

The Limits of Decidability for First Order Logic on CPDA Graphs

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Abstract

Higher-order pushdown automata (HOPDA) are abstract machines equipped with a nested ‘stack of stacks of stacks’. Collapsible pushdown automata (CPDA) extend these devices by adding ‘links’ to the stack and are equi-expressive for tree generation with simply typed λY terms. Whilst the configuration graphs of HOPDA are well understood, relatively little is known about the CPDA graphs. The order-2 CPDA graphs already have undecidable MSO theories but it was only recently shown by Kartzow (in his 2010 STACS paper) that first-order logic is decidable at the second level. In this paper we show the surprising result that first-order logic ceases to be decidable at order-3 and above. We delimit, in terms of quantifier alternation and the orders of CPDA links used, the fragments of the decision problem to which our undecidability result applies. Additionally we exhibit a natural sub-hierarchy to which limited decidability applies.

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1 Introduction

Higher-order pushdown automata generalise traditional pushdown automata by allowing the stack to contain other stacks rather than just atomic elements. These devices are closely related to *recursion schemes*, which are essentially simply typed λY terms that generate a single infinite tree. Enjoying decidable μ -calculus theories, the class of trees generated by recursion schemes shows a lot of promise as a model for verifying higher-order functional programs [12, 13]. Unfortunately n -PDA are believed to expressively coincide with order- n recursion schemes only when the latter satisfy a property called *safety* [10]. It is conjectured that unsafe recursion schemes are strictly more expressive and this is known for level 2 [14]. Hence a more powerful automaton is needed, which motivates order- n *collapsible pushdown automata* (n -CPDA) [7]. Inspired by *panic automata* [11], which can be viewed as the special case at order-2, atomic elements in collapsible stacks emanate ‘links’ that target a component of the stack further below. Their expressive power coincides precisely with unrestricted order- n recursion schemes.

We concern ourselves here with configuration *graphs* of these automata, with states of memory as nodes and transitions as edges. It is particularly fruitful to consider the ‘ ϵ -closures’ of such graphs, which allow to construct a graph whose edges consist of an unbounded number of transitions rather than just single steps. The ϵ -closures of HOPDA graphs form precisely the *Causal Hierarchy* [6, 3, 5], which is defined independently in terms of graph transformations. This deep result has as a consequence that every n -PDA graph has decidable MSO theory.

So how does the addition of links affect this? Unfortunately there is even a 2-CPDA graph that has *undecidable* MSO theory [7]. Nevertheless the local nature of first-order logic meant it was widely assumed the first-order theories would still enjoy decidability. However, the problem remained open for a few years until Kartzow saw that the ϵ -closures of 2-CPDA graphs are *tree automatic* [9] and so do indeed have decidable first-order theory.



	2-CPDA /w ϵ -clos.	3 ₂ -CPDA	3 ₂ -CPDA /w ϵ -clos.	n_n -CPDA ($n \geq 3$)	n_n -CPDA /w ϵ -clos. ($n \geq 3$)	$n_{n,(n-1)}$ -CPDA $n \geq 4$	$n_{n,(n-1)}$ -CPDA /w ϵ -clos. (all n)	n_m -CPDA ($n \geq 4$, $m \leq n - 2$)	n -PDA /w ϵ -clos. (all n)
Σ_1	Dec [9]	Dec [1]	Dec	Dec	Dec	?	?	Und	Dec [5]
Π_2	Dec [9]	Dec [1]	Und	Und	Und	?	?	Und	Dec [5]
FO	Dec [9]	Dec [1]	Und	Und	Und	?	?	Und	Dec [5]
MSO	Und [7]	Und [7]	Und [7]	Und [7]	Und [7]	Und [7]	Und [7]	Und [7]	Dec [5]
μ -calculus	Dec [11]	Dec [7]	Dec [7]	Dec [7]	Dec [7]	Dec [7]	Dec [7]	Dec [7]	Dec [10]

■ **Table 1** Summary of (un)decidability results known to date. Those in bold are from this paper. The notation ‘ $n_{m,m'}$ -CPDA’ means an n -CPDA that only uses links of orders m and m' .

Our first contribution is to show that Kartzow’s result cannot be extended to higher-orders in full generality. At order-3 we get undecidability when we consider Π_2 -sentences, namely those with quantifier alternation of the form $\forall\exists$. If we allow order-3 links we do not even need ϵ -closure for this. This result is surprising in itself, but we also gain some insight into what links ‘mean’ in terms of 3-CPDA *graphs*. On the one hand links can act as ‘place holders’ that allow first-order logic to compare internal components of a single order-3 stack rather than just two order-3 stacks in their entirety. This is the core of the undecidability result, which goes via a reduction from Post’s Correspondence Problem [15]. Additionally, order-3 links provide edges in the graph that are ‘non-local’ in nature, allowing ϵ -closure to be eliminated as a requirement for undecidability. At order-4 we get that even the Σ_1 -theory is undecidable—*viz.* the theory consisting of sentence *without any* quantifier alternation, a particularly expressively weak fragment of the logic.

Our second contribution introduces a technique to tackle the Σ_1 -theories of CPDA graphs. Making use of *logical reflection* [2], which enables CPDA to ‘know’ which μ -calculus sentences they satisfy at any given point, we define a notion of *monotonic CPDA* that can construct all of its reachable configurations in a manner that does not every destroy an order- $(n - 1)$ stack. This has some parallels to Carayol’s work on canonical sequences of operations witnessing the constructibility of HOPDA stacks [4]. Provided that an n -CPDA only has ‘order- n links’, monotonicity allows us to eliminate them, thereby producing an n -PDA with decidable MSO theory, and leading to the decidability of the Σ_1 theory of the original n -CPDA. This can be viewed as a graph analogue of Aehlig *et al.*’s work [8] in which it is shown that links can be eliminated from 2-CPDA graphs to produce an equivalent word-generating 2-PDA at the expense of introducing non-determinism. This decidability result is the first that applies a fragment of first-order logic to n -CPDA of all orders and establishes that restricting links can recover some decidability.

2 Preliminaries

2.1 Higher-Order Stacks

Let us fix a stack-alphabet Γ . For higher-order automata this alphabet must be finite, but it is convenient for definitions to allow it to be infinite. An *order-1* stack over Γ is just a string of the form $[\gamma]$ where $\gamma \in \Gamma^*$. Let us refer to the set of order-1 stacks over Γ as $stack_1(\Gamma)$. For $n \in \mathbb{N}$ the set of *order- $(n + 1)$ -stacks* is: $stack_{n+1}(\Gamma) := stack_1(stack_n(\Gamma))$. In a (higher-order) stack $[s_1 s_2 \cdots s_m]$ we refer to s_i as the *i th component of the stack*. We allow the following operations on an order-1 stack s for every $a \in \Gamma$: $push_1^a([a_1 \cdots a_m]) := [a_1 \cdots a_m a]$, $pop_1([a_1 \cdots a_m a_{m+1}]) := [a_1 \cdots a_m]$, $nop(s) := s$. We allow the following operations on an order- $(n + 1)$ stack s , where θ is any operation that may be performed on an order- n stack: $push_{n+1}([s_1 \cdots s_m]) := [s_1 \cdots s_m s_m]$, $pop_{n+1}([s_1 \cdots s_m s_{m+1}]) := [s_1 \cdots s_m]$,

$\theta([s_1 \cdots s_m]) := [s_1 \cdots \theta(s_m)]$. Operations that we may perform on an order- n stack are collectively referred to as *order- n operations*. Where s is an $(n+1)$ -stack. We also use the notation $top_{n+1}(s)$ to denote the top-most order- n stack and $top_1(s)$ as the top atomic element.

