T exists, it is enough to show that $\sim_i$ is defined. By definition, $\sim_i$ is defined if $\sim_{i-1}$ is defined and $\simeq_T \subseteq \sim_{i-1}$. This is shown in the following lemma.

Lemma 57. *Let G be a graph, S, T be a shapes, $s : G \to S$, $t : G \to T$ be shaping morphisms, and $\beta : T \to S$ be an abstraction morphism such that $s = \beta \circ t$. If s is the neighbourhood shaping of G, then $\sim_{i-1}$ is defined on the nodes of T, and $\simeq_T \subseteq \sim_{i-1}$.*

Lemma 57 will be shown in Section B.3. The proof of this lemma allows to establish the following corollary. This corollary will be used later on for the proof of Statement 1, and also for the proof of Statement 2. Corollary 58 is also shown in Section B.3.

Corollary 58. *Let G be a graph, S, T be a shapes, $s : G \to S$, $t : G \to T$ be shaping morphisms, and $\beta : T \to S$ be an abstraction morphism such that $s = \beta \circ t$. If at least one of these conditions is verified:*

1. *s is the neighbourhood shaping of G,*
2. *β is the neighbourhood shaping of T,*

then for any $0 \leq j \leq i$, and fol all $v, v' \in N_G$ and all $e, e' \in E_G$,

$$v \equiv_j v' \quad \Leftrightarrow \quad t(v) \sim_j t(v') \qquad \textit{and} \qquad e \equiv_j e' \quad \Leftrightarrow \quad t(e) \sim_j t(e').$$

The Abstraction Isomorphism f Exists We show here that there exists a morphism $f : T' \to S$ which is an abstraction isomorphism and such that $\beta = f \circ \beta'$ (see Figure 9). Remind that that $\beta' : T \to T'$ is the neighbourhood shaping of T. We start by defining a mapping f from nodes and edges T' to nodes and edges of S, and we show that this mapping is a morphism, it is bijective and f and f^{-1} are abstraction morphisms.

Define a mapping f such that $\beta = f \circ \beta'$ Remind that the shaping t and the abstraction morphism β' are surjective. Thus, any node (resp. edge) of T' can be written as $t(\beta'(x))$ for some node (resp. edge) x of G. Then f is defined by: for any $t(\beta'(x))$ node or edge of T', $f(t(\beta'(x))) = s(x)$. Then $\beta = f \circ \beta'$ by definition of f and using $s = \beta \circ t$.

Show that f is a morphism The fact that f defined as previously is a morphism is not very difficult to deduce using that t, β, β' are morphisms.

Show that f is a bijection Showing that f is a surjection is easily done using the definition of f and the fact that s is a surjection. Let us show that f is an injection, that is, for any $t(\beta'(v)), t(\beta'(v'))$ nodes of T', if $t(\beta'(v)) \neq t(\beta'(v'))$, then $s(v) \neq s(v')$. Now, $t(\beta'(v)) \neq t(\beta'(v'))$ if, and only if,, by definition, $t(v) \not\sim_i t(v')$ and, using Corollary 58, if, and only if, $v \not\equiv_i v'$, which is equivalent to $s(v) \neq s(v')$ by definition of the neighbourhood shaping s. The same reasoning can be applied to edges.

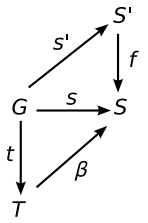


Figure 10. Proof of Statement 2

Show that f and f^{-1} are abstraction morphisms This is not difficult to show using the following facts:

1. for all nodes w, w' of T', $w \simeq_{T'} w'$ if, and only if, $f(w) \simeq_{T'} f(w')$. This follows from the fact that $\simeq_{T'} = \sim_i$ and $\simeq_S = \equiv_i$, and using the dependence and characteristics of the shapings and abstraction morphisms s, t, β, β', f;
2. for all node or edge x of S, $s^{-1}(x) = (t \circ \beta' \circ f)^{-1}(x)$. This fact together with the previous one ensure equality of the multiplicity functions of S and T'.

B.2 Proof of Statement 2

We start by defining f first as a mapping, then showing that it is indeed a morphism, a bijection, and f and f^{-1} are abstraction morphisms.

Define a mapping f such that $s = f \circ s'$ Remind that $s' : G \to S'$ is the neighbourhood shaping of G. As s' is a shaping morphism, it is surjective, thus any node (resp. edge) of S' can be written as $s'(x)$ for x a node (resp. edge) of G. Then f is defined by: for any $x \in NG \cup E_G$, $f(s'(x)) = s(x)$. Thus, $s = f \circ s'$ by definition.

Show that f is a morphism Showing that f is a morphism is not difficult using that s' and s are morphisms.

Show that f is a bijection The morphism f is surjective as s' and s are surjective. For injection, we have to show that for all nodes v, v' of G, if $s'(v) \neq s'(v')$, then $s(v) \neq s(v')$ (and the same for edges, but it easily follows). As s' is the neighbourhood shaping of G, we know that $s'(v) \neq s'(v')$ if, and only if, $v \not\equiv_i v'$. On the other hand, as $s = \beta \circ t$ and β is the neighbourhood shaping of T, we have that $s(v) \neq s(v')$ if, and only if, $t(v) \not\sim_i v'$. Now, by Corollary 58 we know that $v \not\equiv_i v'$ if, and only if, $t(v) \not\sim_i v'$, which shows that f in injective.

Show that f and f^{-1} are abstraction morphisms As for Statement 1, it is not difficult to show using the results that have already been established.

B.3 Proofs of Lemma 57 and Corollary 58

Let us first show Lemma 57, then we will argue how its proof is used for deducing Corollary 58.

Proof of Lemma 57
Lemma 57 *Let G be a graph, S, T be a shapes, $s : G \to S$, $t : G \to T$ be shaping morphisms, and $\beta : T \to S$ be an abstraction morphism such that $s = \beta \circ t$. If s is the neighbourhood shaping of G, then $\sim_{i-1}$ is defined on the nodes of T, and $\simeq_T \subseteq \sim_{i-1}$.*

We show by induction on $0 \leq j \leq i-1$ that

IHA(j): $\sim_j$ is defined,
IHB(j): assuming that IHA(j), $\simeq_T \subseteq \sim_j$,
IHC(j): assuming IHA(j) and IHB(j), $\forall w \in N_G$, $t([w]_{\equiv_j}) = [t(w)]_{\sim_j}$.

