On the structure of graphs in the Caucal hierarchy

Achim Blumensath

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Abstract. We investigate the structure of graphs in the Caucal hierarchy. We provide criteria concerning the degree of vertices or the length of paths which can be used to show that a given graph does not belong to a certain level of this hierarchy. Each graph in the Caucal hierarchy corresponds to the configuration graph of some higher-order pushdown automaton. The main part of the paper consists of a study of such configuration graphs. We provide tools to decompose and reassemble their runs, and we prove a pumping lemma for higher-order pushdown automata.

Keywords. Caucal hierarchy; monadic second-order logic; higher-order pushdown automata

1 Introduction

The Caucal hierarchy is the class of relational structures which one obtains by alternated applications of monadic second-order interpretations and the Muchnik iteration (see [10, 12, 1, 3]) starting with the class of all finite structures. Since these operations preserve decidability of monadic second-order theories it follows that every structure in the Caucal hierarchy has a decidable monadic theory. Originally, Caucal [5] defined the hierarchy only for graphs where the above operations can be replaced by, respectively, inverse rational mappings and unravellings.

The lowest level of the Caucal hierarchy consists of the class of *prefix-recognisable* (also called *tree-interpretable*) structures. Restricted to graphs this is the class of all graphs that can be obtained from the configuration graph of some pushdown automaton by contracting each ε-transition. Recently, Carayol and Wöhrle [4] have extended this characterisation to the whole hierarchy: A graph belongs to the n-th level of the Caucal hierarchy if and only if it can be obtained by contracting ε-transitions from the configuration graph of some *higher-order pushdown automaton* of level n. This automaton model has been introduced by Maslov in [9]. It was used by Damm and Goerdt [6] to characterise the so-called OI-hierarchy which consists of the solutions of higher-order lambda schemes. Due to the connection with the Muchnik iteration and the Caucal hierarchy this work has recently received renewed attention in the study of hierarchies of trees or graphs with decidable monadic theories (see, e.g., [8]).

Naturally, the question arises of which structures are contained in the Caucal hierarchy and at what level they do appear. It is known that each structure in the hierarchy has a finite partition width (see [2] for definitions and details). Whereas the first level, the class of prefix-recognisable structures, is rather well understood, there are few structural results concerning the higher levels of the Caucal hierarchy.

This is the motivation of the results presented in this article. We study graphs in the Caucal hierarchy and we try to derive bounds on their degree or on the length of paths. Much of this work is based on a detailed investigation of configuration graphs of higher-order pushdown automata. We study paths in these graphs and we provide operations to decompose and reassemble them. Our main technical result will be a pumping lemma for higher-order pushdown automata. For *indexed grammars* (which correspond to pushdown automata of level 2), a pumping lemma was already proved by Hayashi [7]. The present article owes much to this paper.

The overview of this article is as follows. In Section 2 we fix notation and give basic definitions. We introduce higher-order pushdown automata in Section 3. Section 4 contains our first major result. We derive a bound on the outdegree of graphs in a given level of the Caucal hierarchy.

Sections 5 to 8 contain an in-depth investigation of configuration graphs of higher-order pushdown automata. In Section 5 we show how to replace, in all configurations of a given run, the bottom of the stack by another stack content without destroying the property of being a run. Usually this substitution operation can be applied only to parts of a run. Therefore, we introduce in Sections 6 and 7 two partial orders on runs, the so-called *weak* and *strong domination* *orders,* that will be used to decompose a given run into such parts. Section 8 contains a more detailed investigation of the strong domination order and a proof that it contains arbitrary long chains. In the Section 9 we apply the tools developed in the second part of the article to prove a pumping lemma for higher-order pushdown automata.

2 Trees and the Caucal hierarchy

Besides (directed) graphs $\mathfrak{G} = (V, E)$ we will also consider relational structures $\mathfrak{A} = (A, R_0, \dots, R_r)$ (with finitely many relations). Note that we do not assume graphs and structures to be finite. In fact, we will mostly consider countably infinite ones.

Definition 2.1. Let Σ be a set. The *prefix ordering* $\preceq$ on Σ^* is defined by

$$x \preceq y \quad :\text{iff} \quad y = xz \text{ for some } z \in \Sigma^* .$$

Definition 2.2. An *unlabelled tree* is a partial order $(T, \preceq)$ where $T \subseteq \omega^*$, $\preceq$ is the prefix ordering, and T satisfies the following closure properties:

- If $u \in T$ and $v \preceq u$ then $v \in T$.
- If $uk \in T$ and $i < k$ then $ui \in T$, for $i, k \in \omega$.

A Λ-*labelled tree* is a function $t : T \to \Lambda$ where the domain $\mathrm{dom}(t) := T \subseteq \omega^*$ forms an unlabelled tree.

To define the Caucal hierarchy we use operations based on *monadic second-order logic* (MSO), the extension of first-order logic by set variables and quantification over sets.

Definition 2.3. (a) The *Muchnik iteration* of a structure $\mathfrak{A} = (A, R_0, \dots, R_r)$ is the structure $\mathfrak{A}^* := (A^*, \mathrm{suc}, \mathrm{cl}, R_0^*, \dots, R_r^*)$ where the universe A^* consists of all finite sequence of elements of A and we have

$$\begin{aligned} \mathrm{suc} &:= \{ (w, wa) \mid w \in A^*,\ a \in A \} , \\ \mathrm{cl} &:= \{ waa \mid w \in A^*,\ a \in A \} , \\ R_i^* &:= \{ (wa_0, \dots, wa_{n-1}) \mid w \in A^*,\ \bar{a} \in R_i \} . \end{aligned}$$

By $\mathfrak{A}^{*n}$ we denote the n-fold iteration of $\mathfrak{A}$

$$\mathfrak{A}^{*0} := \mathfrak{A} \quad \text{and} \quad \mathfrak{A}^{*(n+1)} := (\mathfrak{A}^{*n})^* .$$

(b) An MSO-*interpretation* is a sequence

$$\mathcal{I} = \langle \delta(x), \varphi_0(\bar{x}), \dots, \varphi_r(\bar{x}) \rangle$$

of MSO-formulae. It induces a function on structures that we also denote by $\mathcal{I}$. This function maps a structure $\mathfrak{A}$ to the structure

$$\mathcal{I}(\mathfrak{A}) := (\delta^{\mathfrak{A}}, \varphi_0^{\mathfrak{A}}, \dots, \varphi_r^{\mathfrak{A}}) ,$$

where $\psi^{\mathfrak{A}} := \{ \bar{a} \mid \mathfrak{A} \vDash \psi(\bar{a}) \}$ denotes the relation defined by ψ.

Definition 2.4. The *Caucal hierarchy* $\mathcal{C}_0 \subseteq \mathcal{C}_1 \subseteq \dots$ is the hierarchy whose n-th level consists of all structures of the form $\mathcal{I}(\mathfrak{A}^{*n})$ where $\mathfrak{A}$ is a finite structure.

Note that the Muchnik iteration of a structure is a tree. To investigate the expressive power of monadic second-order logic on iterations Walukiewicz [12] introduced the following kind of tree automaton (see also [1] for an exposition).

Definition 2.5. An MSO-*automaton* is a tuple $\mathcal{A} = (Q, \Sigma, \delta, q_{\mathrm{in}}, \Omega)$ where Q is a finite set of states, Σ is the input alphabet, q_{in} is the initial state, $\Omega : Q \to \omega$ a priority function, and $\delta : Q \times \Sigma \to \mathrm{MSO}$ is the transition function.

Such an automaton takes as input a structure $\mathfrak{A}$ and a labelling $\lambda : A^* \to \Sigma$. A run of $\mathcal{A}$ on $\mathfrak{A}$ and λ is a function $\rho : A^* \to Q$ such that

- $\rho(\langle\rangle) = q_{\mathrm{in}}$ and
- for all $w \in A^*$, we have

  $$(\mathfrak{A}, C, \bar{P}) \vDash \delta(\rho(w), \lambda(w)) ,$$

  where, for each $q \in Q$, we have

  $$P_q := \{ a \in A \mid \rho(wa) = q \} \quad \text{and} \quad C := \begin{cases} \{a\} & \text{if } w = w'a , \\ \varnothing & \text{if } w = \langle\rangle . \end{cases}$$

A run ρ is accepting if it satisfies the parity condition Ω, i.e., on every infinite path the least priority seen infinitely often is even. We say that $\mathcal{A}$ *accepts* a pair $(\mathfrak{A}, \lambda)$ if there exists an accepting run of $\mathcal{A}$ on input $\mathfrak{A}$ and λ.

Theorem 2.6 (Walukiewicz [12]). *For every* MSO-*formula* $\varphi(\bar{X})$, *we can construct an* MSO-*automaton* $\mathcal{A}$ *such that*

$$\mathfrak{A}^* \vDash \varphi(\bar{P}) \quad \text{iff} \quad \mathcal{A} \text{ accepts } (\mathfrak{A}, \lambda_{\bar{P}}) ,$$

where $\lambda_{\bar{P}}(w) := \{ i \mid w \in P_i \}$.

3 Higher-order pushdown automata

We can also characterise the graphs in the Caucal hierarchy in terms of higher-order pushdown automata. The stack of a higher-order pushdown automaton of level n is a list of stacks of level $n-1$. If the innermost stacks, i.e., those of level 1, are words over an alphabet Σ, then we denote the set of level n stacks by Σ^{+n}.

Definition 3.1. Let Σ be an alphabet. We define

$$\Sigma^{+0} := \Sigma\,, \qquad \Sigma^{+(n+1)} := (\Sigma^{+n})^+\,,$$
$$\Sigma^{*0} := \Sigma\,, \qquad \Sigma^{*(n+1)} := (\Sigma^{+n})^*\,.$$

(Note that we use Σ^{+n} instead of Σ^{*n} in the last definition.)

Each word $\xi \in \Sigma^{+n}$ is of the form $\xi = \xi_n(\xi_{n-1}\cdots(\xi_1\xi_0)\cdots)$ where $\xi_i \in \Sigma^{*i}$, for $0 \leq i \leq n$. We can write such words as

$$\xi_n : \xi_{n-1} : \cdots : \xi_1 : \xi_0\,,$$

where $(:) : \Sigma^{*i} \times \Sigma^{+(i-1)} \to \Sigma^{+i}$ with $\xi : a := \xi a$ is the right associative operation that appends a single level i symbol a (i.e., a word of level $i-1$) to a word ξ of level i.

Given a word ξ, we denote by $(\xi)_i$, for $0 \leq i \leq n$, the unique words such that

$$\xi = (\xi)_n : \cdots : (\xi)_0\,.$$

Definition 3.2. A *pushdown automaton* of level n is a tuple

$$\mathcal{A} = (Q, \Sigma, \Gamma, \Delta, q_0, z, F)$$

where Q is the set of states, Σ the input alphabet, Γ the stack alphabet, $q_0 \in Q$ the initial state, $z \in \Gamma$ the initial stack element, $F \subseteq Q$ the set of accepting states, and

$$\Delta \subseteq Q \times (\Sigma \cup \{\varepsilon\}) \times \Gamma \times Q \times \mathrm{Op}$$

the transition relation that consists of tuples $(p, a, c, q, \mathrm{op})$ where op is one of the following operations:

$$\mathrm{pop}_k(\xi_n : \cdots : \xi_0) := \xi_n : \cdots : \xi_k\,,$$
$$\mathrm{push}_a(\xi_n : \cdots : \xi_0) := \xi_n : \cdots : \xi_2 : \xi_1\xi_0 : a\,,$$
$$\mathrm{clone}_k(\xi_n : \cdots : \xi_0) := \xi_n : \cdots : \xi_{k+1} : (\xi_k : \xi_{k-1} : \cdots : \xi_0) : \xi_{k-1} : \cdots : \xi_0\,,$$

where $\xi_i \in \Gamma^{*i}$ and $a \in \Gamma$.

Further, we define the projections $\pi : \Gamma^{+n} \times Q \to \Gamma^{+n}$ and $\rho : \Gamma^{+n} \times Q \to Q$ and a function $\mathrm{top} : \Gamma^{+n} \times Q \to \Gamma \times Q$ by

$$\pi(\xi, q) := \xi\,, \quad \rho(\xi, q) := q\,, \quad \text{and} \quad \mathrm{top}(\xi, q) := ((\xi)_0, q)\,.$$

A configuration (ξ, q) of $\mathcal{A}$ consists of a stack content $\xi \in \Gamma^{+n}$ and a state $q \in Q$. We write $(\xi, q) \vdash^a (\zeta, p)$ if $\mathcal{A}$ enters configuration (ζ, p) when reading the letter $a \in \Sigma \cup \{\varepsilon\}$ in configuration (ξ, q), formally,

$$(\xi, q) \vdash^a (\zeta, p) \quad \text{iff} \quad (q, a, (\xi)_0, p, \mathrm{op}) \in \Delta \text{ and } \zeta = \mathrm{op}(\xi)\,.$$

A *run* of $\mathcal{A}$ is a $(\Gamma^{+n} \times Q)$-labelled tree r such that $(\mathrm{dom}(r), \leq)$ forms a linear order and, for every vertex $u \in \mathrm{dom}(r)$ with immediate $\leq$-successor v, we have $r(u) \vdash r(v)$. We do not require that r starts with the initial configuration $(\varepsilon : \cdots : \varepsilon : z, q_0)$. Instead, we only require that the first configuration of r is reachable, that is, there exists a sequence OP of stack operations such that the stack contents of the first configuration is $\mathrm{OP}(\varepsilon : \cdots : \varepsilon : z)$. We will denote the successor function on $\mathrm{dom}(r)$ by σ.

Example. For every n, there exists an automaton $\mathcal{A}_n$ of level $n+1$ recognising the language

$$L_n := \{\, a^{\beth_n(k)} \mid k < \omega \,\}\,,$$

where $\beth_n(k)$ is the function defined by

$$\beth_0(k) := k \quad \text{and} \quad \beth_{n+1}(k) = 2^{\beth_n(k)}\,.$$

Informally the automaton $\mathcal{A}_n$ starts by guessing the number k and writing an encoding of $\beth_n(k)$ onto its stack. Then it enters a loop where in each iteration it decrements the number stored in the stack and reads one input letter. $\mathcal{A}_n$ stops when the number on the stack becomes 0.

How can we encode such huge numbers into a stack of level $n+1$? For the stack alphabet we choose $\Gamma = \{1, \dots, n, a\}$. The bottom of a stack of level i will be marked by the level $i-1$ word

$$\bar{\imath} := \varepsilon : \cdots : \varepsilon : 12 \dots i \in \Gamma^{+(i-1)}\,.$$

By induction on n, we define a coding function $\kappa_n : \omega \to \Gamma^{+n}$ based on the binary encoding of integers.

$$\kappa_1(m) := \bar{1}a^m\,,$$
$$\kappa_{n+1}(m) := \overline{n+1}\,\kappa_n(i_0)\cdots\kappa_n(i_l)\,,$$
$$\text{where } m = 2^{i_0} + \dots + 2^{i_l} \text{ and } i_0 > \dots > i_l\,.$$

Instead of presenting the actual transition table of the automaton we specify it by pseudo-code. We need a predicate $\mathrm{zero}_i(\xi)$ that is true if the top-most level i stack in ξ is empty, and we need a function $\mathrm{dec}_i(\xi)$ that decrements the top-most level i stack of ξ. zero_i can be defined with the help of the markers $\bar{\imath}$.

$$\mathrm{zero}_i(\xi) \quad :\text{iff} \quad (\xi)_0 = i\,.$$

The decrementation procedure $\mathrm{dec}_i(\xi)$ has to distinguish two cases. If the binary encoding of the number ends with the digit 1 then we change it to 0. Otherwise, the number ends with a sequence of digits 10⋯0 that we have to replace by 01⋯1.