► **Definition 1.** Let $s := [s_1 s_2 \cdots s_m]$ be an n -stack. Then we define the n -height $|s|_n$ of s by $|s|_n := m$. If $1 \leq k < n$, then the k -height $|s|_k$ of s is recursively defined by: $|s|_k := \sum_{i=1}^m |s_i|_k$

► **Definition 2.** Let $s := [s_1 s_2 \cdots s_m]$ and $t := [t_1 t_2 \cdots t_{m'}]$ be two n -stacks. We say that s is an n -prefix of t written $s \sqsubseteq_n t$ just in case $m \leq m'$ and $s_i = t_i$ for $1 \leq i \leq m$. We recursively say that $s \sqsubseteq_k t$ for $k < n$ just in case $m \leq m'$ and $s_i = t_i$ for $1 \leq i < m$ and $s_m \sqsubseteq_k t_m$. We write $s \sqsubset_k t$ to mean that $s \sqsubseteq_k t$ and $s \neq t$.

► **Example 3.** Consider 2-stacks $s := [[ababa][bababa]]$ and $t := [[ababa][bab]]$. Then we have $s \sqsubseteq_1 t$ but we do not have $s \sqsubseteq_2 t$. We also have $|s|_2 = |t|_2 = 2$ but $|s|_1 = 11$ and $|t|_1 = 8$.

► **Definition 4.** Let $s = [s_1 \cdots s_m]$ be a higher-order stack. Then $s_{\leq s_i} := s = [s_1 \cdots s_i]$ for $1 \leq i \leq m$. If t is an occurrence of a stack in s_i , then $s_{\leq t} := [s_1 \cdots s_{i \leq t}]$. We also have a strict version where $s_{< s_i} := s = [s_1 \cdots s_{i-1}]$ and $s_{< t} := s = [s_1 \cdots t_{< s_i}]$.

2.2 Collapsible Pushdown Stacks

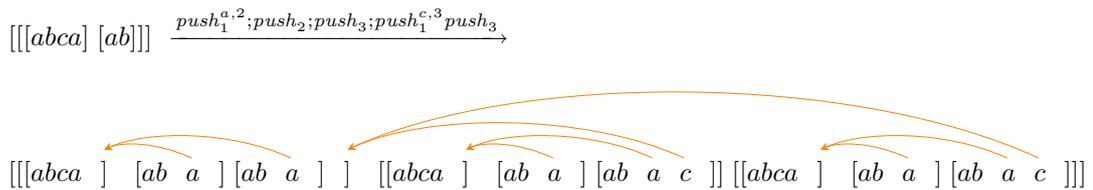
We offer fine control over the orders of links that a collapsible stack may contain—an order- $(n+1)$ link is one that targets an order- n stack within an order- $(n+1)$ stack. We include the orders of links as a subscript, so an order- n_S stack is an order- n stack equipped with order- i links for each $i \in S$. The S -collapsible pushdown alphabet (for $S \subseteq \mathbb{N}$) $\Gamma^{[S]}$ induced by an alphabet Γ is the set $\Gamma \times S \times \mathbb{N}$. The set of order- n_S open collapsible stacks $stack_{n_S}^C(\Gamma)$ is defined by: $stack_{n_S}^C(\Gamma) := stack_n(\Gamma^{[S]})$. The order of a link of an atomic element $(a, l, p) \in \Gamma^{[S]}$ is given by the number in its second component. If $l < n$ the target of a link is the p th component of the l -stack in which the element resides. If $l \geq n$ we say that the link is ‘dangling’.

When we write $top_1(s)$ where s is a collapsible stack with top atomic element (a, l, p) by abuse of notation we usually mean $top_1(s) := a$. If (a, l, p) is intended, it is usually clear from the context. However, we have additional notation to explicitly refer to l .

► **Definition 5.** Let s be a collapsible stack with top atomic element (a, l, p) , which by abuse of notation we denote a . We then define $l_o(a) := l$ (the order of the link) and $l_a(a) := l$ (the absolute target of the link relative to the bottom of the p -stack in which it resides). It is also useful to describe the target of the link in terms of an offset from the top: $l_r(a) := |t|_l - 1$ where t is the l stack within s in which the occurrence a resides.

Note in particular that a $push_k$ operation will preserve the absolute targets of links when copying the $k-1$ stack. We replace the $push_1$ operation to allow the attachment of links: $push_1^{a,k}(s) := push_1^{(a,k,|top_{k+1}(s)|_{k-1})}(s)$ where $top_{k+1}(s) := s$ where s is order- n . The *collapse* operation discards everything above the target of a pointer. This can neatly be described in terms of link offset where θ^m means the m -fold iteration of the operation θ : $collapse(s) := pop_{l_o(top_1(s))}^{l_r(top_1(s))}$. Write Θ_{n_S} to denote the set of order- n_S collapsible stack operations.

► **Example 6.** We exhibit operations on an order-3 collapsible stack, representing links graphically.



2.3 The Automata and their Graphs

► **Definition 7.** Let $n \in \mathbb{N}$ and let $S \subseteq [1..n]$. An n_S -CPDA (order- n_S collapsible pushdown automaton) \mathcal{A} is a tuple:

$$\langle \Sigma, \Pi, Q, q_0, \Gamma, R_{a_1}, R_{a_2}, \dots, R_{a_r}, P_{b_1}, P_{b_2}, \dots, P_{b_{r'}} \rangle$$

where Σ is a finite set of transition labels $\{a_1, a_2, \dots, a_r\}$; Π is a finite set of configuration labels $\{b_1, b_2, \dots, b_{r'}\}$; Q is a finite set of control-states; $q_0 \in Q$ is an initial control-state; Γ is a finite stack alphabet; each R_{a_i} is the a_i -labelled transition relation with $R_{a_i} \subseteq Q \times \Gamma \times \Theta_{n_S} \times Q$; each P_{b_i} is the b_i -labelled unary predicate specified by $P_{b_i} \subseteq Q \times \Gamma$.

We define n -CPDA and n -PDA in a manner consistent with the standard definitions in the literature:

► **Definition 8.** An n -CPDA is an $n_{[n..2]}$ -CPDA and an n -PDA is an n_\emptyset -CPDA.

A *configuration* of an n_S -CPDA is a pair (q, s) where q is a control-state and s is a stack.

► **Definition 9.** Let (q, s) and (q', s') be configurations of an n_S -CPDA \mathcal{A} . We say that (q', s') can be reached from (q, s) in \mathcal{A} with path labeled in \mathcal{L} for some $\mathcal{L} \subseteq \Sigma^*$ just in case:

$$(q, s) \mathbf{a}_{i_1}(q_1, s_1) \mathbf{a}_{i_2}(q_2, s_2) \mathbf{a}_{i_3} \cdots (q_{m-1}, s_{m-1}) \mathbf{a}_{i_m}(q', s')$$

for some configurations $(q_1, s_1), \dots, (q_{m-1}, s_{m-1})$ where $\mathbf{a}_{i_1} \mathbf{a}_{i_2} \mathbf{a}_{i_3} \cdots \mathbf{a}_{i_m} \in \mathcal{L}$. We write $(q, s) \mathbf{r}_{\mathcal{L}}(q', s')$ to mean this. We write $(q, s) \mathbf{r}(q', s')$ to mean $(q, s) \mathbf{r}_{\Sigma^*}(q', s')$.