We start with the following intermediate result.

Fact 59 *For any $k \leq i$, it holds that*

$$\forall v, v' \in N_G, \quad t(v) \simeq_T t(v') \quad \text{implies} \quad v \equiv_k v'$$

Proof. The proof of this fact goes as follows.

$$\begin{array}{ll} t(v) \simeq_T t(v') & \Longrightarrow \text{ (β is an abstraction morphism)} \\ \beta(t(v)) \simeq_S \beta(t(v')) & \Longleftrightarrow \text{ ($s = \beta \circ t$)} \\ s(v) \simeq_s (v') & \Longleftrightarrow \text{ (s is the level i neighbourhood shaping of G)} \\ v \equiv_i v & \Longrightarrow \text{ (holds for any $j \geq i$)} \\ v \equiv_j v' & \end{array}$$

◀

Going back to the proof of the lemma, using Fact 59 and definition of $\subseteq$ for equivalence relations, we can see that for IHB(j) it is enough to show the following

$$\forall v, v' \in N_G, \quad v \equiv_j v' \text{ implies } t(v) \sim_j t(v') \tag{1}$$

Base case For the base case, $j = 0$. For IHA(0), $\sim_0$ is always defined.

For IHB(0), we have to show (1). It is the case that for any nodes $v, v' \in N_G$, $t(v) \sim_0 t(v')$ if, and only if, $v \equiv_0 v'$; this is because $\sim_0$ and $\equiv_0$ only take into account labels for grouping nodes and labels are preserved and reflected by shaping. The same argument allows to see that IHC(0) also holds.

General case Assume that the induction hypotheses IHA(k), IHB(k) and IHC(k) hold for any $k < j$. Let us show that they hold for j.

For IHA(j), by definition $\sim_j$ is defined if $\sim_{j-1}$ is defined and $\simeq_T \subseteq \sim_{j-1}$, thus IHA($j$) follows from IHA($j-1$) and IHB($j-1$).

For IHB(j), we first establish two intermediary results in Fact 60 and Fact 61.

Fact 60 *It holds that*

$$\forall v \in N_G, \quad \forall u \in N_G, \quad \forall \mathsf{a} \in \mathsf{Lab}, \quad \sum_{K \in N_T/\simeq_T \mid K \subseteq [t(u)]_{\sim_{j-1}}}^{\mu} \mathsf{mult}_{\mathsf{out},T}(t(v), \mathsf{a}, K) \;=\; \left| v \rhd\!\rhd^{\mathsf{a}}_G [u]_{\equiv_{j-1}} \right|_\mu .$$

Proof. By definition, $\mathsf{mult}_{\text{out},T}(t(v),\mathsf{a},K)$ is equal to $\left|v \rhd\!\!\rhd^{\mathsf{a}}_G(t^{-1}(K))\right|_\mu$ (for all v,a,K). Note now that the $K \in N_T/\simeq_T$ summed-up above form a partition of the set $[t(u)]_{\sim_{j-1}}$; this comes from the fact that $\simeq_T \subseteq N_T/\sim_{j-1}$ (IHB$(j-1)$). Then, by definition of set multiplicity function,

$$\sum_{K\in N_T/\simeq_T | K\subseteq [t(u)]_{\sim_{j-1}}}^{\mu} \mathsf{mult}_{\text{out},T}(t(v),\mathsf{a},K) \;=\; \left|v \rhd\!\!\rhd^{\mathsf{a}}_G(t^{-1}([t(u)]_{\sim_{j-1}}))\right|_\mu$$

and it holds for all $v \in N_G$, all $u \in N_G$ and all label a. Now by IHC$(j-1)$, $[t(u)]_{\sim_{j-1}} = t([u]_{\equiv_{j-1}})$, therefore $t^{-1}([t(u)]_{\sim_{j-1}}) = t^{-1}(t([u]_{\equiv_{j-1}})) = [u]_{\equiv_{j-1}}$. This terminates the proof of Fact 60. ◀

Fact 61 *It holds that*

$$\forall v,v' \in N_G, \quad v \equiv_j v' \iff t(v) \sim_j t(v')$$

Proof. By definition of the neighbourhood equivalence relations on graphs and shapes,

$$v \equiv_j v' \quad\iff\quad \forall u \in N_G, \quad \forall \mathsf{a} \in \mathsf{Lab}, \quad \left|v \rhd\!\!\rhd^{\mathsf{a}}_G[u]_{\equiv_{j-1}}\right|_\mu = \left|v' \rhd\!\!\rhd^{\mathsf{a}}_G[u]_{\equiv_{j-1}}\right|_\mu$$

and

$$t(v) \sim_j t(v') \quad\iff\quad \sim_{j-1} \text{ is defined and } \forall u \in N_G, \quad \forall \mathsf{a} \in \mathsf{Lab},$$
$$\sum_{K\in N_T/\simeq_T | K\subseteq [t(u)]_{\sim_{j-1}}}^{\mu} \mathsf{mult}_{\text{out},T}(t(v),\mathsf{a},K) = \sum_{K\in N_T/\simeq_T | K\subseteq [t(u)]_{\sim_{j-1}}}^{\mu} \mathsf{mult}_{\text{out},T}(t(v'),\mathsf{a},K).$$

The statement of Fact 61 immediately follows from these definitions and Fact 60. ◀

Back to the proof of IHB(j), we have to show (1). This immediately follows from Fact 59 and Fact 61.

Finally, for IHC(j), we have to show that $\forall w \in N_G$, $t([w]_{\equiv_j}) = [t(w)]_{\sim_j}$. By definition, $t([w]_{\equiv_j})$ is the set

$$\left\{ t(w') \;\middle|\; \forall u \in N_G,\ \forall \mathsf{a} \in \mathsf{Lab},\ \left|w' \rhd\!\!\rhd^{\mathsf{a}}_G[u]_{\equiv_{j-1}}\right|_\mu = \left|w \rhd\!\!\rhd^{\mathsf{a}}_G[u]_{\equiv_{j-1}}\right|_\mu \right\}$$

and $[t(w)]_{\sim_j}$ is the set

$$\left\{ t(w') \;\middle|\; \forall u \in N_G,\ \forall \mathsf{a} \in \mathsf{Lab},\ \sum_{K\in N_T/\simeq_T | K\subseteq [t(u)]_{\sim_{j-1}}}^{\mu} \mathsf{mult}_{\text{out},T}(t(w'),\mathsf{a},K) = \sum_{K\in N_T/\simeq_T | K\subseteq [t(u)]_{\sim_{j-1}}}^{\mu} \mathsf{mult}_{\text{out},T}(t(w),\right.$$

According to Fact 60, these two sets are equal. This terminates the proof for IHC(j), and thus the proof of Lemma 57.