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  dec_1(ξ) := pop_1(ξ) ,
dec_{n+1}(ξ) := if zero_n(ξ) then                 (* last digit is 1 *)
                  return pop_{n+1}(ξ)
                else                               (* last digit is 0 *)
                  ξ := dec_n(ξ)                    (* change 10 to 01 *)
                  while not zero_n(ξ) do
                    ξ := (dec_n ∘ clone_{n+1})(ξ)  (* change 10 to 11 *)
                  end
                  return ξ
                end
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The automaton $\mathcal{A}_n$ works as follows. First, it creates the stack content

$$\overline{n+1} : \dots : \bar{1}\,.$$

Then nondeterministically it performs k push_a-operations. The stack contents now is

$$\overline{n+1} : \dots : \bar{1}a^k = \kappa_{n+1}(\beth_n(k))\,.$$

Finally, it enters a loop where in each iteration it calls dec_n and it reads one input letter.

Our interest in higher-order pushdown automata stems from the following result.

Theorem 3.3 (Carayol, Wöhrle [4]). *A graph $\mathfrak{G}$ belongs to the n-th level $\mathcal{C}_n$ of the Caucal hierarchy if and only if it can be obtained from the configuration graph of a pushdown automaton of level n by contracting all ε-transitions.*

The easy direction of this result is based on the following lemma which we will need in Section 9.

Lemma 3.4. *Let $\mathcal{A} = (Q, \Sigma, \Gamma, \Delta, q_0, z, F)$ be a pushdown automaton of level n with configuration graph $(C, \vdash)$. Let $\mathfrak{A} := (A, (P_a)_{a\in A})$ be the structure with universe $A := Q \cup \Gamma$ and unary predicates $P_a := \{a\}$, for $a \in A$.*

There exist monadic second-order formulae $\varphi_c(x, y)$, for $c \in \Sigma$, such that

$$\mathfrak{A}^{*n} \vDash \varphi_c(\xi : p, \eta : q) \quad \text{iff} \quad (\xi, p) \vdash^c (\eta, q)\,,$$

for all $\xi, \eta \in \Gamma^{*n}$ and $p, q \in Q$.

4 Graphs of finite outdegree

We start our investigation of the structure of graphs in the Caucal hierarchy by computing a bound on their outdegree. Note that the universe of a structure $\mathfrak{A} \in \mathcal{C}_n$ in the n-th level of the hierarchy has the form $A \subseteq \Gamma^{*n}$, for some finite set Γ. We define the following norm on such sets.

Definition 4.1. Let Γ be a finite set. For $\xi = x_0 \cdots x_{r-1} \in \Gamma^{*n}$ and $k \le n$, we define, by induction on k,

$$|\xi|_k := \begin{cases} 0 & \text{if } r = 0\,, \\ |\xi| & \text{if } k = n\,, \\ \max\{\, |x_i|_k \mid i < r \,\} & \text{if } k < n \text{ and } r > 0\,. \end{cases}$$

Lemma 4.2. *Let Γ be a finite set with at least two elements and let $k_1, \dots, k_n$ be numbers. There are less than $|\Gamma|^{k_1\cdots k_n}$ words $\xi \in \Gamma^{*n}$ such that $|\xi|_i < k_i$, for all $i \le n$.*

Proof. The claim follows easily by induction on n. For $n = 1$, we have

$$\sum_{i<k_1} |\Gamma|^i = \frac{|\Gamma|^{k_1} - 1}{|\Gamma| - 1} < |\Gamma|^{k_1}$$

words $\xi \in \Gamma^*$ with $|\xi| < k_1$. For $n > 1$, we can employ the induction hypothesis to obtain the bound

$$\sum_{i<k_n} (|\Gamma|^{k_1 \cdots k_{n-1}})^i < |\Gamma|^{k_1 \cdots k_n}. \qquad \square$$

If $\mathfrak{G} = (V, E)$ is a graph in the n-th level of the Caucal hierarchy then, by definition, there exists a finite structure $\mathfrak{A}$ and two MSO-formulae δ and φ such that

$$V = \{\, \xi \in A^{*n} \mid \mathfrak{A}^{*n} \vDash \delta(\xi) \,\},$$
$$E = \{\, (\xi, \eta) \in A^{*n} \times A^{*n} \mid \mathfrak{A}^{*n} \vDash \varphi(\xi, \eta) \,\}.$$

Therefore, we will consider a structure of the form $\mathfrak{A}^{*n}$ and an MSO-formula $\varphi(x, y)$ with two free first-order variables.

Definition 4.3. Let $\mathfrak{A}$ be a structure and $\varphi(x, y) \in$ MSO a formula. The φ-*outdegree* of $a \in A$ in $\mathfrak{A}$ is the number of elements $b \in A$ such that $\mathfrak{A} \vDash \varphi(a, b)$.

We obtain the following bound on the φ-outdegree.

Theorem 4.4. *For every formula $\varphi(x, y) \in$ MSO and each $n < \omega$, there are constants $c_1, \dots, c_n$ such that, whenever $\mathfrak{A}$ is a finite structure with at least two elements and $a \in A^{*n}$ an element of finite φ-outdegree in $\mathfrak{A}^{*n}$ then*

$$\mathfrak{A}^{*n} \vDash \varphi(a, b) \quad \textit{implies} \quad |b|_i \le L_i(a) \quad \textit{for all } i \le n,$$

where

$$L_i(a) := |a|_i + c_i |A|^{L_1(a) \cdots L_{i-1}(a)}.$$

Proof. Let $\mathcal{A} = (Q, \wp[2], \delta, q_{\mathrm{in}}, \Omega)$ be the nondeterministic MSO-automaton corresponding to φ. Since $\mathfrak{A}$ is fixed we will simplify notation by saying that $\mathcal{A}$ accepts a tree $\lambda : A^{*n} \to \wp[2]$ if it accepts the pair $(\mathfrak{A}^{*(n-1)}, \lambda)$.

W.l.o.g. we may assume that the set of states $Q = Q_\varnothing \cup Q_0 \cup Q_1 \cup Q_{01}$ is partitioned such that starting in a state $q \in Q_C$ the automaton $\mathcal{A}$ accepts only trees λ where the set of occurring labels is exactly C. (If $\mathcal{A}$ is not of this form then we can construct a new automaton with states $Q \times \wp[2]$.) Furthermore, we assume that there exists a unique state $q_1 \in Q_1$ from which $\mathcal{A}$ accepts the tree λ with

$$\lambda(x) := \begin{cases} \{1\} & \text{if } x = \varepsilon, \\ \varnothing & \text{otherwise}. \end{cases}$$

Let ρ be an accepting run of $\mathcal{A}$ on the tree $\lambda : A^{*n} \to \wp[2]$. If $\rho(w) \in Q_1$ then we either have $\lambda(w) = \{1\}$ and $\rho(wa) \in Q_\varnothing$, for all $a \in A^{*(n-1)}$, or we have $\lambda(w) = \varnothing$ and there is some $a \in A^{*(n-1)}$ with $\rho(wa) \in Q_1$ and $\rho(wb) \in Q_\varnothing$, for all $b \neq a$. For $p, q \in Q_1$, we define

$$\psi_{pq}(x, y) := \exists C \exists \bar{P} \Big(\delta(p, \varnothing)(C, \bar{P}) \wedge C = \{x\} \wedge P_q = \{y\} \wedge \bigwedge_{s \in Q \setminus (Q_\varnothing \cup \{q\})} P_s = \varnothing \Big).$$

It follows that, whenever the automaton is in state p at some vertex $wa \in A^{+n}$ with $\lambda(wa) = \varnothing$ then it can go to state q at the vertex wab if and only if $\mathfrak{A} \vDash \psi_{pq}(a, b)$.

Similarly, there exists a formula $\vartheta_{q p_0 p_1}(x, y_0, y_1)$, for $q \in Q_{01}$, $p_0 \in Q_0$, and $p_1 \in Q_1$, such that

$$\mathfrak{A} \vDash \vartheta_{q p_0 p_1}(a, b_0, b_1)$$

if and only if, whenever the automaton $\mathcal{A}$ is in the state q at some vertex $wa \in A^{*n}$ then it can go into the state p_0 at wab_0 and into the state p_1 at wab_1.

Finally, there exists a formula $\chi_p(x, y)$ such that $\chi_p(a, b)$ holds if and only if there exist a sequence of elements $d_0, \dots, d_m \in A^{*(n-1)}$ and a corresponding sequence of states $p_0, \dots, p_m \in Q_1$ such that

- $d_0 = a$ and $p_0 = p$,
- $d_k = b$, for some $k \le m$,
- $p_m = q_1$,
- $\mathfrak{A} \vDash \exists z \bigvee_{q \in Q_0} \vartheta_{p_0 q p_1}(d_0, z, d_1)$, and
- $\mathfrak{A} \vDash \psi_{p_i p_{i+1}}(d_i, d_{i+1})$, for all $0 < i < m$.

Let $\pi : A^{+n} \to A^{*(n-1)}$ be the projection to the last symbol $\pi(wa) := a$. Fix an element $u \in A^{*n}$ such that the set $V := \{\, v \in A^{*n} \mid \mathfrak{A}^* \vDash \varphi(u, v), v \npreceq u \,\}$ is finite. To each $v \in V$ we associate the maximal sequence $v_0, \dots, v_{m(v)}$ such that $u \sqcap v = v_0 \prec v_1 \prec \dots \prec v_{m(v)} = v$. By assumption, the set

$$P := \bigcup \{\, \pi(v_i) \mid v \in V,\ i \le m(v) \,\}$$

is finite. For $v \in V$, we denote the accepting run of $\mathcal{A}$ on the tree $\lambda_{\{u\}\{v\}}$ by ρ_v and we set $p_v := \rho_v(v_0)$. Note that

$$\{\, a \in A^{*(n-1)} \mid \mathfrak{A} \vDash \chi_{p_v}(\pi(v_0), a) \,\} \subseteq P$$

is also finite. By induction hypothesis, there are numbers $c_1, \dots, c_{n-1}$ such that

$$\mathfrak{A} \models \chi_{p_v}(\pi(v_0), a) \quad \text{implies} \quad |a|_i \leq L_i(\pi(v_0)),$$

where

$$L_i(a) := |a|_i + c_i |A|^{L_1(a) \cdots L_{i-1}(a)}.$$

It follows that, for $v \in V$ and $i \leq m(v)$, we have

$$|\pi(v_i)|_l \leq \max \{ L_l(\pi(x)) \mid x \leq u \} \leq L_l(u).$$

Finally, note that, for $v \in V$,

$$\pi(v_i) = \pi(v_l), \quad \text{for } i < l, \qquad \text{implies} \qquad \rho(v_i) \neq \rho(v_l),$$

since, otherwise, the path $\pi(v_i), \dots, \pi(v_{l-1})$ can be repeated an arbitrary number of times and χ_{p_v} defines an infinite set. It follows that

$$m(v) \leq |Q_1| \cdot |A|^{L_1(u) \cdots L_{n-1}(u)}.$$

Consequently, setting $c_n := |Q_1|$ we have

$$|v|_n \leq |u|_n + c_n \cdot |A|^{L_1(u) \cdots L_{n-1}(u)} = L_n(u),$$

and $\quad |v|_i \leq L_i(u), \quad$ for $i < n$. □

Corollary 4.5. *Let $\mathfrak{A}$ be a finite structure and $\varphi(x, y) \in$ MSO some formula that defines a relation $R := \varphi^{\mathfrak{A}^{*n}}$ of finite outdegree on $\mathfrak{A}^{*n}$. If $u_0, u_1, \dots \in A^{*n}$ is an R-path then we have*

$$|u_k|_i \leq |u_0|_i + \beth_{i-1}(\mathcal{O}(k + |u_0|_1 + \dots + |u_0|_{i-1})), \qquad \textit{for all } i \leq n.$$

Proof. By the preceding theorem, we have

$$|u_k|_1 \leq |u_{k-1}|_1 + c_1 \leq |u_0|_1 + c_1 k \leq |u_0|_1 + \beth_0(\mathcal{O}(k)),$$

and, for $i > 1$, it follows by induction that

$$|u_k|_i \leq |u_{k-1}|_i + c_i |A|^{L_1(u_{k-1}) \cdots L_{i-1}(u_{k-1})} \leq |u_0|_i + \sum_{l<k} c_i |A|^{L_1(u_l) \cdots L_{i-1}(u_l)}.$$

Since

$$\begin{aligned}
&L_1(u_l) \cdots L_{i-1}(u_l) \\
&\leq \big(|u_0|_1 + \beth_0(\mathcal{O}(l))\big) \cdots \big(|u_0|_{i-1} + \beth_{i-2}(\mathcal{O}(l + |u_0|_1 + \dots + |u_0|_{i-2}))\big) \\
&\leq (|u_0|_1 + \dots + |u_0|_{i-1} + \beth_{i-2}(\mathcal{O}(l + |u_0|_1 + \dots + |u_0|_{i-2})))^{i-1} \\
&\leq (|u_0|_1 + \dots + |u_0|_{i-1} + \beth_{i-2}(\mathcal{O}(k + |u_0|_1 + \dots + |u_0|_{i-2})))^{i-1} \\
&\leq (k + |u_0|_1 + \dots + |u_0|_{i-1} + \beth_{i-2}(\mathcal{O}(k + |u_0|_1 + \dots + |u_0|_{i-2} + |u_0|_{i-1})))^{i-1} \\
&\leq \beth_{i-2}(\mathcal{O}(k + |u_0|_1 + \dots + |u_0|_{i-2} + |u_0|_{i-1}))^{i-1} \\
&\leq \beth_{i-2}(\mathcal{O}(k + |u_0|_1 + \dots + |u_0|_{i-2} + |u_0|_{i-1}))
\end{aligned}$$

it follows that

$$\begin{aligned}
|u_k|_i &\leq |u_0|_i + \sum_{l<k} c_i 2^{\beth_{i-2}(\mathcal{O}(k+|u_0|_1+\dots+|u_0|_{i-2}+|u_0|_{i-1}))} \\
&\leq |u_0|_i + c_i k \beth_{i-1}(\mathcal{O}(k + |u_0|_1 + \dots + |u_0|_{i-2} + |u_0|_{i-1})) \\
&\leq |u_0|_i + \beth_{i-1}(\mathcal{O}(k + |u_0|_1 + \dots + |u_0|_{i-2} + |u_0|_{i-1})).
\end{aligned}$$ □