The set of *reachable configurations* of \mathcal{A} is given by:

$$\mathbf{R}(\mathcal{A}) := \{ (q, s) : (q_0, \perp_n) \mathbf{r}(q, s) \}$$

► **Definition 10.** Let \mathcal{A} be an n_S -CPDA with transition-labels Σ and configuration-labels Π . The configuration graph of (graph generated by) \mathcal{A} has domain $\mathbf{R}(\mathcal{A})$, unary predicates Π and directed edges Σ between configurations. We write $\mathcal{G}(\mathcal{A})$ to denote this graph.

The ϵ -closure of such a graph $\mathcal{G}^\epsilon(\mathcal{A})$ is induced from $\mathcal{G}(\mathcal{A})$ by taking a -labelled edges between nodes related by $\mathbf{r}_{\epsilon^* a}$.

2.4 Logics

We consider first-order logic **FO** on graphs as is standardly defined. A $\Sigma_0 = \Pi_0 = \Delta_0$ formula $\phi(x_1, \dots, x_k)$ is one without any quantifiers. A Σ_{n+1} formula is one of the form $\exists \vec{y}. \phi(\vec{y}, x_1, \dots, x_k)$ where $\phi(\vec{y}, x_1, \dots, x_k)$ is Π_n and a Π_{n+1} formula is one of the form $\exists \vec{y}. \phi(\vec{y}, x_1, \dots, x_k)$ where ϕ is Σ_n . A Δ_n formula is one that is equivalent to both a Σ_n and Π_n formula on every CPDA graph. MSO is **FO** extended with second-order quantification over set variables. Transitive closure logic **FO(TC)** is **FO** together with a binary predicate $\overline{\phi(x, y)}$ for every formula of **FO** $\phi(x, y)$ with two variables, which defines the relation that is the transitive closure of that defined by $\phi(x, y)$. When the formulae transitively closed are restricted to Δ_1 we call the logic **FO(TC[Δ_1])**. A *sentence* is a formula with no free variables.

3 Undecidability

3.1 Post's Correspondence Problem

All of the undecidability results go via a reduction from Post's Correspondence Problem [15], which is known to be undecidable. Consider a finite-alphabet Σ with $|\Sigma| \geq 2$. An instance of the Post Correspondence Problem (PCP) consists of two finite sets of strings over Σ : u_1, \dots, u_m and v_1, \dots, v_m .

The question to be decided is whether there is a finite sequence $i_1 \dots i_k$ consisting of integers $1 \leq i_j \leq m$ such that $u_{i_1}.u_{i_2} \dots .u_{i_k} = v_{i_1}.v_{i_2} \dots .v_{i_k}$.

► **Example 11.** Consider the following two sets of strings over the alphabet $\{a, b, c\}$:

$$u_1 := ab \quad u_2 := cababcabb \quad u_3 := ca \quad v_1 := ababc \quad v_2 := ab \quad v_3 := bca$$

Then the Post Correspondence Problem has answer ‘yes’ as witnessed by the solution 1123:

$$u_1.u_1.u_2.u_3 = ababcababcabbca = v_1.v_1.v_2.v_3$$

Given an instance of the PCP P we define a pushdown automaton \mathcal{A}_1^P that pushes elements of Σ onto the stack together with indices indicating a partition into strings from the u_i and v_i .

► **Definition 12.** The automaton \mathcal{A}_1^P has stack alphabet: $\Sigma \cup [1_u, 2_u \dots m_u] \cup [1_v, 2_v \dots m_v]$ and behaves by non-deterministically choosing one of the following options:

- Push any member of Σ onto the stack.
- If the Σ symbols in the stack since the last symbol of the form i_u (or the bottom of the stack if there is no such symbol) form the word u_j , then it may push j_u onto the stack.
- If the Σ symbols in the stack since the last symbol of the form i_v (or the bottom of the stack if there is no such symbol) form the word v_j , then it may push j_v onto the stack.

P has a solution just in case \mathcal{A}_1^P can generate a stack with ‘matching’ i_u and i_v subsequences.

► **Lemma 13.** Let P be an instance of Post’s Correspondence Problem. P has a solution just in case the automaton \mathcal{A}_1^P can generate a stack s such that:

- $s_u = s_v$ where s_u is the subsequence of s consisting of elements of the form i_u and s_v of elements of the form i_v and equality is interpreted with respect to the indices i only.
- The top two elements of s form the set $\{i_u, i_v\}$ for some $1 \leq i \leq m$.

► **Example 14.** To continue the running example from Example 11, which we call P , the solution as represented by a stack of \mathcal{A}_1^P is: $[ab\mathbf{1}_u ab\mathbf{1}_u c\mathbf{1}_v ababc\mathbf{1}_v ab\mathbf{2}_v b\mathbf{2}_u ca\mathbf{3}_u \mathbf{3}_v]$

3.2 Post’s Correspondence Problem and 2-CPDA

Hague *et al.* [7] showed that the model-checking problem for MSO on 2-CPDA graphs is undecidable; indeed the 2-CPDA graph that they exhibit witnesses the undecidability of transitive closure logic $FO(TC)$. In order to introduce our basic technique, we first reprove the undecidability of $FO(TC)$ on 2-CPDA graphs by a reduction from PCP—in fact $FO(TC[\Delta_1])$.

The 2-CPDA \mathcal{A}_2^P is very like \mathcal{A}_1^P except that it ensures each index (the elements of the form i_u or i_v) emanate a pointer to a distinct 1-stack in the 2-stack. This will enable first-order logic to ‘ascertain corresponding positions’ in two instances of a 1-stack by comparing the results of collapsing.

► **Definition 15.** Let P be an instance of Post’s Correspondence Problem (using the notation above). The automaton \mathcal{A}_2^P has stack alphabet: $\Sigma \cup [1_u, 2_u \dots m_u] \cup [1_v, 2_v \dots m_v]$. It behaves by non-deterministically choosing one of the following options:

- Push any member of Σ onto the stack.
- If the Σ symbols in the stack since the last symbol of the form i_u in the top 1-stack (or the bottom of the 1-stack if there is no such symbol) form the word u_j , then it may perform $push_2; push_1^{j_u, 2}$.
- If the Σ symbols in the stack since the last symbol of the form i_v in the top 1-stack (or the bottom of the 1-stack if there is no such symbol) form the word v_j , then it may perform $push_2; push_1^{j_v, 2}$.

As with \mathcal{A}_1^P , the finite control-states can enforce the preconditions.

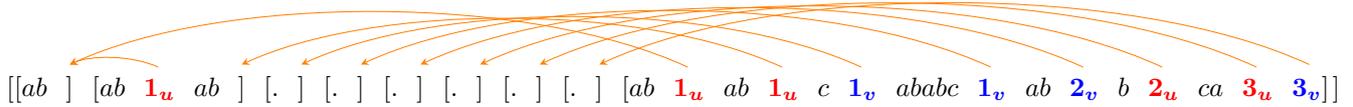
A solution to P can be formulated in terms of \mathcal{A}_2^P in a very similar manner to before:

► **Lemma 16.** Let P be an instance of Post's Correspondence Problem. P has a solution just in case the automaton \mathcal{A}_2^P can generate a stack s such that:

- $s_u = s_v$ where s_u is the subsequence of $\text{top}_2(s)$ consisting of elements of the form i_u and s_v of elements of the form i_v and equality is interpreted with respect to the indices i only.
- The top two elements of s form the set $\{i_u, i_v\}$ for some $1 \leq i \leq m$.