Proof of Corollary 58

Corollary 58 *Let G be a graph, S,T be a shapes, $s : G \to S$, $t : G \to T$ be shaping morphisms, and $\beta : T \to S$ be an abstraction morphism such that $s = \beta \circ t$. If at least one of these conditions is verified:*

1. *s is the neighbourhood shaping of G,*

2. β is the neighbourhood shaping of T,

then for any $0 \leq j \leq i$, and fol all $v, v' \in N_G$ and all $e, e' \in E_G$,

$$v \equiv_j v' \quad \Leftrightarrow \quad t(v) \sim_j t(v') \qquad \textit{and} \qquad e \equiv_j e' \quad \Leftrightarrow \quad t(e) \sim_j t(e').$$

We only show the corollary for nodes, the statement for edges easily follows by definitions. One can notice that the statement of this corollary is very similar to what has been shown in Fact 61. However, there are some small differences either in the hypotheses, or in what has been proved. We will show how the proof of Fact 61 can be completed for showing the corollary.

The first difference is that Fact 61 is shown for $j < i$. However, the proof of Fact 61 can be extended for $j = i$. Figure 11 illustrates what needs to be shown for Fact 61 with $j = i$. That is, for showing Fact 61 with $j = i$, we use Fact 60 with $j = i$; the proof of Fact 60 for j uses IHB$(j-1)$ and IHC$(j-1)$. Thus, it is enough to show that IHC(0) and IHB(j) for all $0 \leq j \leq i-1$ hold. (Here IHC() and IHB() denote the induction hypotheses used for proving Lemma 57).

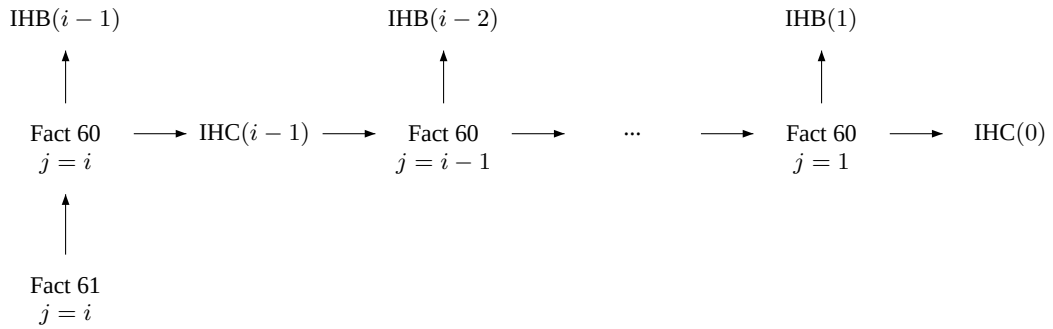


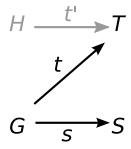
Figure 11. Proof dependence for Fact 61.

Now, if condition 1 of the corollary holds, it corresponds exactly to the hypotheses of Lemma 57. Thus IHC(0) and IHB(j) for all $0 \leq j \leq i-1$ can be shown. If condition 2 of the corollary holds, IHB(j) holds for all $0 \leq j \leq i-1$. Remind that IHB(j) states that $\simeq_T \subseteq \sim_j$, and this is the case because the neighbourhood shaping β of T exists. Moreover, it is immediate that $\forall w \in N_G$, $t([w]_{\equiv_0}) = [t(w)]_{\sim_0}$ (that is, IHC(0)) holds under condition 2.

C Proof of Lemma 24

Lemma 24 *If two neighbourhood shapes have a common concretisation, then they are isomorphic.*

Proof. (Sketch) We show that any shaping to a neighbourhood shape is a neighbourhood shaping. That is, if G is a graph, $s : G \to S$ is its neighbourhood shaping and $t : G \to T$ is some arbitrary shaping with T being a neighbourhood shape (i.e. there exists a graph H with neighbourhood shaping $t' : H \to T$), then T and S are isomorphic. We will consider that S and T are given with their canonical representation (see Section 4.2), and we will show that S and T have the same canonical representation. By Lemma 29, this implies that S and T are isomorphic. Let v be a node of G. Remind



that $s(v)$ and $t(v)$ are canonical names. If we show that $s(v) = t(v)$ (as a canonical name), then it would imply that the set of node canonical names of S and T are the same (remind that the morphisms s and t are surjective). The same is similarly shown for edges.

A level i canonical name is of the form $(C, \mathit{out}, \mathit{in})$, where *out* and *in* are multiplicity functions, and C is a level $i-1$ canonical name. Of course, C has as first component a level $i-2$ canonical name, and so on. Thus, a level i canonical name somehow contains a level j canonical name for any $0 \leq j \leq i$. In the following we call it its level j component.

We show that (for any $v \in N_G$):

- for all $0 \leq j \leq i$, the level j components of $t(v)$ and $s(v)$ (considered as node canonical names) are the same,
- $s(v)$ and $t(v)$ have the same *out* and *in* multiplicity functions.

The proof of these two statements goes by induction on j. We omit it here. □

D Proof of Lemma 29

.