Corollary 4.6. *Let $\mathfrak{A}$ be a finite structure and $\varphi(x, y) \in$ MSO some formula that defines a relation of finite outdegree on $\mathfrak{A}^{*n}$. The k-neighbourhood*

$$N_k(u) := \{ v \in A^{*n} \mid d(u, v) \leq k \}$$

of an element $u \in A^{*n}$ is bounded by

$$|N_k(u)| \leq \beth_n(\mathcal{O}(k + |u|_1 + \dots + |u|_n)).$$

Proof. If $d(u, v) \leq k$ then we know by the preceding corollary that

$$|v|_i \leq |u|_i + \beth_{i-1}(\mathcal{O}(k + |u|_1 + \dots + |u|_{i-1})).$$

It therefore follows from Lemma 4.2 that there are less than

$$\begin{aligned}
&|A|^{(|u|_1+\mathcal{O}(k))\cdots(|u|_n+\beth_{n-1}(\mathcal{O}(k+|u|_1+\dots+|u|_{n-1})))} \\
&\leq |A|^{(|u|_1+\dots+|u|_n+\beth_{n-1}(\mathcal{O}(k+|u|_1+\dots+|u|_{n-1})))^n} \\
&\leq |A|^{\beth_{n-1}(\mathcal{O}(k+|u|_1+\dots+|u|_{n-1}+|u|_n))^n} \\
&\leq |A|^{\beth_{n-1}(\mathcal{O}(k+|u|_1+\dots+|u|_{n-1}+|u|_n))} \\
&= \beth_n(\mathcal{O}(k + |u|_1 + \dots + |u|_n))
\end{aligned}$$

such words v. □

Corollary 4.7. *Let $\mathfrak{A}$ be a finite structure $\varphi(x, y) \in$ MSO, and $u \in A^{*n}$. If the φ-outdegree of u in $\mathfrak{A}^{*n}$ is finite then it is bounded by*

$$\beth_n(\mathcal{O}(|u|_1 + \cdots + |u|_n)) .$$

Example. Let

$$T_k := \{ 0^n i \in \omega^* \mid n < \omega,\ i < \beth_k(n) \}$$

and let $E \subseteq T_k \times T_k$ be the immediate successor relation. The tree (T_{2k}, E) is not contained in the k-th level of the Caucal hierarchy since, if $w_n \in A^{*2k}$ encodes the element $0^n \in T_{2k}$ then

$$|w_n|_i \leq \beth_{i-1}(\mathcal{O}(n))$$

and the outdegree of w_n is bounded by $\beth_{2k-1}(\mathcal{O}(n))$.

Similarly, if we define $T_\omega := \{ 0^n i \in \omega^* \mid i < \beth_{2n}(n) \}$ then (T_ω, E) is not contained in any level of the hierarchy.

5 Substitution of stacks

After having studied the degree of vertices in a graph of the Caucal hierarchy we now turn to the investigation of paths in such graphs. For the remainder of the article we fix a pushdown automaton $\mathcal{A}$ of level n. Let us introduce some additional notation. If r is a run and $x \in \operatorname{dom}(r)$ then the *operation at x* is the operation op such that $\pi r(\sigma x) = \operatorname{op}(\pi r(x))$. We call pop_1 and push_a a *level 1 operation* and, for $k > 1$, pop_k and clone_k a *level k operation*. A push(1)*-operation* is an operation of the form push_a and, for $k > 1$, we call clone_k a push(k)*-operation*.

We start by showing how to replace in a given run the bottom part of all stacks by some other stack content such that the resulting sequence of configurations still forms a run. To do so we define a variant of the prefix relation $\xi \triangleleft_k \zeta$ saying that some stack content ξ is contained in a larger stack ζ. In the constructions of the following sections we will need to also consider operations and relations on just the bottom levels of a stack. Therefore, we have to define all notions depending on a parameter k.

Definition 5.1. For words $\xi, \eta \in \Gamma^{+n}$, we define the prefix relation $\xi \triangleleft_k \eta$ by induction on n.

If $n < k$, in particular if $n = 0$, then $\xi \triangleleft_k \eta$ always holds. For $n \geq k$, suppose that $\xi = x_0 \cdots x_r$ and $\eta = y_0 \cdots y_s$ where $x_i, y_i \in \Gamma^{+(n-1)}$. We define $\xi \triangleleft_k \eta$ iff

$$r \leq s, \quad x_i = y_i, \text{ for } i < r, \quad \text{and} \quad x_r \triangleleft_k y_i, \text{ for } r \leq i \leq s .$$

For notational convenience, if r is a run and $x, y \in \operatorname{dom}(r)$, we define

$$x \triangleleft_k y \quad :\text{iff} \quad \pi r(x) \triangleleft_k \pi r(y) .$$

The following easy observations will frequently be used in the proofs below.

Lemma 5.2. *If we have $\xi_n : \cdots : \xi_0 \triangleleft_k \xi_n \eta : \zeta_{n-1} : \cdots : \zeta_0$ and $\eta \neq \varepsilon$ then $\xi_n : \cdots : \xi_0 \triangleleft_k \xi_n \eta$.*

Proof. Suppose that $\eta = y_0 \ldots y_m$. Then

$$\xi_n : \cdots : \xi_0 \triangleleft_k \xi_n \eta : \zeta_{n-1} : \cdots : \zeta_0$$

implies $\xi_{n-1} : \cdots : \xi_0 \triangleleft_k y_i$, for all $i \leq m$. Hence,

$$\xi_n : \cdots : \xi_0 \triangleleft_k \xi_n y_0 \ldots y_{m-1} : y_m = \xi_n \eta . \qquad \square$$

Lemma 5.3. *If $\xi, \eta, \zeta \in \Gamma^{+n}$ are words such that*

$$\xi \triangleleft_k \eta \triangleleft_{k+1} \zeta , \quad \xi \triangleleft_k \zeta , \quad \textit{and} \quad (\xi)_k = (\eta)_k$$

then we have $\eta \triangleleft_k \zeta$.

Proof. We prove the claim by induction on $n - k$. If $k = n$ then we have $(\eta)_n = (\xi)_n \leq (\zeta)_n$ which implies $\eta \triangleleft_n \zeta$. Suppose that $k < n$ and let

$$\xi = x_0 \cdots x_r , \quad \eta = y_0 \cdots y_s , \quad \zeta = z_0 \cdots z_t , \qquad \text{for } x_i, y_i, z_i \in \Gamma^{+(n-1)} .$$

Let $s \leq i \leq t$. $\eta \triangleleft_{k+1} \zeta$ implies that

$$y_0 \cdots y_{s-1} = z_0 \cdots z_{s-1} \quad \text{and} \quad y_s \triangleleft_{k+1} z_i .$$

Since $x_r \triangleleft_k y_s$, $x_r \triangleleft_k z_i$, and $(x_r)_k = (\xi)_k = (\eta)_k = (y_s)_k$ we can apply the induction hypothesis and it follows that $y_s \triangleleft_k z_i$, for all $s \leq i \leq t$. Hence, we have $\eta \triangleleft_k z$. $\square$

If $\xi \triangleleft_k \eta$ then we can replace ξ by some other value ζ without destroying the structure of the stack.

Definition 5.4. Let $\xi, \eta, \zeta \in \Gamma^{+n}$ where

$$\xi = x_0 \cdots x_r\,, \quad \eta = y_0 \cdots y_s\,, \quad \zeta = z_0 \cdots z_t\,, \qquad \text{for } x_i, y_i, z_i \in \Gamma^{+(n-1)}.$$

If $\xi \lhd_k \eta$ we define, by induction on n, the *substitution*

$$\eta[\xi/\zeta]_k := \begin{cases} \eta & \text{if } k > n\,, \\ z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_s [x_r/z_t]_k & \text{if } k \le n\,. \end{cases}$$

We extend this operation to configurations $(\eta, q) \in \Gamma^{+n} \times Q$ by setting

$$(\eta, q)[\xi/\zeta]_k := (\eta[\xi/\zeta]_k, q)\,.$$

The above definitions of $\lhd_k$ and $\eta[\xi/\zeta]_k$ were chosen to be compatible with the pushdown operations as stated in the following important lemma.

Lemma 5.5. *Let* $\mathrm{op} \in \{\mathrm{push}_b, \mathrm{clone}_j, \mathrm{pop}_j\}$ *be a pushdown operation,* $1 \le k \le n$*, and let* $\xi, \eta, \zeta \in \Gamma^{+n}$ *be words. If*

$$\xi \lhd_k \eta \quad \textit{and} \quad |(\mathrm{op}(\eta))_i| \ge |(\xi)_i|\,, \quad \textit{for all } i \ge k\,,$$

then we have

$$\xi \lhd_k \mathrm{op}(\eta) \quad \textit{and} \quad \mathrm{op}(\eta[\xi/\zeta]_k) = (\mathrm{op}(\eta))[\xi/\zeta]_k\,.$$

Proof. We prove the claims by induction on n. Clearly, we only need to consider the case that $k \le n$. Let

$$\xi = x_0 \cdots x_r\,, \quad \eta = y_0 \cdots y_s\,, \quad \zeta = z_0 \cdots z_t\,, \qquad \text{for } x_i, y_i, z_i \in \Gamma^{+(n-1)}.$$

(A) First we consider the case that $\mathrm{op} = \mathrm{push}_b$. For $n = k = 1$, we have

$$\begin{aligned} \mathrm{push}_b(\eta[\xi/\zeta]_1) &= \mathrm{push}_b(z_0 \cdots z_{t-1} y_r \cdots y_s) \\ &= z_0 \cdots z_{t-1} y_r \cdots y_s b \\ &= (y_0 \cdots y_s b)[\xi/\zeta]_1 \\ &= (\mathrm{push}_b(\eta))[\xi/\zeta]_1\,, \end{aligned}$$

and, for $n > 1$,

$$\begin{aligned} &\mathrm{push}_b(\eta[\xi/\zeta]_k) \\ &\quad = \mathrm{push}_b(z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_s [x_r/z_t]_k) \\ &\quad = z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_{s-1} [x_r/z_t]_k (\mathrm{push}_b(y_s [x_r/z_t]_k)) \\ &\quad = z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_{s-1} [x_r/z_t]_k (\mathrm{push}_b(y_s))[x_r/z_t]_k \\ &\quad = (y_0 \cdots y_{s-1} \mathrm{push}_b(y_s))[\xi/\zeta]_k \\ &\quad = (\mathrm{push}_b(\eta))[\xi/\zeta]_k\,. \end{aligned}$$

(B) Suppose that $\mathrm{op} = \mathrm{clone}_j$. For $n = j$, we have

$$\begin{aligned} \mathrm{clone}_j(\eta[\xi/\zeta]_k) &= \mathrm{clone}_j(z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_s [x_r/z_t]_k) \\ &= z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_s [x_r/z_t]_k y_s [x_r/z_t]_k \\ &= (y_0 \cdots y_s y_s)[\xi/\zeta]_k \\ &= (\mathrm{clone}_j(\eta))[\xi/\zeta]_k\,, \end{aligned}$$

and, for $n > j$,

$$\begin{aligned} &\mathrm{clone}_j(\eta[\xi/\zeta]_k) \\ &\quad = \mathrm{clone}_j(z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_s [x_r/z_t]_k) \\ &\quad = z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_{s-1} [x_r/z_t]_k (\mathrm{clone}_j(y_s [x_r/z_t]_k)) \\ &\quad = z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_{s-1} [x_r/z_t]_k (\mathrm{clone}_j(y_s))[x_r/z_t]_k \\ &\quad = (y_0 \cdots y_{s-1} \mathrm{clone}_j(y_s))[\xi/\zeta]_k \\ &\quad = (\mathrm{clone}_j(\eta))[\xi/\zeta]_k\,. \end{aligned}$$

(C) Finally, consider the case that $\mathrm{op} = \mathrm{pop}_j$. Since

$$r = |(\xi)_n| \le |(\mathrm{pop}_n(\eta))_n| = s - 1\,,$$

we have, for $n = j$,

$$\begin{aligned} \mathrm{pop}_n(\eta[\xi/\zeta]_k) &= \mathrm{pop}_n(z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_{s-1} [x_r/z_t]_k y_s [x_r/z_t]_k) \\ &= z_0 \cdots z_{t-1} y_r [x_r/z_t]_k \cdots y_{s-1} [x_r/z_t]_k \\ &= (y_0 \cdots y_{s-1})[\xi/\zeta]_k \\ &= (\mathrm{pop}_n(\eta))[\xi/\zeta]_k\,, \end{aligned}$$

and, for $n > j$,

$$\begin{aligned}\mathrm{pop}_j(\eta[\xi/\zeta]_k) &= \mathrm{pop}_j(z_0\cdots z_{t-1}y_r[x_r/z_t]_k\cdots y_s[x_r/z_t]_k)\\ &= z_0\cdots z_{t-1}y_r[x_r/z_t]_k\cdots y_{s-1}[x_r/z_t]_k(\mathrm{pop}_j(y_s[x_r/z_t]_k))\\ &= z_0\cdots z_{t-1}y_r[x_r/z_t]_k\cdots y_{s-1}[x_r/z_t]_k(\mathrm{pop}_j(y_s))[x_r/z_t]_k\\ &= (y_0\cdots y_{s-1}\mathrm{pop}_j(y_s))[\xi/\zeta]_k\\ &= (\mathrm{pop}_j(\eta))[\xi/\zeta]_k\,.\end{aligned}$$

(D) In all cases we have $\xi \lhd_k \mathrm{op}(\eta)$ since $(\mathrm{op}(\eta))[\xi/\zeta]_k$ is defined. □

By induction, it follows that each transition of a run can be lifted from η to $\eta[\xi/\zeta]_k$ as long as the word ξ is still contained in η.

Corollary 5.6. *Let $\xi, \zeta, \eta, \eta' \in \Gamma^{+n}$ be words such that $|(\eta')_i| \geq |(\xi)_i|$, for all $i \geq k$. Then*

$$\xi \lhd_k \eta \quad \textit{and} \quad (\eta, q) \vdash^a (\eta', q')$$

implies

$$\xi \lhd_k \eta' \quad \textit{and} \quad (\eta[\xi/\zeta]_k, q) \vdash^a (\eta'[\xi/\zeta]_k, q')\,.$$

Proof. Let $\delta = (q, c, a, q', \mathrm{op}) \in \Delta$ be the transition witnessing $(\eta, q) \vdash^a (\eta', q')$. By definition, we have $(\eta[\xi/\zeta]_k)_0 = (\eta)_0$. Hence

$$\mathrm{top}(\eta[\xi/\zeta]_k, q) = \mathrm{top}(\eta, q) = (a, q)$$

and we can apply δ to $(\eta[\xi/\zeta]_k, q)$. The resulting configuration (μ, q') has the stack contents

$$\mu = \mathrm{op}(\eta[\xi/\zeta]_k) = (\mathrm{op}(\eta))[\xi/\zeta]_k = \eta'[\xi/\zeta]_k\,.$$

The relation $\xi \lhd_k \eta' = \mathrm{op}(\eta)$ follows immediately from the preceding lemma. □

In particular, if we have a run such that the stack content ξ of the first configuration is never touched then we can replace ξ by an arbitrary other word ζ and we obtain again a valid run.