Proof. A consequence of Lemma 13 given that the permissible changes to the top_2 1-stack of the 2-stack of \mathcal{A}_2^P are precisely those that could be made to the 1-stack of \mathcal{A}_1^P . ◀

► **Example 17.** To continue Example 11, the solution as represented by a stack of \mathcal{A}_2^P is:



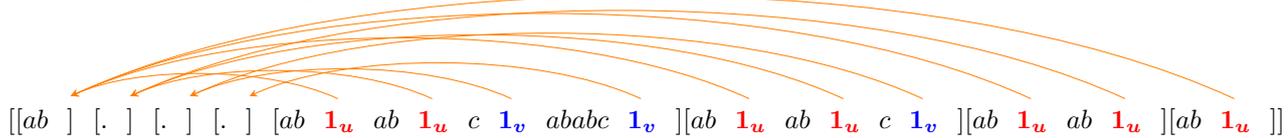
Now consider a variant of \mathcal{A}_2^P which we will call \mathcal{A}_{2+}^P . This behaves as follows:

- It initially behaves as \mathcal{A}_2^P . It may terminate this phase if its top two elements are in $\{i_u, i_v\}$ for some i . When it terminates this phase, it enters a distinguished control-state *guess*.
- It then performs a sequence of operations of the form: $\text{push}_2; \text{pop}_1^{m_1}; \text{push}_2; \text{pop}_1^{m_2}; \text{push}_2; \text{pop}_1^{m_3}; \text{push}_2; \text{pop}_1^{m_4}$ with $m_1, m_2, m_3, m_4 \in \mathbb{N}$. It should ensure that the four 1-stacks so created form a set $\{u_1, u_2, v_1, v_2\}$ (in no particular order) with:
 - $\text{top}_1(u_1) = i_u$ and $\text{top}_1(v_1) = i_v$ for some $1 \leq i \leq m$.
 - Either $\text{top}_1(u_2) = i'_u$ and $\text{top}_1(v_2) = i'_v$ for some $1 \leq i' \leq m$ or else u_2 and v_2 are both empty.
 - Going from u_1 to u_2 can be done with the popping of precisely one symbol of the form j_u (that is the one on top of u_1) and all other symbols popped should be letters.
 - Going from v_1 to v_2 can be done with the popping of precisely one symbol of the form k_v (that is the one on top of v_1).

Compliance with these requirements can be checked using a finite number of control states. If the automaton finds that it cannot avoid violating a requirement (e.g. it reaches the bottom of a stack whilst iterating pop_1) then it just enters a distinguished control-state *fail*. Otherwise it enters one of the following distinguished control-states: $u_1 v_1 u_2 v_2^{\text{start}}$, $v_1 u_1 v_2 u_2^{\text{start}}$ or $u_1 u_2 v_1 v_2$, $u_1 v_1 u_2 v_2$, $u_1 v_1 v_2 u_2$, $v_1 u_1 u_2 v_2$, $v_1 u_1 v_2 u_2$, $v_1 v_2 u_1 u_2$ or $u_1 v_1^{\text{end}}$, $v_1 u_1^{\text{end}}$ specifying the order of creation of these four stacks along with a flag indicating *end* if the u_2 and v_2 are empty and *start* if both u_1 and u_2 have the top-most i_u element of s and both v_1 and v_2 the top-most i_v element. Call these control-states *verifier states*.

- From one of the above verifier states, the automaton may perform any sequence of pop_2 and *collapse* operations via edges labelled pop_2 and *collapse* which all end in control-state *test*.

► **Example 18.** The automaton \mathcal{A}_{2+}^P could reach the stack in Example 17 in control-state *guess*. From here it could, for example, reach control-state $v_1 v_2 u_1 u_2$ with stack:



► **Definition 19.** Let us fix some configuration of \mathcal{A}_{2+}^P with stack s and control-state *guess*. Let us call the configurations reachable from (guess, s) associated with a verifier state the *s-verifier configurations*. Given an *s-verifier* configuration c (with set of top four stacks $\{u_1, u_2, v_1, v_2\}$) we

define its *successor* c^+ to be the configuration (which is unique if it exists) with top four stacks $\{u_1^+, u_2^+, v_1^+, v_2^+\}$ such that $u_1^+ = u_2$ and $v_1^+ = v_2$.

Additionally the unique s -verifier bearing the *start* flag is dubbed 0_s . The unique s -verifier configuration whose control-state bears the *end* flag is dubbed end_s .

We can now produce a version of Lemma 16 in terms of s -verifier configurations.

► **Lemma 20.** *Let $(guess, s)$ be a reachable configuration of \mathcal{A}_{2+}^P for some instance P of Post's Correspondence Problem. Then s represents a solution to P in the sense of Lemma 16 if and only if there exists a chain of stacks s_1, s_2, \dots, s_k such that $s_1 = 0_s$, $s_k = end_s$ and $s_{i+1} = s_i^+$ for each $1 \leq i \leq k-1$ and such that for each i there exists a reachable s_i -verifier.*

We can define the $_ = (_)^+$ relation as a Δ_1 formula. This can be achieved by ensuring that the element on top of u_2 in a verifier-configuration stack s is the same as the element on top of u_1 in the purported s^+ , and likewise for v_1 and v_2 . Because every element in a \mathcal{A}_{2+}^P 1-stack has a pointer to a different location, we can detect this by checking that collapsing on u_1 results in the same stack as collapsing on u_2 . Individual $^+$ steps can be extended to a chain via transitive closure.

► **Lemma 21.** *There exists a Σ_1 sentence ϕ of $\mathbf{FO}(\mathbf{TC}[\Delta_1])$ such that for all instances P of Post's Correspondence Problem we have: $\mathcal{G}(\mathcal{A}_{2+}^P) \models \phi$ iff P has a solution.*

3.3 Undecidability for $\mathfrak{3}_2$ -CPDA

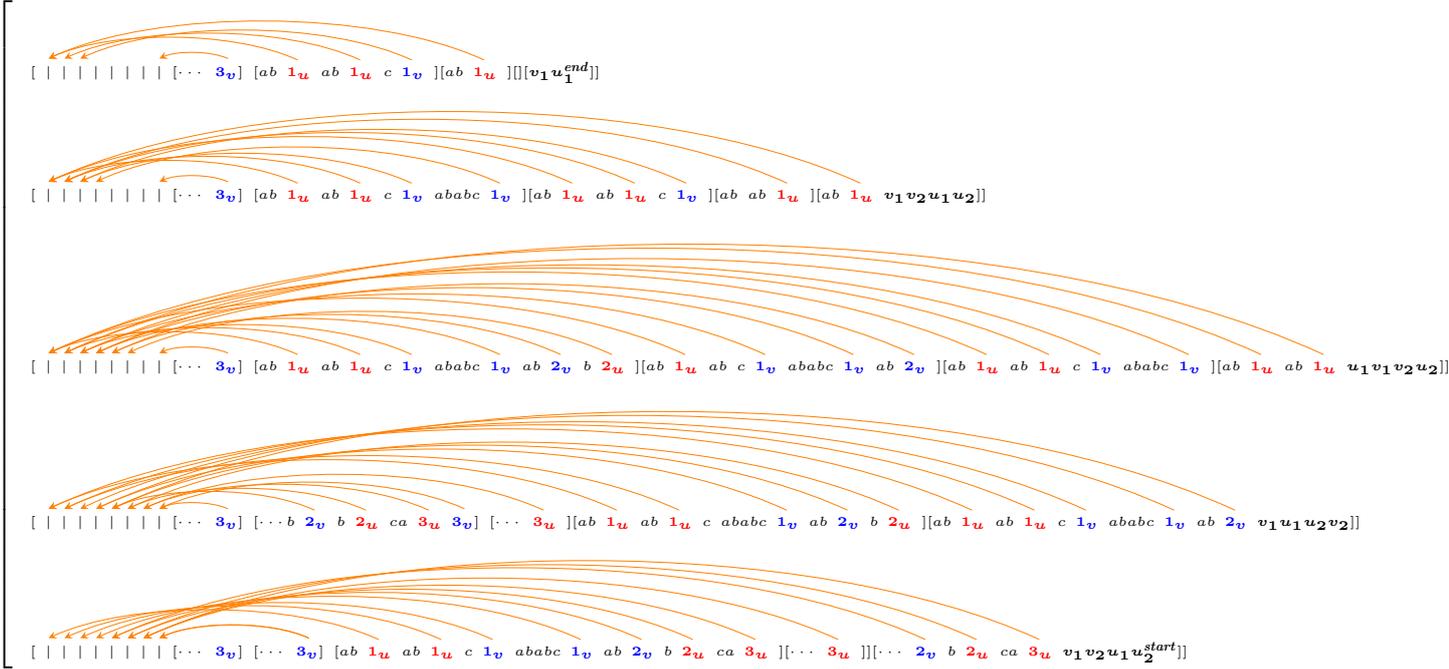
A $\mathfrak{3}_2$ -CPDA can record the chain of 2-stacks mentioned in Lemma 20 directly in its stack—the members of the chain are piled on top of each other. This removes the burden of transitive closure from the logic, although for $\mathfrak{3}_2$ -CPDA we require ϵ -closure.