Lemma 29 *Let G, H be graphs, and let $i \geq 1$. The level i neighbourhood shapes of G and H are isomorphic if, and only if, $\mathcal{C}_G$ and $\mathcal{C}_H$ are equal.*

Proof. For the right-to-left direction, we will show that $\mathcal{C}_G$ defines uniquely a shape S and the shape S is isomorphic to the level i neighbourhood shape of G. Let $S = (G_S, \simeq, \mathsf{mult}_\mathrm{n}, \mathsf{mult}_\mathrm{out}, \mathsf{mult}_\mathrm{in})$ be the shape defined by:

- $N_S = \mathcal{N}$, $E_S = \mathcal{E}$ and for any $e = (C, \mathsf{a}, C')$ in $\mathcal{E}$, $\mathsf{src}_S(e) = C$, $\mathsf{tgt}_S(e) = C'$ and $\mathsf{lab}_S(e) = \mathsf{a}$;
- $\simeq$ is the smallest equivalence relation such that $C \simeq C'$ if C and C' have the same first component. Remind that C and C' are level i canonical names and their first component is a level $i-1$ canonical name;
- $\mathsf{mult}_\mathrm{n} = \mathsf{mult}$;
- for all $C \in N_S$, $\mathsf{a} \in \mathsf{Lab}$, and $K \in \mathsf{NCan}^{i-1}$, $\mathsf{mult}_\mathrm{out}(C, \mathsf{a}, K) = \mathit{out}_C(K, \mathsf{a})$, where out_C is the function second component of C (remind that C is a level i canonical name);
- for all $C \in N_S$, $\mathsf{a} \in \mathsf{Lab}$, and $K \in \mathsf{NCan}^{i-1}$, $\mathsf{mult}_\mathrm{out}(C, \mathsf{a}, K) = \mathit{in}_C(K, \mathsf{a})$, where in_C is the function third component of C (remind that C is a level i canonical name).

Note that S is indeed a shape. We do not show this here, but a similar construction is introduced and shown correct in Section 4.3.

Let us now show that S is isomorphic to the level i neighbourhood shape of G. Consider T, the level i neighbourhood shape of G, and consider the function $f = (f_\mathrm{n}, f_\mathrm{e}), f_\mathrm{n} : N_S \to N_T, f_\mathrm{e} : E_S \to E_T$ defined by:

- $f_\mathrm{n}(C) = \{v \in N_G \mid \mathsf{name}^i_G(v) = C\}$;
- $f_\mathrm{e}(C_\mathrm{e}) = \{e \in E_G \mid \mathsf{name}^i_G(e) = C_\mathrm{e}\}$.

Using Lemma 28, f_{n} and f_{e} are bijections, and it is not difficult to see that f is a graph morphism, thus a graph isomorphism. Showing that f is an abstraction morphism is quite technical, but not difficult, and only uses definitions of S, of T, of abstraction morphism and of neighbourhood shaping. This terminates the proof of the right-to-left direction.

Now, for the left-to-right direction, let S be the level i neighbourhood shape of G with neighbourhood shaping $s : G \to S$, and let T be the level i neighbourhood shape of H with neighbourhood shaping $t : H \to T$. Suppose that S and T are isomorphic with isomorphism $f : S \to T$. We use the modal logic to prove that $\mathcal{C}_G$ and $\mathcal{C}_H$ are equal. We are using the following results on the modal logic.

(1) Neighbourhood shaping preserves and reflects logic formulae (Proposition 53).
(2) For any graph G, any two nodes v, w of G, v, w are level i neighbourhood equivalent if, and only if, v, w have the same level i canonical names, if, and only if, v, w satisfy the same depth i logic formulae (Lemma 28 and Lemma 55).
(3) For any level i canonical name C, there exists a representative formula ϕ_C such that in any graph G, any node v of G, $\mathsf{name}^i_G(v) = C$ if, and only if, $G, v \models \phi_C$ (Lemma 56).
(4) By (1), (2) and (3), we can deduce that for any graph G and $i \geq 1$, if S is the level i neighbourhood shape of G with corresponding shaping $s : G \to S$, and if $C = \mathsf{name}^i_G(v)$ for some v node of G, then $S, s(v) \models \phi_C$.

Let $\mathcal{C}_G = (\mathcal{N}_G, \mathcal{E}_G, \mathsf{mult}_G)$ and $\mathcal{C}_H = (\mathcal{N}_H, \mathcal{E}_H, \mathsf{mult}_H)$. Remark first that the modal logic cannot distinguish isomorphic structures, and this holds both for graph and shapes.This means that $(\star)$ if v is a node of S, then for any level i logic formula ϕ, $S, v \models \phi$ if, and only if, $T, f(v) \models \phi$. Now, let $C \in \mathcal{N}_G$, and let v be a node of G s.t. $\mathsf{name}^i_G(v) = C$. Then, by (3), $G, v \models \phi_C$, and by (4), $S, s(v) \models \phi_C$. Now, by $(\star)$ we deduce that $T, f(s(v)) \models \phi_C$. By preservation and reflection of the logic (by (1)), we have that for any $w \in t^{-1}(f(s(v)))$ node of H, $H, w \models \phi_C$. By (3), we deduce that C is the level i canonical name of $w \in N_H$, thus $C \in \mathcal{N}_H$. That is, we just showed that $\mathcal{N}_G \subseteq \mathcal{N}_H$. Symmetrically we can show that $\mathcal{N}_H \subseteq \mathcal{N}_G$, and thus $\mathcal{N}_G = \mathcal{N}_H$.

It is not difficult to prove that also $\mathcal{E}_G = \mathcal{E}_H$, and the same for the multiplicity functions. □

E Proof of Proposition 51

Proposition 51 *Let $\mathcal{P}$ be a set of atomic propositions, S, T be shapes, $\gamma_S : N_S \to 2^{\mathcal{P}}$ and $\gamma_T : N_T \to 2^{\mathcal{P}}$ be valuation functions such that $\simeq_T$ is compatible with γ_T, and let $\alpha : S \to T$ be an abstraction morphism.*

(preservation): *If α preserves $\mathcal{P}$ under γ_S, γ_T, then α preserves the negation free fragment of $\mathcal{L}_1(\mathcal{P})$ under γ_S, γ_T.*
(reflection): *If α reflects $\mathcal{P}$ under γ_S, γ_T, then α reflects the negation free fragment of $\mathcal{L}_1(\mathcal{P})$ under γ_S, γ_T.*
(preservation and reflection): [7] *If α preserves and reflects $\mathcal{P}$ under γ_S, γ_T, then α preserves and reflects $\mathcal{L}_1(\mathcal{P})$ (possibly with negation) under γ_S, γ_T.*

[7] Preservation for formulae with negation may seem contradictory with the Morphism Preservation Theorem for finite structures [13]. This theorem states that a first-order formula is preserved by morphism if, and only if, it is equivalent to an existential positive formula. Some modal logic formulae cannot be expressed in first-order logic without negation (*e.g.* $\neg\langle\mathsf{a}\rangle^{\lambda}\cdot\mathtt{tt}$.) However, in our case, shapes contain information on interpretation of such negated formulae, by means of the multiplicity functions, which explains this apparent contradiction.