Lemma 5.7. *Let r be a run and $x \in \mathrm{dom}(r)$ its first vertex. Suppose that*

$$\xi := \pi r(x) \lhd_k \pi r(y)\,, \qquad \textit{for all } y \in \mathrm{dom}(r)\,.$$

If $\zeta \in \Gamma^{+n}$ is an arbitrary word then the function r' defined by

$$r'(y) := r(y)[\xi/\zeta]_k\,, \qquad \textit{for } y \in \mathrm{dom}(r)\,,$$

forms a valid run.

Proof. We can use Corollary 5.6 to prove, by induction on $\leq$, that

$$\xi \lhd_k \pi r(y) \quad \text{and} \quad r(y)[\xi/\zeta]_k \vdash r(\sigma y)[\xi/\zeta]_k\,.$$ □

6 Weak domination

In this section we introduce the weak domination order $\sqsubseteq_k^*$ which will be our main tool for decomposing runs.

Definition 6.1. (a) For $\xi, \zeta \in \Gamma^{+n}$ and $0 \leq k \leq n$, we say that ξ *weakly k-dominates* ζ, written $\xi \sqsubseteq_k \zeta$, if there exists a sequence POP of pop-operations such that

$$\mathrm{pop}_k(\xi) = \mathrm{pop}_k(\mathrm{POP}(\zeta))\,.$$

(b) If r is a run and $x, y \in \mathrm{dom}(r)$ then we define

$$\begin{aligned} x \sqsubseteq_k y \quad &:\text{iff} \quad \pi r(x) \sqsubseteq_k \pi r(y)\,,\\ \text{and} \quad x \sqsubseteq_k^* y \quad &:\text{iff} \quad x \leq y \quad \text{and} \quad x \sqsubseteq_k z \quad \text{for all } x \leq z \leq y\,.\end{aligned}$$

The greatest lower $\sqsubseteq_k^*$-bound of x and y will be denoted by $x \sqcap_k y$.

(c) Let r be a run and $x \in \mathrm{dom}(r)$. By $\omega_k(x)$ we denote the $\leq$-minimal element $y \in \mathrm{dom}(r)$ such that $x \leq y$ and $x \not\sqsubseteq_k^* y$. Note that $\omega_k(x)$ might be undefined.

Lemma 6.2. $(\mathrm{dom}(r), \sqsubseteq_k^*)$ *is a forest.*

Remark. Note that the original ordering $\leq$ of a run r coincides with the ordering we obtain when traversing the forest $(\mathrm{dom}(r), \sqsubseteq_k^*)$ in "prefix ordering" (which is not related to the prefix order $\leq$). This is the same as the lexicographic ordering $\leq_{\text{lex}}$ of $(\text{dom}(r), \sqsubseteq_k^*)$ which in this case is defined by

$$x \leq_{\text{lex}} y \quad \text{iff} \quad x \sqsubseteq_k^* y \text{ or } u < v \text{ where } u \text{ and } v \text{ are the immediate } \sqsubseteq_k^*\text{-successors of } x \sqcap_k y \text{ with } u \sqsubseteq_k^* x \text{ and } v \sqsubseteq_k^* y\,.$$

In particular, if $x \sqsubseteq_k^* y$ and $x \not\sqsubseteq_k^* z$ then $z < x \leq y$ or $x \leq y < z$.

Example. Consider the run

$$\begin{aligned} \varepsilon : \varepsilon : a &\vdash \varepsilon : \varepsilon : ab \vdash \varepsilon : ab : ab \vdash \varepsilon : ab : a \vdash (ab : a) : ab : a \\ &\vdash (ab : a) : \varepsilon : ab \vdash (ab : a) : \varepsilon : a \vdash \varepsilon : ab : a \vdash \varepsilon : \varepsilon : ab \\ &\vdash \varepsilon : \varepsilon : a \end{aligned}$$

where we have left out the states for simplicity. The weak domination orderings $\sqsubseteq_3^*$, $\sqsubseteq_2^*$ and $\sqsubseteq_1^*$ are shown in Figure 1.

Lemma 6.3. *Let $\xi, \eta \in \Gamma^{+n}$. If $\xi \triangleleft_k \eta$ then $\xi \sqsubseteq_k \eta$.*

Proof. Let $\xi = x_0 \cdots x_r$ and $\eta = y_0 \cdots y_s$, for $x_i, y_i \in \Gamma^{+(n-1)}$. We prove the claim by induction on n. If $n = k$ then

$$\text{pop}_k(\xi) = x_0 \cdots x_{r-1} = y_0 \cdots y_{r-1} = (\text{pop}_k)^{s-r+1}(\eta)\,.$$

For $n > k$, we have, by definition of $\triangleleft_k$,

$$\xi = x_0 \cdots x_r \triangleleft_k y_0 \cdots y_r = (\text{pop}_n)^{s-r}(\eta)\,.$$

By induction hypothesis, there exists a sequence POP of pop-operations such that

$$\text{pop}_k(x_r) = \text{pop}_k(\text{POP}(y_r))\,.$$

It follows that

$$\text{pop}_k(\xi) = \big(\text{pop}_k \circ \text{POP} \circ \text{pop}_n^{s-r}\big)(\eta)\,. \qquad \square$$

In the following sequence of lemmas we relate the structure of the weak dominance order to the stack contents of the underlying run. First, we consider $\leq$-successors that are not $\sqsubseteq_k^*$-successors.

Lemma 6.4. *Let r be a run and $x, y \in \text{dom}(r)$ vertices such that $x \sqsubseteq_k y$ and $x \not\sqsubseteq_k \sigma y$. Then $\pi r(\sigma y) = \text{pop}_l \pi r(x)$, for some $l \geq k$.*

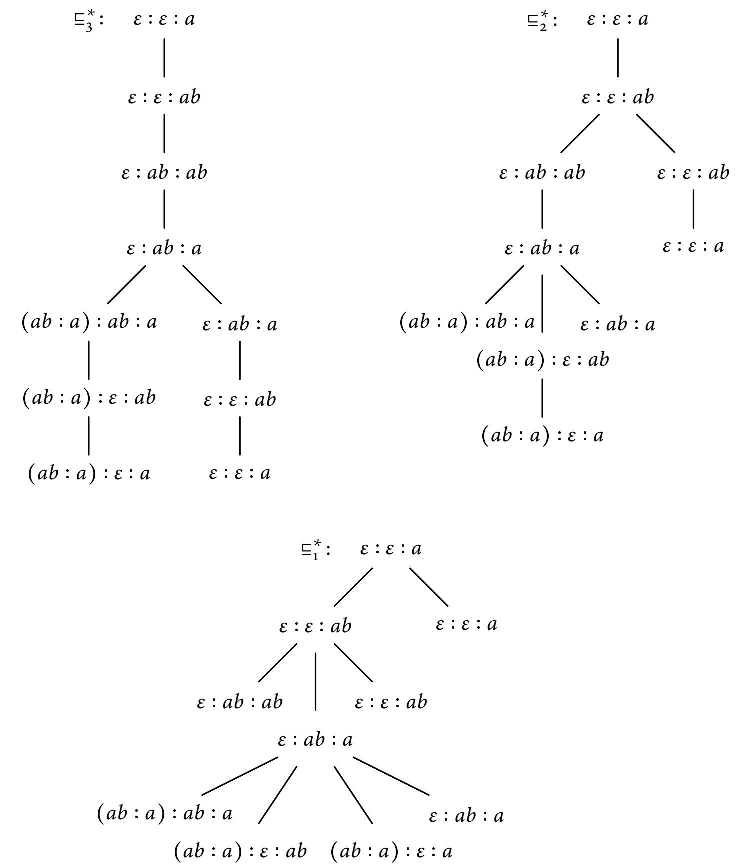

Figure 1: The weak domination orders $\sqsubseteq_3^*$, $\sqsubseteq_2^*$ and $\sqsubseteq_1^*$.

Proof. Let $\pi r(x) = \xi_n : \dots : \xi_0$. Since $x \sqsubseteq_k y$ we have, for some $i \geq k$,

$$\pi r(y) = \xi_n : \dots : \xi_{i+1} : \xi_i \eta_i : \eta_{i-1} : \dots : \eta_0 ,$$

where either $\xi_i : \dots : \xi_0 \sqsubseteq_k \xi_i \eta_i$, or $i = k$ and $\eta_k = \varepsilon$. Since $x \not\sqsubseteq_k \sigma y$ there exist some index $l \geq i \geq k$ such that

$$\pi r(\sigma y) = \mathrm{pop}_l \pi r(y) = \xi_n : \dots : \xi_l = \mathrm{pop}_l \pi r(x) . \qquad \square$$

A configuration with several immediate $\sqsubseteq^*_k$-successors must perform a clone_i-operation and the stack contents of the successors have a certain format.

Lemma 6.5. *Let r be a run, $k > 1$, and $x \in \mathrm{dom}(r)$ a vertex with several immediate $\sqsubseteq^*_k$-successors $y_0, \dots, y_m$, $m \geq 1$. Set $\xi_n : \dots : \xi_1 = \pi r(x)$.*

There exists an index $i \geq k$ satisfying the following conditions.

(a) *There is a $\mathrm{push}(i)$-operation at x.*

(b) *There are indices*

$$1 = l(0) \leq k \leq l(1) \leq \dots \leq l(m) \leq i$$

and words $\zeta_0 \sqsubseteq_0 \xi_{l(0)}, \dots, \zeta_m \sqsubseteq_0 \xi_{l(m)}$ such that, for all $s < m$, we have

$$\pi r(y_s) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{l(s)+1} : \zeta_s$$

and $\pi r(y_{s+1}) = \mathrm{pop}_l \pi r(y_s)$, for some $k \leq l < i$.

(c) *$y_s \sqsubseteq^*_i y_t$, for all $s \leq t < m$, and $y_s \sqsubseteq^*_i y_m$ iff $\pi r(y_m) \neq \pi r(x)$.*

(d) *$x \sqsubseteq^*_l y_s$, for all $s \leq m$ and every $l \leq n$. Furthermore, $y_0, \dots, y_m$ are immediate $\sqsubseteq^*_l$-successors of x, for all $l \leq k$.*

Proof. (a) If $\pi r(\sigma x) = \mathrm{pop}_i \pi r(x)$, for some i, then $x \sqsubseteq^*_k z$ implies $\sigma x \sqsubseteq^*_k z$. Hence, x has at most one immediate $\sqsubseteq^*_k$-successor. The same is the case for a $\mathrm{push}(i)$-operation with with $i < k$.

(b) We proceed by induction on s. For $s = 0$, the claim follows from (a) since $y_0 = \sigma x$. Suppose that $s > 0$ and

$$\pi r(y_{s-1}) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{l(s-1)+1} : \zeta_{s-1} ,$$

where $l(s-1) \leq i$.

(A) If $\pi r(\sigma^{-1} y_s) = \pi r(y_{s-1})$ then $x \sqsubseteq^*_k y_s$ and $\sigma^{-1} y_s \not\sqsubseteq^*_k y_s$ imply that,

$$\pi r(y_s) = \mathrm{pop}_l \pi r(\sigma^{-1} y_s) = \mathrm{pop}_l \pi r(y_{s-1}) ,$$

for some $k \leq l < i$. Hence, if $l > l(s-1)$ then

$$\pi r(y_s) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_l ,$$

and, for $l \leq l(s-1)$, we have

$$\pi r(y_s) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{l(s-1)+1} : \zeta_s ,$$

where $\zeta_s := \mathrm{pop}_l(\zeta_{s-1})$.

(B) If $\pi r(\sigma^{-1} y_s) \neq \pi r(y_{s-1})$ we fix the maximal index h such that

$$(\pi r(\sigma^{-1} y_s))_h \neq (\pi r(y_{s-1}))_h .$$

We claim that $h < i$. Suppose otherwise. Since $y_{s-1} \sqsubseteq^*_k \sigma^{-1} y_s$ we have

$$\pi r(\sigma^{-1} y_s) = \xi_n : \dots : \xi_{h+1} : \xi_h \eta_h : \eta_{h-1} : \dots : \eta_1$$

for some words $\eta_h, \dots, \eta_1$ such that

$$\begin{aligned} &\xi_h : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{l(s-1)+1} : \zeta_{s-1} \\ &\sqsubseteq^*_k \xi_h \eta_h : \eta_{h-1} : \dots : \eta_1 . \end{aligned}$$

Furthermore, by choice of h we have $\eta_h \neq \varepsilon$, and if $h = i$ then

$$\eta_h = (\xi_{i-1} : \dots : \xi_1) \eta'_h ,$$

for some $\eta'_h \neq \varepsilon$. Hence,

$$(*) \qquad \xi_h : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{l(s-1)+1} : \zeta_{s-1} \sqsubseteq^*_k \xi_h \eta_h .$$

Since $x \sqsubseteq^*_k y_s$ and $\sigma^{-1} y_s \not\sqsubseteq^*_k y_s$ it follows that

$$\pi r(y_s) = \mathrm{pop}_j \pi r(\sigma^{-1} y_s) = \xi_n : \dots : \xi_{h+1} : \xi_h \eta_h : \eta_{h-1} : \dots : \eta_j ,$$

for some $k \leq j \leq h$. But $(*)$ implies

$$\begin{aligned} \pi r(y_{s-1}) &= \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{l(s-1)+1} : \zeta_{s-1} \\ &\sqsubseteq^*_k \xi_n : \dots : \xi_{h+1} : \xi_h \eta_h : \eta_{h-1} : \dots : \eta_j = \pi r(y_s) , \end{aligned}$$

that is, $y_{s-1} \sqsubseteq_k^* y_s$. Contradiction.

(c) Consequently, we have $h < i$. If $h > l(s-1)$ then $y_{s-1} \sqsubseteq_k^* \sigma^{-1} y_s$ implies

$$\pi r(\sigma^{-1} y_s) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{h+1} : \\ \xi_h \eta_h : \eta_{h-1} : \dots : \eta_1 .$$

Again, by $x \sqsubseteq_k^* y_s$ and $\sigma^{-1} y_s \not\sqsubseteq_k^* y_s$ it follows that

$$\pi r(y_s) = \mathrm{pop}_l \pi r(\sigma^{-1} y_s)$$

for some $k \le l < i$. If $l \le h$ then

$$\pi r(y_s) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{h+1} : \\ \xi_h \eta_h : \eta_{h-1} : \dots : \eta_l$$

and as above it follows that $y_{s-1} \sqsubseteq_k^* y_s$. Contradiction. Therefore, $l > h$ and

$$\pi r(y_s) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_l = \mathrm{pop}_l r(y_{s-1})$$

as desired.

It remains to consider the case that $h \le l(s-1)$. Let $\zeta_s = \mu_{l(s-1)} : \dots : \mu_1$. Since $y_{s-1} \sqsubseteq_k^* \sigma^{-1} y_s$ we have

$$\pi r(\sigma^{-1} y_s) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{l(s-1)+1} : \\ \mu_{l(s-1)} : \dots : \mu_{h+1} : \mu_h \eta_h : \eta_{h-1} : \dots : \eta_1 ,$$

As above, there is some $h < l \le i$ such that $\pi r(y_s) = \mathrm{pop}_l \pi r(\sigma^{-1} y_s)$ which implies

$$\pi r(y_s) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \xi_{i-1} : \dots : \xi_{l(s-1)+1} : \mu_{l(s-1)} : \dots : \mu_l \\ = \mathrm{pop}_l \pi r(y_{s-1}) .$$

(D) Finally, if $s < t$ then $y_s \not\sqsubseteq_k^* y_t$ implies that $l(s) \le l(t)$ and $l(t) \ge k$.