► **Definition 22.** The $\mathfrak{3}_2$ -CPDA $\mathcal{A}_{\mathfrak{3}_2}^P$ behaves as follows:

- It begins by behaving in the same way as \mathcal{A}_{2+}^P , performing only 2-stack operations until it reaches the control-state $u_1 u_2 v_1 v_2^{start}$ or $v_1 v_2 u_1 u_2^{start}$. If it is unable to reach such a state, it goes into a distinguished *fail* state and aborts.
- The automaton then pushes a record of its $\mathcal{A}_{\mathfrak{3}_2}^P$ control-state on to the stack and performs: $push_3; pop_2; pop_2; pop_2; pop_2$. This will return the stack to the original \mathcal{A}_{2+}^P *guess*-configuration. It then behaves from here as though it were \mathcal{A}_2^P in the *guess* control state (with a stack s) until it reaches an s -verifier-configuration (or finds it is unable to, in which case it aborts).
- The previous step is repeated until an end_s configuration is reached, at which point the CPDA pushes the $\mathcal{A}_{\mathfrak{3}_2}^P$ control-state onto the stack and enters a distinguished *guess* $_{\mathfrak{3}_2}$ control-state.

This gives the essence of the automaton, although some extra edges do have to be added to the graph for technical reasons. Let us continue with the running example:

► **Example 23.** Recall the stack of \mathcal{A}_2^P in Example 17. $\mathcal{A}_{\mathfrak{3}_2}^P$ extends this upwards to form a 3-stack with contents dissecting each stage in the i_u and i_v subsequences. In control-state *guess* $_{\mathfrak{3}_2}$:

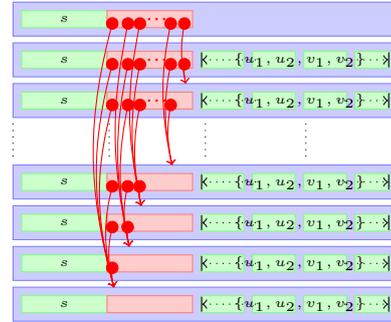


A stack in a $guess_{3_2}$ configuration of $\mathcal{A}_{3_2}^P$ fixes not only the 2-stack representing a guess at the solution (as is done by $\mathcal{A}_{2_+}^P$) but also a sequence of 2-stacks alleged to witness the correctness of this guess. With the aid of ϵ -closure we can perform an arbitrary number of pop_3 operations to quantify over the 2-stacks belonging to this alleged chain.

► **Lemma 24.** *There exists a Σ_2 sentence ϕ of FO such that for all instances P of Post's Correspondence Problem we have: $\mathcal{G}^\epsilon(\mathcal{A}_{3_2}^P) \models \phi$ iff P has a solution.*

3.4 The Non-Locality of 3_3 -CPDA

Adapting $\mathcal{A}_{3_2}^P$ to become a 3_3 -CPDA is straightforward—we can simply replace the 2-links with 3-links and replace the initial $push_2$ operations with $push_3$ operations to ensure different targets. Moreover, the undecidability result for 3_3 -CPDA is stronger; the non-locality of additional 3-links is exploited to alleviate the need for ϵ -closure. We illustrate this idea of exploiting non-locality in Figure 1. We can access all elements z in the chain with a first-order formula along the lines of:



■ **Figure 1** Exploiting the non-locality of 3-links

$(\exists x.x \text{ is a candidate stack})(\forall y.y \text{ is a candidate stack after some } pop_1\text{'s} \wedge pop_3(y) = pop_3(x)).z = collapse(y)$

In this way we can construct a 3_3 -CPDA $\mathcal{A}_{3_3}^P$ such that:

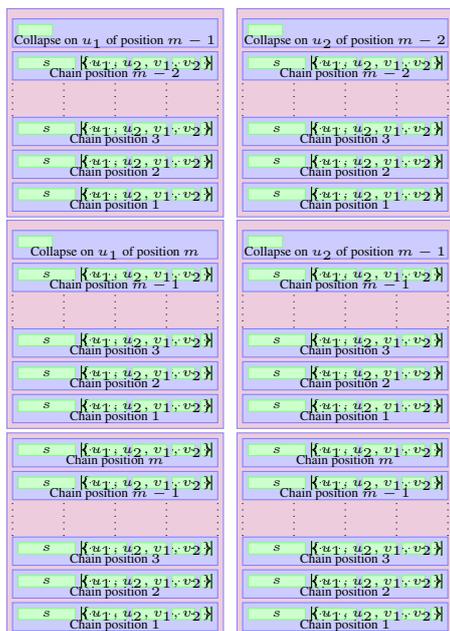
► **Lemma 25.** *Let P be an instance of Post's Correspondence Problem. Then there exists a Σ_2 sentence ϕ of FO such that: $\mathcal{G}(\mathcal{A}_{3_3}^P) \models \phi$ (note no ϵ -closure) if and only if P has a solution.*

3.5 Σ_1 Undecidability for 4_2 -CPDA

The Σ_2 -sentence witnessing undecidability on 3_2 graphs universally quantifies over elements in an alleged chain under the $_ = (_)^+$ relation in order to verify that it really is a chain. This is done

by verifying that the result of *collapse* on adjacent 2-stacks is the same. However, with a 4_2 -CPDA it is possible to construct two 4-stacks where the 3-stacks to be compared are in corresponding positions. This is illustrated in Figure 2. Unfortunately it is only possible to make this work for half of the definition of successor. The figure demonstrates the u_1/u_2 comparison, but we cannot simultaneously do the v_1/v_2 comparison. This can be circumvented by revising the definition of chain, successor and automaton to one where only one such comparison is sufficient. This is slightly more fiddly than the definition presented here, but it works in a similar manner. This allows us to construct an automaton $\mathcal{A}_{4_2}^P$ such that:

► **Lemma 26.** *There exists a Σ_1 -sentence ϕ such that for every instance P of Post's Correspondence Problem we have $\mathcal{G}(\mathcal{A}_{4_2}^P) \models \phi$ iff P has a solution.*



■ **Figure 2** The idea behind $\mathcal{A}_{4_2}^P$.

final configuration. This is illustrated in Figure 3.