The rest of the section is devoted to the proof of this proposition.

Let $\mathcal{M}(\mathcal{P})$ be the set of logic formulae defined by the symbol ϕ in the following syntax:

$$\phi ::= \mathtt{tt} \mid \rangle \mathsf{a} \langle^{\lambda} \cdot \psi \mid \langle \mathsf{a} \langle^{\lambda} \cdot \psi \mid \phi \vee \phi \mid \phi \wedge \phi \mid \neg \phi$$
$$\psi ::= \mathsf{p} \mid \psi \vee \psi \mid \psi \wedge \psi \mid \neg \psi \mid \mathtt{tt}$$

The set of propositions defined by ψ above is denoted $Bool(\mathcal{P})$. It is not difficult to see that ϕ defines a grammar for $\mathcal{L}_1(\mathcal{P})$, thus $\mathcal{M}(\mathcal{P})$ is exactly the logic $\mathcal{L}_1(\mathcal{P})$. We will use this grammar in the proof for an induction on the structure of a $\mathcal{L}_1(\mathcal{P})$ formula.

Let us state Proposition 51 using the previous notations. Let $\mathcal{P}$ be a set of atomic propositions and S, T be shapes, $\gamma_S : N_S \to 2^{\mathcal{P}}$ and $\gamma_S : N_S \to 2^{\mathcal{P}}$ be valuations such that $\simeq_T$ is compatible with γ_T, and $\alpha : S \to T$ be an abstraction morphism. If α preserves $\mathcal{P}$, then for any node v in N_S and for any $\mathcal{M}(\mathcal{P})$ formula ϕ without negation

$$\text{(preservation)} \quad S, v, \gamma_S \models \phi \text{ implies } T, \alpha(v), \gamma_T \models \phi$$

If α reflects $\mathcal{P}$, then for any node v in N_S and for any $\mathcal{M}(\mathcal{P})$ formula ϕ without negation

$$\text{(reflection)} \quad T, \alpha(v), \gamma_T \models \phi \text{ implies } S, v, \gamma_S \models \phi$$

If moreover α preserves and reflects $\mathcal{P}$, then for any node v it N_S, and for any $\mathcal{M}(\mathcal{P})$ formula ϕ (possibly with negation), both (preservation) and (reflection) hold.

For brevity, we will omit the valuations γ_S and γ_T, as they are fixed for each of the shapes.

We first show some preliminary lemmas.

Lemma 62 (α preserves / reflects $Bool(\mathcal{P})$). *If α preserves $\mathcal{P}$, then α preserves $Bool(\mathcal{P})$, that is, for any $Bool(\mathcal{P})$ formula ψ without negation and for any node v in N_S, if $S, v \models \psi$, then $T, \alpha(v) \models \psi$.*

If α reflects $\mathcal{P}$, then α reflects $Bool(\mathcal{P})$ without negation, that is, for any $Bool(\mathcal{P})$ formula ψ without negation and for any node v in N_S, if $T, \alpha(v) \models \psi$, then $S, v \models \psi$.

If α preserves and reflects $\mathcal{P}$, then α preserves and reflects $Bool(\mathcal{P})$, that is, for any $Bool(\mathcal{P})$ formula ψ and for any node v in N_S, $S, v \models \psi$, if, and only if, $T, \alpha(v) \models \psi$.

Proof. The proof is an easy induction on the structure of ψ that we will omit. □

Lemma 63 ($\simeq_T$ is compatible with $Bool(\mathcal{P})$). *If $\simeq_T$ is compatible with γ_T, for any two nodes v, w in N_T and for any formula ψ in $Bool(\mathcal{P})$ if $v \simeq_T w$, then $T, v, \gamma_T \models \psi$ if, and only if, $T, w, \gamma_T \models \psi$.*

Proof. By induction on the structure of ψ; the base case for $\phi = \mathsf{p}$ uses the fact that $\simeq_T$ is compatible with $\mathcal{P}$.

We call this property $\simeq_T$ *is compatible with* $Bool(\mathcal{P})$, in the sense that two $\simeq_T$-equivalent nodes satisfy the same $Bool(\mathcal{P})$ formulae.

Let us now go to the proof of Proposition 51. Consider a node v in N_S fixed from now on. We first show preservation.

E.1 Preservation

Assume that α preserves $\mathcal{P}$, and let ϕ be a $\mathcal{M}(\mathcal{P})$ formula without negation s.t. $S, v \models \phi$. We will show that $T, \alpha(v) \models \phi$ and the proof goes by induction on the structure of ϕ. For the base case, either $\phi = \mathtt{tt}$, and then the proposition is trivial, or ϕ is in $Bool(\mathcal{P})$ without negation, in which case the proposition follows from Lemma 62. For the induction step, if $\phi = \phi_1 \vee \phi_2$ or $\phi = \phi_1 \wedge \phi_2$, then, by definition of satisfaction and by induction hypothesis, preservation property easily follow. Let us now show the preservation for $\phi = \langle \mathsf{a} \rangle^{\lambda} \cdot \psi$ for some ψ in $Bool(\mathcal{P})$ without negation. By definition, $S, v \models \langle \mathsf{a} \rangle^{\lambda} \cdot \psi$ if, and only if,

$$\sum_{D \in X}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, D) \geq \lambda$$

and $T, \alpha(v) \models \langle \mathsf{a} \rangle^{\lambda} \cdot \psi$ if, and only if,

$$\sum_{C \in Y}^{\mu} \mathsf{mult}_{\text{out},T}(\alpha(v), \mathsf{a}, C) \geq \lambda$$

where $X_{S,\psi}$ and $X_{T,\psi}$ are the sets

$$X = \{D \in N_S/{\simeq_S} \mid \forall w \in D.\ S, w \models \psi\}$$
$$Y = \{C \in N_T/{\simeq_T} \mid \forall w \in C.\ T, w \models \psi\}$$