(c) By induction on t, we have $y_s \sqsubseteq_i^* y_{t-1} \sqsubseteq_k^* \sigma^{-1} y_t$ which implies $y_s \sqsubseteq_i^* \sigma^{-1} y_t$. By (b), we also have $y_s \sqsubseteq_i y_t$. Together it follows that $y_s \sqsubseteq_i^* y_t$. If $\pi r(y_m) \neq \pi r(x)$ then $x \sqsubseteq_k^* y_m$ implies

$$\pi r(y_m) = \xi_n : \dots : \xi_{i+1} : (\xi_i : \dots : \xi_1) : \eta_{i-1} : \dots : \eta_1 ,$$

and the claim follows as above.

(d) By (a), we have $x \sqsubseteq_l^* y_s$, for all $s \le m$ and every $l \le n$. Furthermore, if there were some element $x \sqsubset_l^* z \sqsubset_l^* y_s$, for $l \le k$, then this would imply $x \sqsubset_k^* z \sqsubset_k^* y_s$ which is impossible. □

Finally, we collect some basic facts about the function ω_k.

Lemma 6.6. *Let r be a run, $x \in \mathrm{dom}(r)$, and $y := \omega_k(x)$. The element $x \sqcap_k y$ is the immediate $\sqsubseteq_k^*$-predecessor of y and*

$$\pi r(y) = \mathrm{pop}_l \pi r(x) \qquad \text{for some } l \ge k .$$

Proof. Suppose that there is some element z such that $x \sqcap_k y \sqsubset_k^* z \sqsubset_k^* y$. Then $x < z < y$ and, by choice of y, we have $x \sqsubseteq_k^* z$. Hence, $x \sqsubseteq_k^* z \sqsubseteq_k^* y$. A contradiction. The second claim is a special case of Lemma 6.4. □

Lemma 6.7. *Let r be a run and $x \in \mathrm{dom}(r)$. If $i < k$ then*

$$\omega_k(x) = \omega_i(x) \quad \text{or} \quad \omega_k(x) = \omega_k(\omega_i(x)) .$$

Proof. Let $y := \omega_i(x)$ and $z := \omega_k(x)$. If $z < y$ then $x \sqsubseteq_i^* z$ which implies $x \sqsubseteq_k^* z$. A contradiction.

Suppose that $y < z$. By Lemma 6.6, there exist indices $l \ge i$ and $m \ge k$ such that

$$\pi r(y) = \mathrm{pop}_l \pi r(x) \qquad \text{and} \qquad \pi r(z) = \mathrm{pop}_m \pi r(x) .$$

If $y < z$ then we have $l < k$. Consequently,

$$\pi r(z) = \mathrm{pop}_m \pi r(x) = \mathrm{pop}_m \pi r(y) ,$$

and it follows that $y \not\sqsubseteq_k^* z$. Hence, $\omega_k(y) \le z$. On the other hand, we have

$$\pi r(\omega_k(y)) = \mathrm{pop}_h \pi r(y) = \mathrm{pop}_h \pi r(x) , \qquad \text{for some } h \ge k .$$

Therefore, we have $x \not\sqsubseteq_k^* \omega_k(y)$ which implies $z \le \omega_k(y)$. Together, it follows that $z = \omega_k(y)$. □

7 Strong domination and holes

Remember that we want to decompose a given run r into parts such that in each subrun s we can apply a substitution, that is, if x is the first element of $\mathrm{dom}(s)$ we would like to have $x \lhd_k y$, for all $y \in \mathrm{dom}(s)$. Therefore, we define a second domination order by combining the relations $\lhd_k$ and $\sqsubseteq_k^*$.

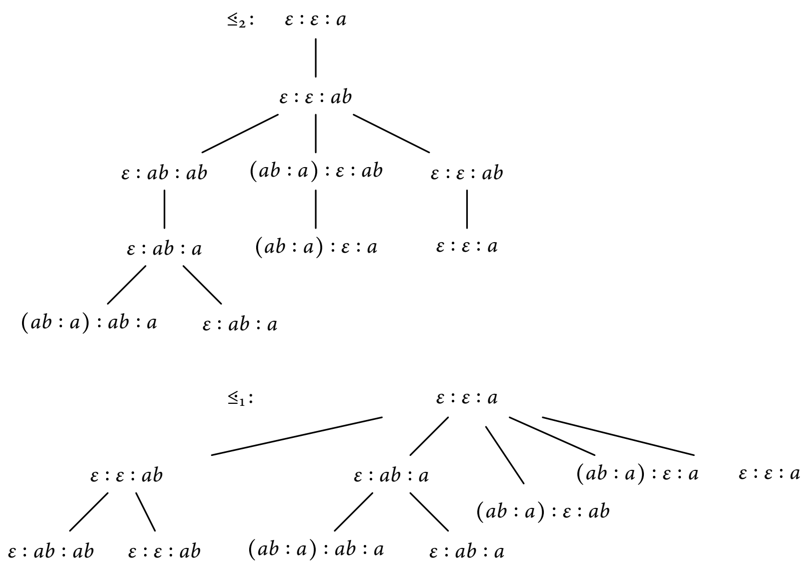

Figure 2: The strong domination orders $\leq_2$ and $\leq_1$.

Definition 7.1. For a run r, elements $x, y \in \mathrm{dom}(r)$, and a number $1 \leq k \leq n$, we define the *strong domination order* $\leq_k$ by

$$x \leq_k y \quad :\text{iff} \quad x \sqsubseteq_k^* y \quad \text{and} \quad x \triangleleft_i z \quad \text{for all } i \geq k \text{ and } x \sqsubseteq_i^* z \sqsubseteq_i^* y\,.$$

The greatest lower $\leq_k$-bound of x and y will be denoted by $x \sqcap_k y$.

Example. Figure 2 shows the strong domination orderings $\leq_2$ and $\leq_1$ corresponding to the run whose weak domination order is depicted in Figure 1.

Let us collect some basic properties of the strong domination order.

Lemma 7.2. *Let $x \leq_k y$. We have $x \leq_k \sigma y$ iff $x \sqsubseteq_k \sigma y$ and $x \triangleleft_k \sigma y$.*

Proof. ($\Rightarrow$) follows immediately from the definition.

($\Leftarrow$) Suppose $x \nleq_k \sigma y$. By definition, we either have $x \not\sqsubseteq_k^* \sigma y$ or there is some $x \sqsubseteq_i^* z \sqsubseteq_i^* \sigma y$, for $i \geq k$, with $x \ntriangleleft_i z$. In the first case, $x \sqsubseteq_k^* y$ implies $x \not\sqsubseteq_k y$. For the second case, note that, if $z \sqsubset_i^* \sigma y$ then $z \sqsubseteq_i^* y$, and $x \leq_i y$ implies $x \triangleleft_i z$. Consequently, $z = \sigma y$ and $x \ntriangleleft_k \sigma y$. □

Lemma 7.3. *Suppose that $x \leq_{k+1} \sigma x$ and $x \nleq_k \sigma x$.*

(a) *There is a pop_k-operation at x.*

(b) *There is a $\mathrm{push}(i)$-operation at $w := x \sqcap_k \sigma x$, for some $i \geq k$.*

(c) *If $u \in \mathrm{dom}(r)$ is some element with $u \leq_k x$ and $u \nleq_k \sigma x$ then there are words $\xi_n, \dots, \xi_0$ and $\mu_n, \dots, \mu_{k+1}$ such that*

$$\pi r(u) = \xi_n : \dots : \xi_0 \quad \text{and} \quad \pi r(\sigma x) = \xi_n \mu_n : \dots : \xi_{k+1}\mu_{k+1} : \xi_k\,.$$

Proof. (a) Since $x \leq_{k+1} \sigma x$ and $x \nleq_k \sigma x$ we have

$$\pi r(\sigma x) = \mathrm{pop}_k(\pi r(x))\,.$$

(b) If the operation at w were a $\mathrm{push}(i)$ or a pop_i with $i < k$ then $w \leq_k x, \sigma x$ would imply $\sigma w \leq_k x, \sigma x$ and we would have $w \neq x \sqcap_k \sigma x$. If there were a pop_i-operation at w with $i \geq k$ then w would have no $\leq_k$-successor. Consequently, the operation at w is a $\mathrm{push}(i)$ with $i \geq k$.

(c) Let $\pi r(u) = \xi_n : \dots : \xi_0$. $u \leq_k x$ implies $u \triangleleft_k x$. Hence, there are words $\mu_n : \dots : \mu_0$ such that

$$\pi r(x) = \xi_n \mu_n : \dots : \xi_k \mu_k : \mu_{k-1} : \dots : \mu_0\,,$$

and $\quad \pi r(\sigma x) = \mathrm{pop}_k \pi r(x) = \xi_n \mu_n : \dots : \xi_k \mu_k\,.$

We claim that $\mu_k = \varepsilon$. Suppose otherwise. Then $u \triangleleft_k \sigma x$ and it follows that $u \not\sqsubseteq_k^* \sigma x$. Since $u \sqsubseteq_k^* x$ this implies $u \nleq_k \sigma x$. Consequently, $\mu_i = \varepsilon$, for all $k \leq i \leq n$. Contradiction. □

We will study decompositions of a run into parts of the following form.

Definition 7.4. For a run r and a vertex $x \in \mathrm{dom}(r)$ we define

$$D_k(x) := \{\, y \in \mathrm{dom}(r) \mid x \leq_k y \,\}\,,$$
$$E_k(x) := \{\, y \in \mathrm{dom}(r) \mid x \sqsubseteq_k^* y \,\}\,.$$

Remark. Note that $D_k(x)$ is an initial segment of $E_k(x)$.

Lemma 7.5. $x \leq_k y$ *iff* $D_k(y) \subseteq D_k(x)$.

Proof. ($\Leftarrow$) By definition, $y \in D_k(y) \subseteq D_k(x)$ implies $x \leq_k y$.

($\Rightarrow$) If $z \in D_k(y)$ then $y \leq_k z$. Hence, $x \leq_k y \leq_k z$ and $z \in D_k(x)$. □

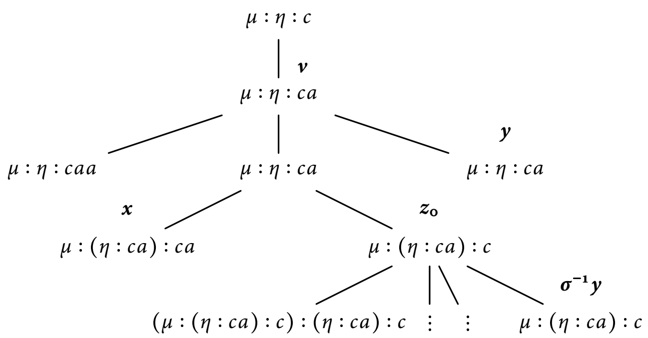

Figure 3: A hole in $D_1(v)$ between x and y.

It will turn out that a good way to construct such a decomposition is by considering subruns whose domain is of the form $D_k(v)$. But in doing so we face the problem that such subruns might contain *holes*, that is, there might be vertices $x, y \in D_k(v)$, $x \prec y$, such that all vertices $x \prec z \prec y$ are not contained in $D_k(v)$. In the remainder of this section we study the structure of such a hole.

Definition 7.6. Let r be a run, $v \in \mathrm{dom}(r)$, and $1 \leq k \leq n$.

(a) If z is the $\preceq$-maximal element of $E_k(v)$ we define

$$\Omega_k(v) := \{(*, \rho r(z))\} \cup \{ (h, q) \mid r(z) \vdash (\mathrm{pop}_h \pi r(v), q),\ h \geq k \}.$$

(b) $D_k(v)$ has a *hole* at x if $x \in D_k(v)$ and $\sigma x \in E_k(v) \setminus D_k(v)$. In this case we define

$$H(x) := \{ y \in \mathrm{dom}(r) \mid z \in E_k(v) \setminus D_k(v) \text{ for all } x \prec z \preceq y \}.$$

We say that the hole is *between* x and y if

$$H(x) = \{ z \mid x \prec z \prec y \}.$$

If such an element y exists then we call the hole *properly terminated*. The maximal element y such that

$$\{ z \mid x \prec z \prec y \} \subseteq H(x)$$

is the *end point* of the hole. Note that the end point is contained in $H(x)$ if and only if the hole is not properly terminated.

(c) An *exit point* of $D_k(v)$ is a $\leq_k$-minimal element of $E_k(v) \setminus D_k(v)$. The set of all exit points of $D_k(v)$ is denoted by $X_k(v)$. The *order* of an exit point x is the number k such that

$$\pi r(x) = \mathrm{pop}_k(\pi r(\sigma^{-1}(x))),$$

and its *type* is the triple

$$(k, \rho r(x), \Omega_{k+1}(x))$$

where k is the order of x.

(d) Suppose that there is a hole in $D_k(v)$ at x with end point y. The *principal sequence* $z_0, \dots, z_m$ of this hole and the *associated sequence* $l(0), \dots, l(m)$ of indices is defined inductively as follows. $z_0 := \sigma x$ and $l(0)$ is the index such that $\pi r(z_0) = \mathrm{pop}_{l(0)} \pi r(x)$. Suppose that z_j and $l(j)$ are already defined. If $z_j \not\sqsubseteq^*_{l(j)+1} y$ then we define $z_{j+1} := \omega_{l(j)+1}(z_j)$, and $l(j+1)$ is the index such that $\pi r(z_{j+1}) = \mathrm{pop}_{l(j+1)} \pi r(z_j)$. We continue this construction until we reach a vertex with $z_j \sqsubseteq^*_{l(j)+1} y$.

If $z_j \neq y$ then we call the element z_j a *principal exit point* of $D_k(v)$. Its *order* is the number $l(j)$. By $P_{kl}(v)$ we denote the set of all principal exit points of $D_k(v)$ of order l.

(e) Suppose there is a hole at x with principal sequence $z_0, \dots, z_m$ and associated sequence of indices $l(0), \dots, l(m)$. Set $h := m - 1$ if the hole is properly terminated and $h := m$, otherwise. The *type* of the hole is the sequence

$$\big(l(0), \rho r(z_0), \Omega_{l(0)+1}(z_0)\big), \dots, \big(l(h), \rho r(z_h), \Omega_{l(h)+1}(z_h)\big),$$

of the types of $z_0, \dots, z_h$

Lemma 7.7. *Let r be a run, $v \in \mathrm{dom}(r)$ and suppose that there is a hole in $D_k(v)$ at x.*

$$H(x) = \dot{\bigcup} \{ D_k(z) \mid z \in H(x) \cap X_k(v) \}$$

$$\textit{and} \quad E_k(z) = D_k(z) \cup \dot{\bigcup} \{ D_k(z) \mid z \in X_k(v) \}.$$

Proof. Since the second equation follows from the first one we only need to prove the first equation.