This leads to the notion of a *monotonic n -CPDA*, which witnesses the reachability of all configurations in its graph without destroying $(n - 1)$ stacks during its run. The relationship between the graphs of an CPDA \mathcal{A} and its monotonic counterpart is one of *strong isomorphism*. We say that an isomorphism L between two configuration graphs \mathcal{G} and \mathcal{G}' is *strong*, written $L : \mathcal{G} \cong \mathcal{G}'$, if it maps a configuration (q, s) to one of the form $(q, L(s'))$ where L preserves stack structure and respects \sqsubseteq_1 prefixes.

The construction of monotonic CPDA is given in terms of devices called μ CPDA. A μ CPDA operates

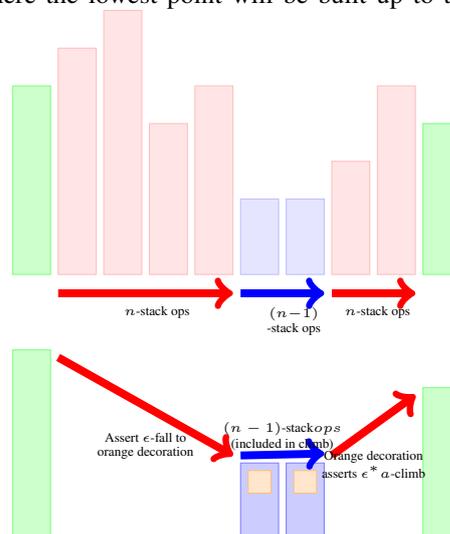
As a consequence of all these reductions:

- **Theorem 27. 1.** *For every $n \geq 4$ and $2 \leq m \leq n - 2$ the Σ_1 -FO model-checking problem for n_m -CPDA graphs (even without ϵ -closure) is undecidable.*
- 2. *For every $n \geq 3$ and $m \geq 3$ the Π_2 -FO model-checking problem for n_m -CPDA graphs (even w/o ϵ -closure) is undecidable.*
- 3. *For every $n \geq 3$ and $m \geq 2$ the Π_2 -FO model-checking problem for the ϵ -closures of n_m -CPDA graphs is undecidable.*

4 Σ_1 Decidability on n_n -CPDA

4.1 Monotonic CPDA

We wish to decompose ϵ^*a -labelled runs of an automaton between two configurations into an ϵ -fall and an ϵa -climb, which we will describe as a *bounce*. The fall is the first part of the run during which the stack will reach its lowest point, whilst the climb is the part of the run where the lowest point will be built up to the



■ **Figure 3** Asserting the existence of a bounce without performing any stack operations.

on an underlying CPDA, which it manipulates indirectly, determining transitions on the basis of ‘tests’ for the satisfaction of a μ -calculus sentence at the current configuration of the underlying CPDA. In particular, μ CPDA are able to ‘predict the future’ and consequently avoid the need to actually perform certain transitions, facilitating monotonicity. Logical reflection [2] implies every μ CPDA is strongly isomorphic to some CPDA.

► **Definition 28.** Let \mathcal{A} be an n -CPDA. An ϵ^* -*a-climb* of \mathcal{A} from a configuration (q, s) to a configuration (q', s') , written $(q, s) \mathbf{r}_{\epsilon^* a}^\uparrow(q', s')$, is an ϵ^* - a -labelled run from the first configuration to the second such that each stack occurring in the run (including s') has stack t such that $\text{pop}_n(s) \sqsubset_n t$.

We say that an n -CPDA is *monotonic via r* just in case no r -transition performs a *collapse* on an n -link or a pop_n operation. That is, when transitioning using r -edges, the number of $(n - 1)$ -stacks in an n -stack increases monotonically. The following Lemma constructs an automaton monotonic via an edge r_ϵ such that ϵ^* -climbs are precisely captured by standard *reachability* using r_ϵ -edges. Write $\mathcal{A} \upharpoonright_{\Pi, \Sigma}$ for the automaton formed from \mathcal{A} by deleting all unary predicates not labelled in Π and deleting all transitions not labelled in $\Sigma \cup \{\epsilon\}$.

► **Lemma 29.** Let \mathcal{A} be an n -CPDA with edge alphabet Σ and unary predicates Π . Then there exists an n -CPDA \mathcal{A}^\uparrow such that $\mathcal{G}^\epsilon(\mathcal{A}) \cong \mathcal{G}^\epsilon(\mathcal{A}^\uparrow \upharpoonright_{\Sigma, \Pi})$ but whose additional distinguished edge labels include $r_\epsilon \notin \Sigma$ such that \mathcal{A}^\uparrow is monotonic via r_ϵ and $(q, s) \mathbf{r}_{\epsilon^* a}^\uparrow(q', s')$ just in case $(q, s) \mathbf{r}_{r_\epsilon a}^\uparrow(q', s')$.

The dual of an ϵ -climb is an ϵ -fall; a configuration with a higher stack reaching a configuration with a lower stack such that no configuration in the run descends below the lower stack.

► **Definition 30.** Let \mathcal{A} be an n -CPDA. An ϵ -fall of \mathcal{A} from a configuration (q, s) to a configuration (q', s') is an ϵ^* -labelled run from (q, s) to (q', s') such that for every stack t occurring in the run (including s) we have $\text{pop}_n(s') \sqsubset_n t$.

The quasi-analogue of \mathcal{A}^\uparrow for falls is \mathcal{A}^\downarrow . However, we avoid needing to perform any destructive operations (including *collapse*) by instead making \mathcal{A}^\downarrow aware of the predicates that \mathcal{A} could satisfy after performing an ϵ -fall.

► **Lemma 31.** Let \mathcal{A} be an n -CPDA with unary predicates Π . Then there exists an n -CPDA \mathcal{A}^\downarrow with stack-alphabet Γ^\downarrow and control-state space Q^\downarrow such that $\mathcal{G}(\mathcal{A}) \cong \mathcal{G}(\mathcal{A}^\downarrow \upharpoonright_{\Pi^\downarrow})$ and that also has a predicate P^\downarrow for each $P \in \Pi$ such that P holds of precisely those configurations c from which \mathcal{A} has an ϵ -fall to a configuration c' satisfying P .

► **Definition 32.** Let \mathcal{A} be an n -CPDA. An a -bounce in \mathcal{A}^\uparrow from (q, s) to (q', s') in \mathcal{A}^\uparrow is a run consisting of an ϵ -fall from (q, s) to some configuration (q'', s'') followed by an $r_{\epsilon^* a}$ -climb from (q'', s'') to (q', s') . Let us write $(q, s) \mathbf{b}_a(q', s')$ to indicate the existence of such a bounce.

The significance of bounces is summed up in the following lemma. Whilst we strictly only need to consider \mathcal{A}^\uparrow we state the Lemma in terms of $\mathcal{A}^{\uparrow\downarrow}$ as when we come to make use of it (with meta-annotations) we will need to reference predicates holding at the bottom of the bounce:

► **Lemma 33.** Let (q, s) and (q', s') be two configurations of a CPDA \mathcal{A} and let $(q, L(s))$ and $(q', L(s'))$ be the corresponding configurations in $\mathcal{A}^{\uparrow\downarrow}$ via the strong isomorphism. Then $(q, s) \mathbf{r}_{\epsilon^* a}^\uparrow(q', s')$ just in case $(q, L(s)) \mathbf{b}_a L(q', L(s'))$.