By definition of abstraction, $\sum_{C \in Y}^{\mu} \mathsf{mult}_{\text{out},T}(\alpha(v), \mathsf{a}, C)$ is equal to

$$\sum_{C \in Y}^{\mu} \quad \sum_{D \in (\alpha^{-1}(C))/{\simeq_S}}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, D) \tag{2}$$

Now, for any two different C_1 and C_2 group-equivalent classes in Y, the sets of nodes $\alpha^{-1}(C_1)$ and $\alpha^{-1}(C_2)$ are different (as α is functional on N_S). Then, by commutativity associativity of μ-sum, the sum in (2) is equal to

$$\sum_{D \in (\alpha^{-1}(\bigcup_{C \in Y} C))/{\simeq_S}}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, D). \tag{3}$$

Consider now the set of nodes

$$Y' = \{w \in N_T \mid T, w \models \psi\}.$$

As $\simeq_T$ is compatible with $Bool(\mathcal{P})$ (Lemma 63) and ψ is a formula in $Bool(\mathcal{P})$, we have that if two nodes w, w' are in some $C \in N_T/{\simeq_T}$, then $T, w \models \psi$ if, and only if, $T, w' \models \psi$. We deduce that if Y' contains some node w of the group-equivalence class C, then $C \subseteq Y'$. Thus, $Y = Y'/{\simeq_T}$, or, equivalently, $\bigcup_{C \in Y} C = Y'$. Now, α being a morphism, $\alpha^{-1}(Y')$ is the set of nodes X':

$$X' = \{w \in N_S \mid T, \alpha(w) \models \psi\}.$$

Therefore, the sum in (3) is equivalent to

$$\sum_{D \in X'/{\simeq_S}}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, D). \tag{4}$$

Now, by preservation of $Bool(\mathcal{P})$, we have that $D \in X$ implies that D is in the set

$$\left\{ D' \in N_S/{\simeq_S} \,\middle|\, \forall w \in D'.T, \alpha(w) \models \psi \right\}$$

and it is easy to see that then $D \in X'/{\simeq_S}$. That is, the sum in (4) has more components than the sum $\sum_{D \in X}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, D)$, which by hypothesis we know being greater than λ. As the sum in (4) is equivalent to $\sum_{C \in Y}^{\mu} \mathsf{mult}_{\text{out},T}(\alpha(v), \mathsf{a}, C)$, we conclude that this latter is greater than λ, thus ϕ is preserved.

E.2 Reflection

Assume that α reflects $\mathcal{P}$, and let ϕ be a $\mathcal{M}(\mathcal{P})$ formula without negation s.t. $T, \alpha(v) \models \phi$. We will show that $S, v \models \phi$ and the proof goes by induction on the structure of ϕ. For the cases $\phi = \mathtt{tt}$, ϕ in $Bool(\mathcal{P})$, $\phi = \phi_1 \vee \phi_2$ and $\phi = \phi_1 \wedge \phi_2$, the proof goes as for preservation.

For ϕ being a modality formula, the proof is close to the proof of preservation. However, there is a particular point on which one has to pay attention, due to the asymmetry in the hypotheses of the proposition, namely, we have a hypothesis for compatibility of $\simeq_T$ with γ_T, but there is no a similar hypothesis for $\simeq_S$ and γ_S. Therefore, we briefly remind the steps of the proof that are common with the proof for preservation, and then do the remaining part.

Let $\phi = \langle \mathsf{a} \rangle^{\lambda} \psi$ for some ψ in $Bool(\mathcal{P})$ without negation. We have to show that $\sum_{D \in X}^{\mu} \mathsf{mult}_{\text{out},S}(v, \mathsf{a}, D) \geq \lambda$ using that $\sum_{C \in Y}^{\mu} \mathsf{mult}_{\text{out},T}(\alpha(v), \mathsf{a}, C) \geq \lambda$, where the sets X and Y are as for preservation. As for preservation, we can establish that $\sum_{C \in Y}^{\mu} \mathsf{mult}_{\text{out},T}(\alpha(v), \mathsf{a}, C)$ is equal to the sum in (4). It is then enough to show that

$$(\star) \qquad \text{if } D \in X'/{\simeq_S}, \text{ then } D \in X.$$

Consider the set X''

$$X'' = \{ w \in N_S \mid S, w \models \psi \text{ and } T, \alpha(w) \models \psi \}.$$

By reflection of $Bool(\mathcal{P})$, and ψ being a $Bool(\mathcal{P})$ formula, we deduce that $D \in X'/{\simeq_S}$ implies $D \in X''/{\simeq_S}$. Using the definition of X, one can see that then for $(\star)$ it is enough to show

$$(\star\star) \qquad \text{if } D \in X''/{\simeq_S}, \text{ then } D \in N_S/{\simeq_S}.$$

This remains to show that the set X'' contains only entire classes of nodes for $\simeq_S$. That is where the condition $T, \alpha(w) \models \psi$ in the definition of X'', which may seem redundant, is used to compensate the asymmetry of the hypotheses pointed out before. Let us show that if $w \simeq_S w'$, and $S, w \models \psi$, and $T, \alpha(w) \models \psi$, then $S, w' \models \psi$, which is sufficient for $(\star\star)$.

By α being an abstraction morphism, we know that $w \simeq_S w'$ implies $\alpha(w) \simeq_T \alpha(w')$. By compatibility of $\simeq_T$ with $Bool(\mathcal{P})$ (Lemma 63), it follows that $T, \alpha(w) \models \psi$ if, and only if, $T, \alpha(w') \models \psi$. By hypothesis, $T, \alpha(w) \models \psi$, then also $T, \alpha(w') \models \psi$. Finally, by reflection of ψ, we deduce that $S, w' \models \psi$.