($\subseteq$) If $y \in H(x)$ then $z \leq_k y$, for some exit point z. If $z \notin H(x)$ then we have $z \prec x \prec y$ and $z \sqsubseteq^*_k y$, and it follows that $z \sqsubseteq^*_k x$. Hence, $x \in D_k(v)$ implies $z \in D_k(v)$. A contradiction.

(⊇) Let $y \in D_k(z)$ for some exit point $z \in H(x)$. Then $z \sqsubseteq_k^* y$ and $z \in E_k(v) \setminus D_k(v)$ implies $y \in E_k(v) \setminus D_k(v)$. It remains to show that there is no element $w \in D_k(v)$ with $x \prec w \preceq y$. Suppose otherwise. Since $z \in H(x)$ we have $z \prec w \preceq y$. Hence, $z \sqsubseteq_k^* y$ implies $z \sqsubseteq_k^* w$. But $v \sqsubseteq_k^* z \sqsubseteq_k^* w$ and $v \leq_k w$ implies $v \leq_k z$. A contradiction. □

The following lemma investigates the structure of a hole and it clarifies the role of the principal sequence.

Lemma 7.8. *Let r be a run, $v \in \mathrm{dom}(r)$, $1 \leq k \leq n$. Suppose that there is a hole in $D_k(v)$ at x with end point y, let $z_0, \dots, z_m$ be its principal sequence, and $l(0), \dots, l(m)$ the sequence of indices such that*

$$\pi r(z_j) = \mathrm{pop}_{l(j)} \pi r(z_{j-1}) .$$

Suppose that $\pi r(v) = \xi_n : \dots : \xi_0$ and $\pi r(x) = \xi_n \eta_n : \dots : \xi_k \eta_k : \eta_{k-1} : \dots : \eta_0$.

(a) *If $z_j \neq y$ then $z_j \in E_k(v) \setminus D_k(v)$.*

(b) *$k \leq l(0) < \dots < l(m)$, in particular $m < n$.*

(c) *If u_j is the immediate $\sqsubseteq_k^*$-predecessor of z_j then $u_j \in D_k(v)$.*

(d) *We have*

$$\pi r(z_j) = \mathrm{pop}_{l(j)} \pi r(x) = \xi_n \eta_n : \dots : \xi_{l(j)+1} \eta_{l(j)+1} : \xi_{l(j)} \eta_{l(j)} .$$

Furthermore, if $z_j \neq y$ then $\eta_{l(j)} = \varepsilon$.

(e) *If the hole is properly terminated then $z_m = y$.*

Proof. (a) $x \prec z_j \prec y$ implies, by definition of y, that $z_j \in H(x) \subseteq E_k(v) \setminus D_k(v)$.

(b) Since $v \lhd_k x$ and $v \ntriangleleft_k \sigma x$ we have, by Lemma 7.3 (a),

$$\pi r(z_0) = \pi r(\sigma x) = \mathrm{pop}_{l(0)} \pi r(x) \qquad \text{with } l(0) \geq k .$$

Furthermore, Lemma 6.6 implies that $l(j+1) \geq l(j) + 1$, for $j < m$.

(c) We claim that $v \sqsubseteq_k^* u_{j+1} \sqsubseteq_k^* u_j$, for all $j < m$. Then the result follows by induction on j since $v \sqsubseteq_k^* u_0 \sqsubseteq_k^* x \in D_k(v)$ implies $u_0 \in D_k(v)$ and $v \sqsubseteq_k^* u_{j+1} \sqsubseteq_k^* u_j \in D_k(v)$ implies $u_{j+1} \in D_k(v)$.

Note that $v \leq x \prec z_{j+1}$ and $v \sqsubseteq_k^* z_{j+1}$ implies $v \sqsubset_k^* z_{j+1}$ and, hence, $v \sqsubseteq_k^* u_{j+1}$. Therefore, we only need to prove that $u_{j+1} \sqsubseteq_k^* u_j$.

By Lemma 6.6, the immediate $\sqsubseteq_{l(j)+1}^*$-predecessor of z_{j+1} is

$$w_{j+1} := z_j \sqcap_{l(j)+1} z_{j+1} .$$

As w_{j+1} has at least two immediate $\sqsubseteq_{l(j)+1}^*$-successors it follows by Lemma 6.5 (d) that z_{j+1} is an immediate $\sqsubseteq_l^*$-successor of w_{j+1}, for all $l \leq l(j) + 1$. Because $k \leq l(j) + 1$ we therefore have $u_{j+1} = w_{j+1} = z_j \sqcap_{l(j)+1} z_{j+1}$. Consequently, we have $u_{j+1} \prec z_j \prec z_{j+1}$ and, together with $u_{j+1} \sqsubseteq_k^* z_{j+1}$, it follows that $u_{j+1} \sqsubseteq_k^* z_j$. Hence, by definition of u_j, we have $u_{j+1} \sqsubseteq_k^* u_j$.

(d) First, consider the case that $l(j) = 1$. By (b), this implies $k = 1$ and $j = 0$. Since $z_0 = \sigma x$ we have $\pi r(z_0) = \mathrm{pop}_{l(0)} \pi r(x)$, by definition of $l(0)$. Finally, we have $\eta_1 = \varepsilon$, by Lemma 7.3 (c).

For $l(j) > 1$, we prove the claim by induction on j. For $j = 0$, we have, by definition,

$$\pi r(z_0) = \pi r(\sigma x) = \mathrm{pop}_{l(0)} \pi r(x) = \xi_n \eta_n : \dots : \xi_{l(0)} \eta_{l(0)} ,$$

and, for $j > 0$, the induction hypothesis implies that

$$\begin{aligned} \pi r(z_j) &= \mathrm{pop}_{l(j)} \pi r(z_{j-1}) \\ &= \mathrm{pop}_{l(j)} (\xi_n \eta_n : \dots : \xi_{l(j-1)} \eta_{l(j-1)}) \\ &= \xi_n \eta_n : \dots : \xi_{l(j)} \eta_{l(j)} . \end{aligned}$$

Suppose that $\eta_{l(j)} \neq \varepsilon$. We claim that $z_j = y$.

$$\xi_n : \dots : \xi_0 \lhd_k \pi r(x) = \xi_n \eta_n : \dots : \xi_k \eta_k : \eta_{k-1} : \dots : \eta_0$$

implies, by Lemma 5.2, that

$$\xi_n : \dots : \xi_0 \lhd_k \xi_n \eta_n : \dots : \xi_{l(j)} \eta_{l(j)} = \pi r(z_j) .$$

Furthermore, by (c), we have $u_j \in D_k(v)$ for the immediate $\sqsubseteq_k^*$-predecessor u_j of z_j. Together with $z_j \in E_k(v)$ it therefore follows that $z_j \in D_k(v)$. This implies $z_j = y$.

(e) Suppose that $z_m \neq y$. We define a sequence $w_0, \dots, w_s$ of vertices as follows. Set $w_0 := z_m$. For $j > 0$, fix the maximal index h such that $w_{j-1} \not\sqsubseteq_h^* y$ and let $w_j := \omega_h(w_{j-1})$. The construction stops when we reach a vertex $w_s \sqsubseteq_k^* y$. Since the hole is properly terminated we have $y \in D_k(v)$. Hence, $v \sqsubseteq_k^* w_s \sqsubseteq_k^* y$ implies $w_s \in D_k(v)$ and it follows that $w_s = y$.

Let $l := l(m)$. We prove by induction on j that

$$\pi r(w_j) = \xi_n\eta_n : \cdots : \xi_{l+1}\eta_{l+1} : \mu_j\,, \qquad \text{for some } \mu_j \sqsubseteq_0 \xi_l \text{ with } \mu_j \neq \varepsilon\,.$$

For $j = 0$, we have $\pi r(w_0) = \pi r(z_m)$ and $\mu_0 = \xi_l$ as desired. By Lemma 6.6, for every $j > 0$, there is some index h such that

$$\pi r(w_j) = \mathrm{pop}_h \pi r(w_{j-1})\,.$$

If $h > l$ then

$$\pi r(w_j) = \mathrm{pop}_h(\xi_n\eta_n : \cdots : \xi_{l+1}\eta_{l+1} : \mu_{j-1}) = \xi_n\eta_n : \cdots : \xi_h\eta_h\,,$$

which implies $z_m \not\sqsubseteq^*_h w_j$. Hence, $z_m \not\sqsubseteq^*_{l+1} w_j$ and, therefore, $z_m \not\sqsubseteq^*_{l(m)+1} y$. Contradiction. Thus, we have $h \leq l$ and

$$\begin{aligned}\pi r(w_j) &= \mathrm{pop}_h(\xi_n\eta_n : \cdots : \xi_{l+1}\eta_{l+1} : \mu_{j-1}) \\ &= \xi_n\eta_n : \cdots : \xi_{l+1}\eta_{l+1} : \mu_j\end{aligned}$$

with $\mu_j = \mathrm{pop}_h(\mu_{j-1})$.

Since $\mu_s \sqsubseteq_0 \xi_l$ implies $\xi_l : \cdots : \xi_0 \not\trianglelefteq_k \mu_s$, it follows that

$$\xi_n : \cdots : \xi_0 \not\trianglelefteq_k \xi_n\eta_n : \cdots : \xi_{l+1}\eta_{l+1} : \mu_s = \pi r(y)$$

in contradiction to $y \in D_k(v)$. □

Lemma 7.9. *Every principal exit point is an exit point.*

Proof. Let $z \in P_{kl}(v)$. Clearly, $z \in E_k(v) \setminus D_k(v)$. Suppose there is some $y \in E_k(v) \setminus D_k(v)$ with $y \lessdot_k z$. By Lemma 7.8 (c), $y \sqsubset^*_k z$ implies $y \in D_k(v)$. Contradiction. □

8 Expansion sequences

In order to perform the pumping construction in the next section we need to find a pair of vertices $u \lessdot_1 v$ with certain properties. As an intermediate step to prove the existence of such pairs we show in the current section that, if the run is long enough then we can find arbitrary long chains $u_0 \lessdot_1 \cdots \lessdot_1 u_m$.

In order to prove the existence of long chains $u_0 \lessdot_1 \cdots \lessdot_1 u_m$ it is sufficient to bound the branching factor of the forest $(\mathrm{dom}(r), \leq_1)$. To do so we employ the following device.

Definition 8.1. Let r be a run. An *expansion sequence* of r is a sequence of injections $t_k \to \cdots \to t_n$ between forests where $t_n := r$ and, for $i < n$, we have $t_i := (C, \leq_{i+1})$ where $C \subseteq \mathrm{dom}(t_{i+1})$ is a maximal chain in t_{i+1}.

We want to prove that each forest in an expansion sequence is binary. The following lemmas collect basic properties about the vertices in such a forest.

Lemma 8.2. *Let $t_k \to \cdots \to t_n$ be an expansion sequence of r and let $x \in \mathrm{dom}(t_k)$. If y is an immediate successor of x with $(\pi t_k(y))_{k+1} = (\pi t_k(x))_{k+1}$ then there exist no immediate successors z of x with $y < z$.*

Proof. Denote the first embedding by $\iota : t_k \to t_{k+1}$. We show that, for all $z \in \mathrm{dom}(t_k)$ with $x \leq_{k+1} z$, we have $y \leq_{k+1} z$. The proof proceeds by induction on the number of elements w such that $\iota y \leq w \leq \iota z$.

Since

$$x \lhd_{k+1} y \lhd_{k+2} z\,, \quad x \lhd_{k+1} z\,, \quad \text{and} \quad (\pi t_k(x))_{k+1} = (\pi t_k(y))_{k+1}\,,$$

it follows by Lemma 5.3 that $y \lhd_{k+1} z$. Consequently, $y \sqsubseteq_{k+1} z$ and, by induction hypothesis, we have $y \sqsubseteq^*_{k+1} z$.

Let w be some element such that $y \sqsubseteq^*_{k+1} w \sqsubseteq^*_{k+1} z$. We have to show that $y \lhd_{k+1} w$. Since $x \sqsubseteq^*_{k+1} w \sqsubseteq^*_{k+1} z$ and $x \leq_{k+1} z$ we have $x \lhd_{k+1} w$. Similarly, $y \sqsubseteq^*_{k+2} w \sqsubseteq^*_{k+2} z$ implies $y \lhd_{k+2} w$. Since $(\pi t_k(x))_{k+1} = (\pi t_k(y))_{k+1}$ we can again apply Lemma 5.3 to infer that $y \lhd_{k+1} w$. Together with $y \leq_{k+2} z$ it therefore follows that $y \leq_{k+1} z$. □

Lemma 8.3. *Let $t_k \to \cdots \to t_n$ be an expansion sequence of r. Denote the embedding $t_k \to t_n$ by ι and let $x \in \mathrm{dom}(t_k)$.*

(a) *If the operation at x is a level i operation with $i \leq k$ and x has an immediate successor y then $\iota y = \sigma\iota x$. In particular, y is the only immediate successor of x.*

(b) *If there is a pop_i-operation at x with $i > k$ then x is a leaf.*

Proof. (a) follows from Lemma 8.2 by induction on k, and (b) follows immediately from the definition. □

Lemma 8.4. *Let $t_k \to \cdots \to t_n$ be an expansion sequence of r and $x \in \mathrm{dom}(t_k)$ a vertex with several immediate successors $y_0, \ldots, y_{m-1}$, $m \geq 2$.*

(a) *The operation at x is a $\mathrm{push}(k+1)$-operation.*

(b) *There are words* $\xi_n, \dots, \xi_0$ *and* $\mu_n, \dots, \mu_{k+2}$ *such that*

$$\pi t_k(x) = \xi_n : \dots : \xi_0 ,$$
$$\pi t_k(y_0) = \begin{cases} \text{clone}_{k+1}(\pi t_k(x)) & \text{if } k > 0 , \\ \text{push}_a(\pi t_k(x)) & \text{if } k = 0 , \end{cases}$$
$$\pi t_k(y_1) = \xi_n \mu_n : \dots : \xi_{k+2}\mu_{k+2} : \xi_{k+1} : \dots : \xi_0 .$$

(c) *x has exactly two immediate successors.*

Proof. We prove the claims by induction on k. Denote the embedding $t_k \to t_i$ by ι_i and set $C := \text{rng}(\iota_{k+1})$.

(a) Lemma 8.3 (a) and (b) imply that there is a push(i)-operation at x with $i > k$. Suppose that $i > k+1$. Let z be the element such that $\iota_{i-1}z$ is the immediate successor of $\iota_{i-1}x$. By construction of t_k, z is the first immediate successor of x. By induction hypothesis we have $(\pi t_k(z))_{k+1} = (\pi t_k(x))_{k+1}$. Therefore, it follows from Lemma 8.2 that z is also the last immediate successor of x. Hence, x has only one immediate successor. Contradiction.