4.2 Link Trails: Towards Link Elimination for Graphs

Part of our technique addressing the Σ_1 model-checking problem for CPDA graphs involves the elimination of outer-most links. The operational part of the simulation will make use of bouncing

(Lemma 33). But it is not enough just to simulate collapse; even if links are never used operationally, they still provide a feature by which stacks may be distinguished. For example the stacks

$[[abc] [ab c]]$ and $[[abc] [a b c]]$ are different although removing the link from either gives us the same: $[[abc] [abc]]$. We introduce the idea of *link-trails* in order to capture the differences created by links after they have been removed. Stacks and atomic elements are ‘coloured’ in a manner that is unique to a particular arrangement of n -links.

► **Definition 34.** We overload the $l_\alpha(s)$ operator to apply to stacks s as well as individual elements. Let $s = [s_1 s_2 \cdots s_m]$ be a k -stack with $2 \leq k$ (located within an n -stack for $k \leq n$). Define $l_\alpha(s)$ to be the position of the highest $(n-1)$ -stack pointed to by an n -link: $l_\alpha(s) = \max(\{ l_\alpha(s_i) : 1 \leq i \leq m \} \cup \{ 0 \})$ and when $s = [a_1 a_2 \cdots a_m]$ is an order-1 stack: $l_\alpha(s) = \max(\{ l_\alpha(a_i) : l_o(a_i) = n \text{ and } 1 \leq i \leq m \} \cup \{ 0 \})$

So in particular $l_\alpha(s) = 0$ when s contains no element with an n -link.

We now describe how stacks and atomic elements can be ascribed one of four colours in $\{ c_<, c_=:, c_>, \perp \}$.

► **Definition 35.** We ascribe colours to stacks and atomic elements via a function $\mathbf{col}(_)$. Let $s = [a_1 a_2 \cdots a_m]$ be a 1-stack located in an n -stack. Suppose that $l_o(a_i) = n$ for some i :

$$\mathbf{col}(a_i) := \begin{cases} \perp & \text{if } l_o(a_i) \neq n \\ c_> & \text{if for every } j < i \text{ such that } l_o(a_j) = n \text{ we have} \\ & l_\alpha(a_i) > l_\alpha(a_j) \\ c_=: & \text{if } l_o(a_i) = n \text{ and the greatest } j < i \text{ such that} \\ & l_o(a_j) = n \text{ satisfies } l_\alpha(a_j) = l_\alpha(a_i) \end{cases}$$

Note that for constructible stacks the above is exhaustive (it is impossible to construct a stack containing a link with target lower than the target of a link below it in the same 1-stack).

Now let $s := [s_1 s_2 \cdots s_m]$ be an order- k stack in an order- n stack for $n \geq k \geq 2$ (in particular we allow $k = n$ in which case s is the whole n -stack). We then set $\mathbf{col}(s_i)$ by:

$$\mathbf{col}(s_i) := \begin{cases} c_> & \text{if } l_\alpha(s_i) > \max(\{ l_\alpha(s_j) : 1 \leq j < i \}) \\ c_=: & \text{if } l_\alpha(s_i) = \max(\{ l_\alpha(s_j) : 1 \leq j < i \}) \\ c_< & \text{if } l_\alpha(s_i) < \max(\{ l_\alpha(s_j) : 1 \leq j < i \}) \end{cases}$$

For an n -stack s let us write $\mathbf{stripln}(s)$ to denote the n -stack that results from deleting all of the n -links from s . The colouring uniquely specifies the n -links that it contains:

► **Lemma 36.** Consider two constructible n -stacks s and s' with $\mathbf{stripln}(s) = \mathbf{stripln}(s')$. Assume for every stack or atomic element a contained within s and corresponding element a' in s' we have $\mathbf{col}(a) = \mathbf{col}(a')$. Then $s = s'$.

► **Lemma 37.** Let \mathcal{A} be an n_n -CPDA. Then there exists an n_n -CPDA $\mathbf{lum}(\mathcal{A})$ such that $\mathcal{G}^\epsilon(\mathbf{lum}(\mathcal{A})) \cong \mathcal{G}^\epsilon(\mathcal{A})$ and further such that for any reachable configurations $(q, s), (q, s')$ of $\mathbf{lum}(\mathcal{A})$ we have $s = s'$ iff $\mathbf{stripln}(s) = \mathbf{stripln}(s')$.

4.3 Meta-Annotations

Having enabled link removal whilst preserving equality between configurations, we now add a mechanism by which we can simulate edges in the graph without needing to actually perform the *collapse* operations. Indeed it will remove the need to perform any stack operations at all. This is achieved

by decorating $(n - 1)$ -stacks within an n -stack with information about the control-states from which a complete n -stack could be reached via an ϵ^*a -climb. Because this requires quantification over multiple runs and a CPDA can only perform one run at a time, it is necessary for the CPDA to guess the appropriate annotations and to externally verify them. It turns out that this can be done using MSO over $\mathbf{lum}(\mathcal{A})^{\uparrow\downarrow}$ since Lemma 29 allows climbs to be expressed in terms of r_ϵ -edges; we have $cr_{\epsilon^*a}^\uparrow c'$ iff $cr_{r_\epsilon^*a}^\uparrow c'$, and r_σ can always be expressed in MSO. Moreover, the reachability of a particular meta-annotation via an ϵ -fall can be asserted by MSO over $\mathbf{lum}(\mathcal{A})^{\uparrow\downarrow}$ due to Lemma 31. This MSO formula makes an assertion of the ‘consistency’ of k -tuples of configurations $(q_1, s_1), \dots, (q_k, s_k)$ with the constituent $(n - 1)$ stacks of each n -stack decorated with a ‘meta-annotation’. A meta-annotation is a $|\Sigma| \cdot k$ -tuple $((Q_1^a)_{a \in \Sigma}, \dots, (Q_k^a)_{a \in \Sigma})$ where each component is a subset of control-states Q . The k -tuple is deemed *consistent* if for every $(n - 1)$ stack s' in s_i , the meta-annotation on top of $s_{i \leq s'}$ satisfies $q \in Q_j^a$ iff there is an ϵ^*a climb from $(q, s_{i \leq s'})$ to (q_j, s_j) .

By asserting the (non-)existence of a suitable ϵ -fall to such a decoration, we can assert the (non-)existence of a bounce witnessing (non-)reachability, as illustrated in Figure 3. This corresponds to reachability in the original automaton due to Lemma 33. Since MSO is decidable on n -PDA:

► **Theorem 38.** *Let \mathcal{A} be an n_n -CPDA. Then the Σ_1 theory of $\mathcal{G}^\epsilon(\mathcal{A})$ is decidable.*

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A

 Undecidability

A.1 Post's Correspondence Problem

Lemma 13

Let P be an instance of Post's Correspondence Problem. P has a solution just in case the automaton \mathcal{A}_1^P can generate a stack s such that:

- $s_u = s_v$ where s_u is the subsequence of s consisting of elements of the form i_u and s_v of elements of the form i_v and equality is interpreted with respect to the indices i only.
- The top two elements of s form the set $\{i_u, i_v\}$ for some $1 \leq i \leq m$.

Proof. This is a quick consequence of definitions. Suppose that there is a solution $\sigma = u_{i_1}u_{i_2} \cdots u_{i_k} = v_{i_1}v_{i_2} \cdots v_{i_k}$ to P . Then \mathcal{A}_1^P may construct a stack meeting the criteria by pushing the letters in σ onto the stack whilst also pushing i_{ru} onto the stack after completing the pushing of u_{i_r} and likewise pushing i_{rv} after completing v_{i_r} .

Conversely suppose that there is a stack s meeting the criteria. Let $\sigma := \pi_\Sigma(s)$, which we claim is a string generated by a solution to P . Let i_{ru} be the r th element of the form j_u in the stack. Let i_{rv} be the r th element of the form j_v in the stack. Note that this is well defined since the first criterion requires the subsequences of j_u and j_v to be the same. Let k be the length of these two sequences.