E.3 Preservation and reflection

We finally show preservation and reflection in presence of the additional hypothesis that α preserves and reflects $\mathcal{P}$. The proof is very similar as for the previous cases, and goes by induction on the structure of ϕ. More precisely, we show that for any formula ϕ, $S, v \models \phi$ if, and only if, $T, \alpha(v) \models \phi$. For the base case, if ϕ is $\mathtt{tt}$ it is trivial, and if ϕ is a formula from $Bool(\mathcal{P})$, the result follows from Lemma 62. For the induction, if ϕ is a forward or backward modality formula, the proof goes on the

same way that the proof for preservation and reflection. For $\phi = \phi_1 \vee \phi_2$, the result is an immediate consequence of the definition of satisfaction. The only remaining case is $\phi = \neg\phi'$, for which we use that preservation of the negated formula $\neg\phi'$ is equivalent to reflection of the sub-formula ϕ'. That is, $S, v \models \neg\phi$ if, and only if, $S, v \not\models \phi$ if, and only if,, by induction hypothesis, $T, \alpha(v) \not\models \phi$ if, and only if, $T, \alpha(v) \models \neg\phi$.

F Proof of Lemma 45

The result of the following lemma is used without proof in Lemma 45.

Lemma 64. *Let U'' be a shape that admits a level i neighbourhood shaping, and let the shape U' be obtained from U'' by removing some unique node labels. Then U' also admits a level i neighbourhood shaping. Moreover, for all node v in $N_{U'}$ and for all $1 \leq j \leq i$, $[v]_{\sim_j}$ in U'' is included into $[v]_{\sim_j}$ in U'.*

Proof. We denote N the set of nodes of U' and U'', and we denote $[v]^U_j$ the equivalence class of the node v for the equivalence relation $\sim_j$ in the shape U, where U may be one of U' or U''. We show, by induction on j for $j \in 1..i$, that

$$IH(j) \qquad \sim_j \text{ is defined on } U' \text{ and for all } v \text{ in } N,\ [v]^{U''}_{\sim_j} \subseteq [v]^{U'}_{\sim_j}$$

For the base case, $IH(0)$ immediately follows from definitions of $\sim_0$ and the shapes U' and U''.

For the induction step, let $j > 0$. Remind that $\sim_j$ is defined in U' if $\simeq_{U'} \subseteq \sim_{j-1}$, or, equivalently, for all node v, $[v]_{\simeq_{U'}} \subseteq [v]^{U'}_{\sim_{j-1}}$. By definition of U'' we know that $[v]_{\simeq_{U'}} = [v]_{\simeq_{U''}}$. As U'' admits a level i neighbourhood shaping, we have $[v]_{\simeq_{U''}} \subseteq [v]^{U'}_{\sim_{j-1}}$, and by $IH(j-1)$, $[v]^{U''}_{\sim_{j-1}} \subseteq [v]^{U'}_{\sim_{j-1}}$.

Next we have to show that $[v]^{U''}_{\sim_j} \subseteq [v]^{U'}_{\sim_j}$. Suppose $v \sim_j v'$ in U'' and let's show that also $v \sim_j v'$ in U'. By definition, this latter holds if, and only if, for all $C \in N \,/\, \sim_{j-1}$, and for all label a,

$$\sum_{K \in N/\simeq_{U'} \mid K \subseteq C}^{\mu} \mathsf{mult}_{\mathsf{out}}(w, \mathsf{a}, K) = \sum_{K \in N/\simeq_{U'} \mid K \subseteq C}^{\mu} \mathsf{mult}_{\mathsf{out}}(w', \mathsf{a}, K)$$

and analogously for incoming edges multiplicity function. By $IH(j-1)$, the set C is the union of disjoint sets $C_1, \ldots, C_n$ that are all equivalence classes for $\sim_{j-1}$ in U'', *ie*

$$\sum_{K \in N/\simeq_{U'} \mid K \subseteq C}^{\mu} \mathsf{mult}_{\mathsf{out},U'}(w, \mathsf{a}, K) = \sum_{l \in 1..n}^{\mu} \sum_{K \in N/\simeq_{U''} \mid K \subseteq C_l}^{\mu} \mathsf{mult}_{\mathsf{out},U''}(w, \mathsf{a}, K)$$

and the same for w'. This is well defined because the shapes U' and U'' have the same nodes and edges, the same multiplicities, and the same grouping relation. As $\sim_j$ is defined on U'', for any C_l the equality

$$\sum_{K \in N/\simeq_{U''} \mid K \subseteq C_l}^{\mu} \mathsf{mult}_{\mathsf{out},U''}(w, \mathsf{a}, K) = \sum_{K \in N/\simeq_{U''} \mid K \subseteq C_l}^{\mu} \mathsf{mult}_{\mathsf{out},U''}(w', \mathsf{a}, K)$$

holds, thus the equality of the whole sum holds.

Consider now the shape T'' as described in the sketch of the proof. We have to show that T'' admits a level i neighbourhood shaping. That is, it is enough to show that $\sim_j$ is defined in T'' for all $j \in 1..i$ ($\sim_0$ being always defined). We will show that for all $v \in N_{S''}$, $[v]_{\sim_j}$ in T'' is equal to $[v]_{\sim_j}$ in S''. It is enough as $\simeq_{T''}$ and $\simeq_{S''}$ coincide on nodes in $N_{S''}$, thus $\simeq_{S''} \subseteq \sim_j$ in S'' would imply $\simeq_{T''} \subseteq \sim_j$ in T'', and nodes in N^{new} have also singleton classes for the equivalence relations $\simeq_{T''}$ and $\sim_j$ (the latter because they contain fresh labels).

The proof that $[v]_{\sim_j}$ in T'' is equal to $[v]_{\sim_j}$ in S'' is quite technical, but does not use any difficult idea. We rather present it in an intuitive way. Suppose that $v \sim_j v'$ in S''. Then

1. either v and v' are both at distance j or less from some node in $c(L'') \cup N^{\text{new}}$ and their equivalence class is influenced by one or more of the fresh labels,
2. or v and v' are both far away from $c(L'') \cup N^{\text{new}}$.

Remark now that if a node w is at distance d from $c(L'')$ in S'', then it is at distance at least d from $c(L'') \cup N^{\text{new}}$ in T''. So, such a node may join the equivalence class of some other nodes.

G Proof of Lemma 55

Lemma 55 *Two nodes v, v' of a graph G are i-neigborhood equivalent if, and only if, the same $\mathcal{L}_i(\mathsf{Lab})$ formulae hold in v and in v'.*

The proof goes by induction on i. For brevity, we will write $v \models \phi$ instead of $G, v, \gamma \models \phi$ as the graph G and the valuation γ are fixed.