(b) By Lemma 8.3 (a), we know that $\iota_n y_0 = \sigma\iota_n x$. Hence, (a) implies that

$$\pi t_k(y_0) = \begin{cases} \text{clone}_{k+1}(\pi t_k(x)) & \text{if } k > 0 , \\ \text{push}_a(\pi t_k(x)) & \text{if } k = 0 . \end{cases}$$

By construction of t_k, $\iota_{k+1}y_1$ is the minimal element of $C \setminus \{\iota_{k+1}x\}$ such that

$$y_0 \not\trianglelefteq_{k+1} y_1 .$$

Let z be the element such that $\iota_{k+1}z$ is the immediate predecessor of $\iota_{k+1}y_1$ in C. Since $\iota_{k+1}z$ is not a leaf of t_{k+1}, Lemma 8.3 (b) implies that the operation at z is not a pop$_i$ with $i > k+1$. Since

$$y_0 \trianglelefteq_{k+1} z ,$$

the operation at z must therefore be a pop$_{k+1}$ and, by Lemma 8.3 (a), we have $\iota_n y_1 = \sigma\iota_n z$. Furthermore, it follows that there are words $\mu_n, \dots, \mu_0$ such that

$$\pi t_k(z) = \xi_n\mu_n : \dots : \xi_{k+2}\mu_{k+2} : \xi_{k+1}(\xi_k : \dots : \xi_0)\mu_{k+1} : \mu_k : \dots : \mu_0 .$$

Consequently, $y_0 \not\trianglelefteq_{k+1} y_1$ implies that $\mu_{k+1} = \varepsilon$ and

$$\pi t_k(y_1) = \text{pop}_{k+1}(\pi t_k(z)) = \xi_n\mu_n : \dots : \xi_{k+2}\mu_{k+2} : \xi_{k+1} : \dots : \xi_0 .$$

(c) By (b) and Lemma 8.2 it follows that y_1 is the last immediate successor of x. □

Corollary 8.5. *Every forest in an expansion sequence is binary.*

Using this corollary we can prove that every sufficiently long run contains a sequence $u_0 \trianglelefteq_1 \dots \trianglelefteq_1 u_m$.

Lemma 8.6. *Let t be a binary tree with $|\text{dom}(t)| \geq 2^m$ vertices. Then there exists a chain $C \subseteq \text{dom}(t)$ of size $|C| > m$.*

Proof. If every chain is of size at most m then $\text{dom}(t) \subseteq \{0,1\}^{<m}$ which implies

$$|\text{dom}(t)| \leq \sum_{i<m} 2^i = 2^m - 1 .$$

Contradiction. □

We only consider the case of runs starting at the initial configuration. This ensures that the expansion sequence constructed below consists of trees instead of forests. The restriction will be lifted below.

Lemma 8.7. *Let r be a run that starts at the initial configuration. For every set $M \subseteq \text{dom}(r)$ of size $|M| \geq \beth_n(m)$ there exists a sequence $u_0 \trianglelefteq_1 \dots \trianglelefteq_1 u_m$ of vertices of length strictly greater than m such that,*

$$M \cap (D_1(u_i) \setminus D_1(u_{i+1})) \neq \varnothing , \quad \textit{for all } i < m .$$

Proof. We construct an expansion sequence $t_0 \to \dots \to t_n$ and two sequences $C_0, \dots, C_n$ and $M_0, \dots, M_n$ of sets as follows. We start with $t_n := r$ and $M_n := M$. To construct t_k suppose that we have already defined $t_{k+1} = (\text{dom}(t_{k+1}), \leq)$ and a subset $M_{k+1} \subseteq \text{dom}(t_{k+1})$. Choose a chain $C'_{k+1} \subseteq M_{k+1}$ of maximal length in the tree $(M_{k+1}, \leq)$, and let $C_{k+1} \subseteq \text{dom}(t_{k+1})$ be a maximal chain in t_{k+1} with $C'_{k+1} \subseteq C_{k+1}$. We set

$$t_k := (C_{k+1}, \trianglelefteq_{k+1}) \quad \text{and} \quad M_k := C_{k+1} \cap \{ u \wedge v \mid u, v \in M_{k+1} \} ,$$

where $\wedge$ denotes the greatest lower bound in t_k. Finally, we also choose some chain $C'_0 \subseteq M_0$ of maximal length and a corresponding maximal chain $C_0 \subseteq \text{dom}(t_0)$ with $C'_0 \subseteq C_0$.

Let x be the first element of $\text{dom}(r)$. Since x is initial we have $\pi r(x) = \varepsilon : \dots : \varepsilon : a$, for some letter a, which implies, by Corollary 5.6, that $x \triangleleft_1 y$, for all

$y \in \mathrm{dom}(r)$. Therefore, x is the unique minimal element of each t_k and all t_k are binary trees. Since the sets M_k are closed under greatest lower bounds it follows that the subforests induced by them also form binary trees. Consequently, we can apply the preceding lemma. By induction on k, it follows that $|C'_k| > \beth_k(m)$, for $k < n$. Let $u_0 < \cdots < u_m$ be an enumeration of (a subset of) C'_0. The sequence $\iota_n u_0, \dots, \iota_n u_m$ has the desired property. □

By an automaton construction we can generalise this result to arbitrary runs. Unfortunately, this introduces a dependence on the size of the stack contents of the first configuration.

Definition 8.8. For $\xi = x_0 \dots x_m \in \Gamma^{+n}$ we define, by induction on n,

$$\|\xi\| := \begin{cases} |\xi| & \text{if } n = 1\,, \\ \sum_{i \le m} \|x_i\| & \text{if } n > 1\,. \end{cases}$$

Corollary 8.9. *Let r be a run with first element w and set $k := 2\|\pi r(w)\|$. For every set $M \subseteq \mathrm{dom}(r)$ of size $|M| \ge \beth_n(m + k)$ there exists a sequence $u_0 \preceq_1 \cdots \preceq_1 u_m$ of vertices of length strictly greater than m such that,*

$$M \cap (D_1(u_i) \setminus D_1(u_{i+1})) \neq \varnothing\,, \quad \textit{for all } i < m\,.$$

Proof. Let $\xi := \pi r(w)$. There exists a sequence op of at most $k := 2\|\xi\|$ stack operations such that $\xi := \mathrm{op}(\varepsilon : \cdots : \varepsilon : a)$. We construct an automaton $\mathcal{B}$ by modifying the given automaton $\mathcal{A}$ such that, starting at the initial configuration $\mathcal{B}$ executes the operations op until it reaches the configuration $r(w)$. Then it continues in exactly the same way as $\mathcal{A}$ would. Let $r' = sr$ be the run of $\mathcal{B}$ starting at the initial configuration. The preceding lemma implies that there exists a sequence $u_0 \preceq_1 \cdots \preceq_1 u_{m+k}$ with the desired properties in $\mathrm{dom}(r')$. Since $|\mathrm{dom}(s)| = k$ it follows that $u_i \in \mathrm{dom}(r)$, for $i \ge k$. Hence, $u_k \preceq_1 \cdots \preceq_1 u_{m+k}$ is the desired sequence. □

9 A pumping lemma

Using the structure theory developed in Sections 5 to 8 we prove a pumping lemma for higher-order pushdown automata. For the construction below we need to find two vertices $u \lessdot_1 v$ such that the same types of holes appear in $D_1(u)$ and in $D_1(v)$. Such vertices u, v will be called a *pumping pair*. The formal definition is based on the equivalence relation $\sim_{km}$.

Definition 9.1. (a) Let $\xi = \xi_n : \cdots : \xi_k$. We define the set

$$\tilde{\chi}_k(\xi) \subseteq \Gamma^{*n} \times \cdots \times \Gamma^{*(k+1)} \times Q \times \{*, k+1, \dots, n\} \times Q$$

by the following conditions. For $l \in \{k+1, \dots, n\}$, we have

$$(\mu_n, \dots, \mu_{k+1}, p, l, q) \in \tilde{\chi}_k(\xi)\,,$$

iff there is a run r and an element $x \in \mathrm{dom}(r)$ such that

$$r(x) = (\xi_n\mu_n : \cdots : \xi_{k+1}\mu_{k+1} : \xi_k,\ p)\,,$$

and $r(\omega_{k+1}(x)) = (\xi_n\mu_n : \cdots : \xi_l\mu_l,\ q)$,

and we have

$$(\mu_n, \dots, \mu_{k+1}, p, *, q) \in \tilde{\chi}_k(\xi)$$

iff there is a run r and elements $x, y \in \mathrm{dom}(r)$ with $y \in E_{k+1}(x)$ such that

$$r(x) = (\xi_n\mu_n : \cdots : \xi_{k+1}\mu_{k+1} : \xi_k,\ p)\,, \quad \text{and} \quad \rho r(y) = q\,.$$

(b) For $\xi, \zeta \in \Gamma^{+n}$ and $k, m \le n$, we define an equivalence relation $\sim_{km}$ by

$$\begin{aligned} \xi \sim_{km} \zeta \quad :\text{iff} \quad & \text{for all } \mu_i \in \Gamma^{*i},\ p, q \in Q, \text{ and } l \in \{*, k+1, \dots, n\}, \\ & (\mu_n^\xi, \dots, \mu_{k+1}^\xi, p, l, q) \in \tilde{\chi}_k(\mathrm{pop}_k(\xi)) \\ & \Leftrightarrow (\mu_n^\zeta, \dots, \mu_{k+1}^\zeta, p, l, q) \in \tilde{\chi}_k(\mathrm{pop}_k(\zeta))\,, \end{aligned}$$

where, for $\lambda = \lambda_n : \cdots : \lambda_0$, we set

$$\mu_i^\lambda := \begin{cases} \varepsilon & \text{if } \mu_i = \varepsilon\,, \\ \mu_i[\varepsilon : \cdots : \varepsilon : (\mu_i)_0/\varepsilon : \lambda_{i-1} : \cdots : \lambda_0]_m & \text{otherwise}\,. \end{cases}$$

(c) Let r be a run. Two vertices $u, v \in \mathrm{dom}(r)$ form a *pumping pair* if

$$u \lessdot_1 v\,, \quad \rho r(u) = \rho r(v)\,, \quad \text{and} \quad \pi r(u) \sim_{k1} \pi r(v)\,, \quad \text{for all } k \le n\,.$$

Given a pumping pair $u \lessdot_1 v$ we can perform the following pumping construction.

Lemma 9.2. *Let r be a run with a pumping pair $u \lessdot_1 v$ and suppose*

$$\pi r(u) = \xi = \xi_n : \dots : \xi_0 \quad \textit{and} \quad \pi r(v) = \zeta = \zeta_n : \dots : \zeta_0 \,.$$

There exists a run s whose first configuration is the same as that of r and there are vertices $u', v', w' \in \operatorname{dom}(s)$ such that

$$\pi s(u') = \xi\,, \quad \pi s(v') = \zeta\,, \quad \pi s(w') = \zeta[\xi/\zeta]_1\,,$$

$u' \lessdot_1 v'$ form a pumping pair, and $|D_1(v')| = |D_1(u)|$.

Proof. Define

$$s_0 := r|_{\operatorname{dom}(r) \smallsetminus E_1(v)}\,, \quad \text{and} \quad s_1 := (r|_{D_1(u)})[\xi/\zeta]_1\,.$$

Let u' be the copy of u in $\operatorname{dom}(s_0)$ and denote the copies of u and v in $\operatorname{dom}(s_1)$ by v' and w', respectively. For each principal exit x of some hole in $\operatorname{dom}(s_1) = D_1(u)$ we construct a run s_x of the same type as x. We obtain the desired run s by inserting s_1 into s_0 and each s_x into the corresponding hole of s_1.

It remains to find s_x. If x is of order k then, by Lemma 7.8 (d), there are words $\mu_n, \dots, \mu_{k+1}$ such that

$$\pi r(x) = \xi_n\mu_n : \dots : \xi_{k+1}\mu_{k+1} : \xi_k\,.$$

Since $\xi \sim_{k1} \zeta$ we can find a run s_x of the same type as x such that

$$\pi s_x(y) = \zeta_n\tilde{\mu}_n : \dots : \zeta_{k+1}\tilde{\mu}_{k+1} : \zeta_k\,,$$

where y is the first element of $\operatorname{dom}(s_x)$ and

$$\tilde{\mu}_i := \begin{cases} \varepsilon & \text{if } \mu_i = \varepsilon\,, \\ \mu_i[\varepsilon : \xi_{i-1} : \dots : \xi_0/\varepsilon : \zeta_{i-1} : \dots : \zeta_0]_1 & \text{otherwise}\,. \end{cases}$$ □

It remains to prove the existence of a pumping pair. We start by showing that $\tilde{\chi}_k(\xi)$ is closed under $\sim_{i,k+1}$.

Lemma 9.3. *Let $\xi = \xi_n : \dots : \xi_k \in \Gamma^{+n}$ and $\mu_i, \eta_i \in \Gamma^{+i}$, for $k < i \le n$. If*

$$\xi_n\mu_n : \dots : \xi_{k+1}\mu_{k+1} : \xi_k \sim_{i,k+1} \xi_n\eta_n : \dots : \xi_{k+1}\eta_{k+1} : \xi_k\,,$$

for all $k < i \le n$, then we have

$$(\mu_n, \dots, \mu_{k+1}, p, l, q) \in \tilde{\chi}_k(\xi) \quad \text{iff} \quad (\eta_n, \dots, \eta_{k+1}, p, l, q) \in \tilde{\chi}_k(\xi)\,.$$

Proof. Let r be a run of minimal length witnessing the fact that

$$(\mu_n, \dots, \mu_{k+1}, p, l, q) \in \tilde{\chi}_k(\xi)\,.$$

Denote the first and last elements of $\operatorname{dom}(r)$ by x and y, respectively. By minimality of r, we have

$$r(x) = (\xi_n\mu_n : \dots : \xi_{k+1}\mu_{k+1} : \xi_k,\ p)$$

and either

$$l \neq *\,, \quad y = \omega_{k+1}(x)\,, \quad \text{and} \quad r(y) = (\xi_n\mu_n : \dots : \xi_l\mu_l,\ q)\,,$$

or

$$l = *\,, \quad y \in E_{k+1}(x)\,, \quad \text{and} \quad \rho r(y) = q\,.$$

We construct a witness s for

$$(\eta_n, \dots, \eta_{k+1}, p, l, q) \in \tilde{\chi}_k(\xi)$$

as follows. Let

$$t := (r|_{D_{k+1}(x)})[\xi_n\mu_n : \dots : \xi_{k+1}\mu_{k+1} : \xi_k/\xi_n\eta_n : \dots : \xi_{k+1}\eta_{k+1} : \xi_k]_{k+1}\,.$$

If $l \neq *$ then we add the element y as last element to t by setting

$$t(y) := (\xi_n\eta_n : \dots : \xi_l\eta_l, q)\,.$$

Clearly, t is a partial run of the right type with

$$t(x) = (\xi_n\eta_n : \dots : \xi_{k+1}\eta_{k+1} : \xi_k, p)\,.$$

If t does not contain holes then we have already found the desired witness.

Suppose that there is a hole in $\operatorname{dom}(t) = D_{k+1}(x)$ and let w be one of its principal exits. If w is of order i then

$$\pi r(w) = \xi_n\mu_n\beta_n : \dots : \xi_{i+1}\mu_{i+1}\beta_{i+1} : \xi_i\mu_i\,,$$

for some words $\beta_n, \dots, \beta_{i+1}$. We construct a run t_w of the same type as w that be inserted into t to fill the hole. Since

$$\xi_n\mu_n : \dots : \xi_{k+1}\mu_{k+1} : \xi_k \sim_{i,k+1} \xi_n\eta_n : \dots : \xi_{k+1}\eta_{k+1} : \xi_k$$

there exists a run t_w with first and last element u and v, respectively, such that

$$\pi t_w(u) = \xi_n \eta_n \tilde{\beta}_n : \dots : \xi_{i+1}\eta_{i+1}\tilde{\beta}_{i+1} : \xi_i \eta_i ,$$

where

$$\tilde{\beta}_j := \begin{cases} \varepsilon & \text{if } \beta_j = \varepsilon , \\ \beta_j[\varepsilon : \xi_{j-1}\mu_{j-1} : \dots : \xi_{k+1}\mu_{k+1} : \xi_k / \varepsilon : \xi_{j-1}\eta_{j-1} : \dots : \xi_{k+1}\eta_{k+1} : \xi_k]_{k+1} \\ & \text{otherwise} . \end{cases}$$

Furthermore, if $l \neq *$ then

$$\pi t_w(v) = \xi_n \eta_n \tilde{\beta}_n : \dots : \xi_h \eta_h \tilde{\beta}_h ,$$

and, otherwise, we have $\rho t_w(v) = \rho r(v)$. □

We can use the preceding result to compute a bound on the index of $\sim_{km}$.

Lemma 9.4. *The index of $\sim_{km}$ is bounded by*

$$|\Gamma^{+n}/\sim_{km}| \leq \beth_{n-k+1}\big(3^{n-k}|Q|^2(n-k+1)!\big) .$$

Proof. Let $s := |Q|$. We prove the claim by induction on k. For $k = n$, we have

$$\tilde{\chi}_n(\xi) \subseteq Q \times \{*\} \times Q$$

which implies $\xi \sim_{nm} \zeta$ iff $\tilde{\chi}_n(\xi) = \tilde{\chi}_n(\zeta)$. Hence, there are at most 2^{s^2} $\sim_{nm}$-classes.

Suppose that $k < n$. For $\lambda = \lambda_n : \dots : \lambda_k \in \Gamma^{+n}$ and $\mu_i, \eta_i \in \Gamma^{*i}$, we define

$$\begin{aligned} & (\mu_n, \dots, \mu_{k+1}) \equiv_\lambda (\eta_n, \dots, \eta_{k+1}) \\ \text{iff} \quad & \lambda_n\mu_n : \dots : \lambda_{k+1}\mu_{k+1} : \lambda_k \sim_{i,k+1} \lambda_n\eta_n : \dots : \lambda_{k+1}\eta_{k+1} : \lambda_k , \quad \text{for all } i > k . \end{aligned}$$

By Lemma 9.3, $(\mu_n, \dots, \mu_{k+1}) \equiv_\lambda (\eta_n, \dots, \eta_{k+1})$ implies

$$(\mu_n, \dots, \mu_{k+1}, p, l, q) \in \tilde{\chi}_k(\lambda) \quad \text{iff} \quad (\eta_n, \dots, \eta_{k+1}, p, l, q) \in \tilde{\chi}_k(\lambda) .$$

By induction hypothesis, there are at most

$$\begin{aligned} \prod_{i=1}^{n-k} \beth_i(3^{i-1}s^2 i!) &\leq \beth_{n-k}\big((n-k)3^{n-k-1}s^2(n-k)!\big) \\ &\leq \beth_{n-k}\big(3^{n-k-1}s^2(n-k+1)!\big) \end{aligned}$$

$\equiv_\lambda$-classes. Set

$$\begin{aligned} & (\mu_n, \dots, \mu_{k+1}) \equiv (\eta_n, \dots, \eta_{k+1}) \\ \text{iff} \quad & (\mu^\xi_n, \dots, \mu^\xi_{k+1}) \equiv_{\mathrm{pop}_k(\xi)} (\eta^\xi_n, \dots, \eta^\xi_{k+1}) \\ & \text{and } (\mu^\zeta_n, \dots, \mu^\zeta_{k+1}) \equiv_{\mathrm{pop}_k(\zeta)} (\eta^\zeta_n, \dots, \eta^\zeta_{k+1}) , \end{aligned}$$

where, as above,

$$\mu^\xi_i := \begin{cases} \varepsilon & \text{if } \mu_i = \varepsilon , \\ \mu_i[\varepsilon : \dots : \varepsilon : (\mu_i)_0 / \varepsilon : \xi_{i-1} : \dots : \xi_0]_m & \text{otherwise} . \end{cases}$$

By Lemma 9.3, we have $\xi \sim_{km} \zeta$ if and only if, for every $\equiv$-class $[\mu_n, \dots, \mu_{k+1}]$ we have

$$\begin{aligned} & (\mu^\xi_n, \dots, \mu^\xi_{k+1}, p, l, q) \in \tilde{\chi}_k(\mathrm{pop}_k(\xi)) \\ \text{iff} \quad & (\mu^\zeta_n, \dots, \mu^\zeta_{k+1}, p, l, q) \in \tilde{\chi}_k(\mathrm{pop}_k(\zeta)) . \end{aligned}$$

Hence, there are at most

$$\begin{aligned} 2^{\beth_{n-k}(3^{n-k-1}s^2(n-k+1)!)^2 \cdot s^2 \cdot (n-k+1)} &\leq \beth_{n-k+1}\big(3 \cdot 3^{n-k-1}s^2(n-k+1)!\big) \\ &= \beth_{n-k+1}\big(3^{n-k}s^2(n-k+1)!\big) \end{aligned}$$

$\sim_{km}$-classes. □

The existence of a pumping pair immediately follows from the previous lemma and Corollary 8.9.

Lemma 9.5. *Let r be a run with first element w and set $k := 2\|\pi r(w)\|$. For every set $M \subseteq \mathrm{dom}(r)$ of size*

$$|M| \geq \beth_{2n}\big(n3^{n-1}|Q|^3 n! + k\big)$$

there exists a pumping pair $u \lessdot_1 v$ such that

$$M \cap (D_1(u) \setminus D_1(v)) \neq \varnothing .$$

Proof. By Corollary 8.9, there exists a sequence $u_0 \lessdot_1 \dots \lessdot_1 u_m$ of length strictly greater than

$$m := \beth_n\big(n3^{n-1}|Q|^3 n!\big) \geq |Q| \cdot \prod_{1 \leq i \leq n} \beth_{n-i+1}\big(3^{n-i}|Q|^2(n-i+1)!\big)$$

such that

$$M \cap (D_1(u_i) \setminus D_1(u_{i+1})) \neq \varnothing\,, \quad \text{for all } i < m\,.$$

By Lemma 9.4, it therefore follows that there are two indices $i < j$ such that u_i and u_j form a pumping pair. □

We apply the technical Lemma 9.2 to show that, if there exists a run of a certain length then there are infinitely many different runs.

Theorem 9.6 (Pumping Lemma). *Let $\mathcal{A}$ be a pushdown automaton of level n and let r be a run of $\mathcal{A}$ with first element w.*

(a) *If*

$$|\mathrm{dom}(r)| \geq \beth_{2n}\big(n3^{n-1}|Q|^3 n! + 2\|\pi r(w)\|\big)$$

then there exists a sequence $r_0, r_1, \dots$ of runs, each starting with w, where $r_0 = r$ and

$$|\mathrm{dom}(r_i)| < |\mathrm{dom}(r_{i+1})|\,, \qquad \textit{for all } i < \omega\,.$$

(b) *Similarly, if r contains at least*

$$\beth_{2n}\big(n3^{n-1}|Q|^3 n! + 2\|\pi r(w)\|\big)$$

non-ε-transitions then there exists a sequence $r_0, r_1, \dots$ of runs, each starting at w, where $r_0 = r$ and r_{i+1} contains more non-ε-transitions than r_i.

Proof. (a) Let $M := \mathrm{dom}(r)$. By Lemma 9.5, there exists a pumping pair $u \lessdot_1 v$ in r. We define a sequence of runs $r'_0, r'_1, \dots$ inductively. For each run r_i, we will also choose a pumping pair $u_i \lessdot_1 v_i$. We start with $r'_0 := r$, $u_0 := u$, and $v_0 := v$. Suppose that r'_i is already defined. By Lemma 9.2, we can construct a new run r'_{i+1} that contains elements u_{i+1} and v_{i+1} such that $u_{i+1} \lessdot_1 v_{i+1}$ forms a pumping pair and $|D_1(v_{i+1})| = |D_1(u_i)| > |D_1(v_i)|$. To obtain the desired sequence $r_0, r_1, \dots$ we delete from $r'_0, r'_1, \dots$ all runs r'_i such that $|\mathrm{dom}(r'_l)| \geq |\mathrm{dom}(r'_i)|$, for some $l < i$. The condition $|D_1(v_i)| < |D_1(v_{i+1})|$ ensures that the resulting sequence is still infinite.

(b) Let $M \subseteq \mathrm{dom}(r)$ be the set of all configurations with an outgoing non-ε-transition. If we perform the same construction as in the proof of (a) we obtain a sequence of runs r_i, $i < \omega$, such that the number of non-ε-transitions in each run is strictly increasing. □

Corollary 9.7. *Let $\mathcal{A}$ be a pushdown automaton of level n. If $\mathcal{A}$ accepts a word of length at least*

$$\beth_{2n}\big(n3^{n-1}|Q|^3 n!\big)$$

then the language recognised by $\mathcal{A}$ is infinite.

One immediate consequence of this theorem is the fact that finiteness is decidable for languages recognised by a higher-order pushdown automaton.

Corollary 9.8. *The problem whether the language recognised by a given higher-order pushdown automaton is finite is decidable.*

We apply the theorem to prove that a given graph does not belong to a certain level of the Caucal hierarchy.

Example. Let $\mathfrak{T}_k := (T_k, \preceq)$ where $T_k := \{\, 0^i 1^l \mid i < \omega,\ l < \beth_k(i) \,\}$. We claim that $\mathfrak{T}_{3n} \notin \mathcal{C}_n$. For a contradiction, suppose otherwise. By Theorem 3.3, there exists a pushdown automaton $\mathcal{A}$ of level n whose configuration graph becomes isomorphic to $\mathfrak{T}_{3n}$ when we contract all ε-transitions. Furthermore, we can use Lemma 3.4 to find a finite structure $\mathfrak{A}$ with universe $Q \cup \Gamma$ such that the configuration graph of $\mathcal{A}$ is definable in $\mathfrak{A}^{*n}$.

Let $w_k \in A^{*n}$ be the word encoding the element $0^k 1 \in T_{3n}$. In the same way as in the example on page 13 it follows that

$$|w_k|_i \leq \beth_{i-1}(\mathcal{O}(k))\,.$$

Hence, $\|w_k\| \leq \beth_{n-1}(\mathcal{O}(k))$. The unique path starting at w_k has length $\beth_{3n}(k)-1$. Thus, the run of $\mathcal{A}$ corresponding to this path has at least that much non-ε-transitions. Since

$$\begin{aligned}\beth_{2n}\big(n3^{n-1}|Q|^3 n! + 2\|w_k\|\big) &\leq \beth_{2n}\big(n3^{n-1}|Q|^3 n! + 2\beth_{n-1}(\mathcal{O}(k))\big)\\ &\leq \beth_{3n-1}(\mathcal{O}(k))\\ &\leq \beth_{3n}(k) - 1\end{aligned}$$

it follows from part (b) of the theorem that, for large enough k, there are runs starting at w_k with arbitrarily many non-ε-transitions. But this implies that $\mathfrak{T}_{3n}$ contains arbitrarily long paths starting at w_k. Contradiction.

10 Conclusion

In the present article we have started to develop a structure theory for structures in the Caucal hierarchy and for configuration graphs of higher-order pushdown automata. Our main technical results were Theorem 4.4 bounding the outdegree of definable relations and Theorem 9.6 containing a pumping lemma for higher-order pushdown automata. We have used these results to prove that certain graphs are not contained in a given level of the Caucal hierarchy. There are several directions in which this work can be continued.

(a) Theorem 9.6 makes no statements about the length of the runs r_i. We conjecture that the optimal bound is $|\mathrm{dom}(r_i)| \leq \beth_{n-1}(\mathcal{O}(i))$. At least it should be possible to prove the weaker statement that $|\mathrm{dom}(r_{i+1})| \leq 2^{|\mathrm{dom}(r_i)|}$. Note that a lower bound of $\beth_{n-1}(i)$ is provided by the languages L_n defined in Section 2.

(b) After the proof of Sénizergues [11] that language equivalence is decidable for deterministic pushdown automata there have been attempts to extend this result to higher-order automata. The proof is based on a rewriting system for configurations. For the higher-order case, one can try to base the rewriting rules on the substitution operation defined in Section 5.

References

[1] D. Berwanger and A. Blumensath, *The Monadic Theory of Tree-like Structures*, in Automata, Logic, and Infinite Games, E. Grädel, W. Thomas, and T. Wilke, eds., LNCS 2500, Springer Verlag, 2002, pp. 285–301.

[2] A. Blumensath, *Structures of Bounded Partition Width*, Ph. D. Thesis, RWTH Aachen, Aachen, 2003.

[3] A. Blumensath and S. Kreutzer, *An Extension to Muchnik's Theorem*, Journal of Logic and Computation, 15 (2005), pp. 59–74.

[4] A. Carayol and S. Wöhrle, *The Caucal Hierarchy of Infinite Graphs in Terms of Logic and Higher-order Pushdown Automata*, in Proc. 23rd Conf. on Foundations of Software Technology and Theoretical Computer Science, FSTTCS, LNCS 2914, 2004.

[5] D. Caucal, *On Infinite Terms Having a Decidable Monadic Theory*, in Proc. 27th Int. Symp. on Mathematical Foundations of Computer Science, MFCS, 2002, pp. 165–176.

[6] W. Damm and A. Goerdt, *An Automata-Theoretical Characterization of the OI-Hierarchy*, Information and Control, 71 (1986), pp. 1–32.

[7] T. Hayashi, *On derivation trees of indexed grammars: An extension of the $uvwxy$-theorem*, Publ. RIMS, Kyoto Univ., 9 (1973), pp. 61–92.

[8] T. Knapik, D. Niwiński, and P. Urzyczyn, *Higher-order pushdown trees are easy*, 5th Int. Conf. on Foundations of Software Science and Computation Structures, FoSSaCS 2002, LNCS, 2303 (2002), pp. 205–222.

[9] A. N. Maslov, *Multilevel stack automata*, Problemy Peredachi Informatsii, 12 (1976), pp. 55–62.

[10] A. L. Semenov, *Decidability of monadic theories*, LNCS, 176 (1984), pp. 162–175.

[11] G. Sénizergues, *$L(A) = L(B)$? A Simplified Decidability Proof*, Theoretical Computer Science, 281 (2002), pp. 555–608.

[12] I. Walukiewicz, *Monadic second-order logic on tree-like structures*, Theoretical Computer Science, 275 (2002), pp. 311–346.