For the base case We have $i = 0$. For the $\Rightarrow$ direction, assume that $v \equiv_0 v'$. Then, by definition, $\mathsf{lab}(v) = \mathsf{lab}(v')$. Let ϕ be a $\mathcal{L}_0$ formula; by easy induction on the structure of ϕ one can show that $v \models \phi$ if, and only if, $v' \models \phi$. For the $\Leftarrow$ direction, assume that it is not the case that $v \equiv_0 v'$. Then we easily deduce that there is formula ϕ which holds in one of v, v' but not in the other; it is sufficient to take $\phi = \mathsf{a}$ where a is a label in $\mathsf{lab}(v) \cup \mathsf{lab}(v')$ but not in $\mathsf{lab}(v) \cap \mathsf{lab}(v')$ and we know by assumption that this label exists.

For the induction We have $i > 0$. For the $\Rightarrow$ direction, assume that $v \equiv_i v'$. We will show that for any $\mathcal{L}_i$ formula ϕ, $v \models \phi$ if, and only if, $v' \models \phi$ and the proof goes by induction on the structure of ϕ. The only interesting cases are for ϕ being $\langle a \rangle^{\lambda} \cdot \phi'$ and $\langle a \langle^{\lambda} \cdot \phi'$. Let us show it for $\langle a \rangle^{\lambda} \cdot \phi'$, the other case is symmetrical. So, let ϕ be the formula $\langle a \rangle^{\lambda} \cdot \phi'$. Then, by definition of the satisfaction relation, $v \models \phi$ if, and only if, $\left| v \rhd^{\mathsf{a}} \cap S_{\phi'} \lhd^{\mathsf{a}} \right|_{\mu} \geq \lambda$ and $v' \models \phi$ if, and only if, $\left| v' \rhd^{\mathsf{a}} \cap S_{\phi'} \lhd^{\mathsf{a}} \right|_{\mu} \geq \lambda$, where $S_{\phi'}$ denotes the set of nodes of G in which ϕ' holds. We will show that $\left| v \rhd^{\mathsf{a}} \cap S_{\phi'} \lhd^{\mathsf{a}} \right|_{\mu} = \left| v' \rhd^{\mathsf{a}} \cap S_{\phi'} \lhd^{\mathsf{a}} \right|_{\mu}$, which allows us to conclude that $v \models \phi$ if, and only if, $v' \models \phi$.

Let $N /\equiv_{i-1}$ denote the set of equivalence classes of nodes of G induced by the $\equiv_{i-1}$ equivalence relation. Let, for any C in $N /\equiv_{i-1}$, F_C denote the set of $\mathcal{L}_{i-1}$ formulae that hold in the nodes in C : $F_C = \{\psi \in \mathcal{L}_{i-1} \mid \forall v \in C : v \models \psi\}$. Then, as ϕ' is an $\mathcal{L}_{i-1}$ formula and using the induction hypothesis on i, it is easy to see that $S_{\phi'}$ is the set $\bigcup_{C \in N/\equiv_{i-1} \mid \phi' \in F_C} C \lhd^{\mathsf{a}}$. In this case, by distributivity of the multiplicity function over set union, we deduce that $\left| v \rhd^{\mathsf{a}} \cap S_{\phi'} \lhd^{\mathsf{a}} \right|_{\mu} = \sum^{\mu}_{C \in N/\equiv_{i-1} \mid \phi' \in F_C} |v \rhd^{\mathsf{a}} \cap C \lhd^{\mathsf{a}}|_{\mu}$. Now, by assumption we have that $v \equiv_i v'$, so by definition of the $\equiv_i$ equivalence relation we have that for any C in $N /\equiv_{i-1}$, $|v \rhd^{\mathsf{a}} \cap C \lhd^{\mathsf{a}}|_{\mu} = |v' \rhd^{\mathsf{a}} \cap C \lhd^{\mathsf{a}}|_{\mu}$. Thus, $\left| v \rhd^{\mathsf{a}} \cap S_{\phi'} \lhd^{\mathsf{a}} \right|_{\mu} = \sum^{\mu}_{C \in N/\equiv_{i-1}} |v' \rhd^{\mathsf{a}} \cap C \lhd^{\mathsf{a}}|_{\mu}$ and this last quantity is equal to $|v' \rhd^{\mathsf{a}} \cap C \lhd^{\mathsf{a}}|_{\mu}$.

For the $\Leftarrow$ direction,

Assume $v \not\equiv_{i+1} v'$. If this is the case, we know that there exist a label $\mathsf{a} \in \mathsf{Lab}$ and an equivalence class $C \in N_G /\equiv_i$ for which either $o_v = |v \rhd^{\mathsf{a}} \cap C \lhd^{\mathsf{a}}|_\mu \neq |v' \rhd^{\mathsf{a}} \cap C \lhd^{\mathsf{a}}|_\mu = o_{v'}$ or $i_v = |v \lhd^{\mathsf{a}} \cap C \rhd^{\mathsf{a}}|_\mu \neq |v' \lhd^{\mathsf{a}} \cap C \rhd^{\mathsf{a}}|_\mu = i_{v'}$. For the moment, let us believe that there exists a formula $\psi \in \mathcal{L}_i$ that only one such C satisfies. Let ϕ be:

$$\begin{array}{l} \rangle\mathsf{a}\rangle^{max(o_v, o_{v'})} \cdot \psi \text{ if } o_v \neq o_{v'} \\ \langle\mathsf{a}\langle^{max(i_v, i_{v'})} \cdot \psi \quad \text{otherwise} \end{array}$$

As a) no other $\equiv_i$-equivalence class satisfies ψ, and b) all nodes in C satisfy ψ (by inductive hypothesis); we can deduce that C is exactly the set of nodes that satisfies ψ. Thereby, ϕ is satisfied by only one of v or v'. To show that such a ψ exists, consider the following: for each $C' \in N_G /\equiv_i$, s.t. $C' \neq C$, we can find a $\psi_{C'} \in \mathcal{L}_i$ s.t. $C \models \psi$ and $C' \not\models \psi$[8], due to ind. hypothesis too. So we can take ψ to be $\psi = \bigwedge_{C' \in N_G/\equiv_i \mid C' \neq C} \psi_{C'}$

[8] Slight abuse of notation.