Define i_{0u} and i_{0v} to be the bottom of the stack. Divide σ into segments u'_r (for $1 \leq r \leq k$) where u_{r+1} is the subsequence of letters (in Σ) from s that begins immediately after i_{ru} and ends immediately before i_{r+1u} . Define v'_r in a similar manner using i_{rv} . The first criterion ensures that $u'_r = u_{i_r}$ and that $v'_r = v_{i_r}$ for every $1 \leq r \leq k$. Moreover the second criterion ensures that $u'_1u'_2 \cdots u'_k = v'_1v'_2 \cdots v'_k = s$. That is $u_{i_1}u_{i_2} \cdots u_{i_k} = v_{i_1}v_{i_2} \cdots v_{i_k} = s$ and so we do indeed have a solution to P . ◀

A.2 Post's Correspondence Problem and 2-CPDA

Lemma 20

Let $(guess, s)$ be a reachable configuration of \mathcal{A}_{2+}^P for some instance P of Post's Correspondence Problem. Then s represents a solution to P in the sense of Lemma 16 if and only if there exists a chain of stacks s_1, s_2, \dots, s_k such that $s_1 = 0_s$, $s_k = \mathit{end}_s$ and $s_{i+1} = s_i^+$ for each $1 \leq i \leq k-1$ and such that for each i there exists a reachable s_i -verifier.

Proof. From the definitions of $+$ and the relationship between u_1 and u_2 in each verifier configuration, it follows that the top element of u_2 is the element coming after the top element of u_2^+ in the subsequence of elements in $\mathit{top}_2(s)$ consisting of elements of the form i_u . The same holds for v_2 and v_2^+ and the subsequence of elements in $\mathit{top}_2(s)$ consisting of elements of the form i_v .

Also note that the top elements of u_2 and v_2 in 0_s will respectively be the last i_u and i_v in each of these subsequences and the top elements of u_1 and v_1 in end_s will be the first (since by definition of end_s there cannot be any i_u or i_v lying below the top element of u_1 and v_1 respectively).

Now we can get by an easy induction on r that if there is a chain s_1, s_2, \dots, s_r such that $s_1 = 0_s$ and $s_{i+1} = s_i^+$ for each $1 \leq i < r$, then the following three assertions are true:

- The top element of the u_2 of s_r is the r th element from the end of the subsequence of $\mathit{top}_2(s)$ consisting of elements of the form i_u .
- The top element of the v_2 of s_r is the r th element from the end of the subsequence of $\mathit{top}_2(s)$ consisting of elements of the form i_v .
- If the top element of the u_2 of s_j for $1 \leq j \leq r$ is i_{j_u} , then the top element of the v_2 of s_j is i_{j_v} .

As a consequence, we get that the existence of such a chain implies that the final r elements of the subsequence of $top_2(s)$ consisting of elements of the form i_u matches the last r elements of the subsequence of $top_2(s)$ consisting of elements of the form i_v .

So suppose there exists a chain s_1, s_2, \dots, s_k such that $s_1 = 0_s$, $s_k = \mathit{end}_s$ and $s_{i+1} = s_i^+$ for each $1 \leq i \leq k-1$. The observations above ensure that s meets the conditions of Lemma 16 and so we may conclude that s does indeed witness a solution to P .

Conversely let us begin by assuming that s witnesses a solution to P . It must then be the case that $top_2(s)$ satisfies the properties laid out in Lemma 16. It is again an easy induction on r to see that under such circumstances one can generate a sequence s_1, s_2, \dots, s_r where $s_1 = 0_s$ and $s_{i+1} = s_i^+$ for each $1 \leq i < r$ so long as r does not exceed the length of the subsequence of $top_2(s)$ consisting of elements of the form i_u (which is the same as that consisting of elements of the form i_v). The induction step just needs to observe that we should order the $u_1^+, u_2^+, v_1^+, v_2^+$ with decreasing height, to enable the next to be formed from pop_1 ing from the previous.

Finally observe that when r reaches the length of the subsequences, the u_2 and v_2 of s_r will have top elements corresponding to the initial i_u and i_v in the subsequences of $top_2(s)$ given by Lemma 16. This means that s_r^+ will have u_1 and v_1 with these same initial elements and so u_2 and v_2 must be empty. That is $s_r^+ = \mathit{end}_s$. Hence we construct a chain of the required form. \blacktriangleleft

Lemma 21

There exists a Σ_1 sentence ϕ of $\mathbf{FO}(TC)$ containing only derived predicates $\bar{\psi}$ formed from Δ_1 formulae such that for all instances P of Post's Correspondence Problem we have:

$$\mathcal{G}(\mathcal{A}_{2+}^P) \models \phi \text{ iff } P \text{ has a solution.}$$

Proof. Let us first exhibit formulae witnessing the fact that the relation ‘for some stack s x is an s -verifier and $y = x^+$ ’ is Δ_1 -definable. The following is a Σ_1 formula representing the relation:

$$\begin{aligned} & \exists z. (\exists w_1 w_2 w_3. (\mathit{pop}_2(x, w_1) \wedge \mathit{pop}_2(w_1, w_2) \wedge \mathit{pop}_2(w_2, w_3) \wedge \mathit{pop}_2(w_3, z))) \\ & \exists w'_1 w'_2 w'_3. (\mathit{pop}_2(y, w'_1) \wedge \mathit{pop}_2(w'_1, w'_2) \wedge \mathit{pop}_2(w'_2, w'_3) \wedge \mathit{pop}_2(w'_3, z))) \wedge \\ & \bigvee_{\substack{\{a,b,c,d\} \\ = \{u_1, u_2, v_1, v_2\}}} \mathit{abcd}(x) \wedge \bigvee_{\substack{\{a,b,c,d\} \\ = \{u_1, u_2, v_1, v_2\}}} \mathit{abcd}(y) \wedge \\ & ((\mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_1 \mathbf{v}_2(x) \wedge \mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_1 \mathbf{v}_2(y)) \rightarrow ((\exists w_1 w_2. \exists w'_1 w'_2 w'_3. \exists c_u. \\ & \mathit{pop}_2(x, w_1) \wedge \mathit{pop}_2(w_1, w_2) \wedge \mathit{collapse}(w_2, c_u) \\ & \mathit{pop}_2(y, w'_1) \wedge \mathit{pop}_2(w'_1, w'_2) \wedge \mathit{pop}_2(w'_2, w'_3) \wedge \mathit{collapse}(w'_3, c_u)) \\ & \wedge (\exists w'_1. \exists c_v. \mathit{collapse}(x, c_v) \wedge \mathit{pop}_2(y, w'_1) \wedge \mathit{collapse}(w'_1, c_v)))))) \wedge \dots \\ & \dots \wedge ((\mathbf{v}_1 \mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_2(x) \wedge \mathbf{u}_1 \mathbf{v}_1 \mathbf{u}_2 \mathbf{v}_2(y)) \rightarrow ((\exists w_1. \exists w'_1 w'_2 w'_3. \exists c_u. \\ & \mathit{pop}_2(x, w_1) \wedge \mathit{collapse}(w_1, c_u) \wedge \\ & \mathit{pop}_2(y, w'_1) \wedge \mathit{pop}_2(w'_1, w'_2) \wedge \mathit{pop}_2(w'_2, w'_3) \wedge \mathit{collapse}(w'_3, c_u)) \\ & \wedge (\exists w'_1 w'_2. \exists c_v. \mathit{collapse}(x, c_v) \wedge \\ & \mathit{pop}_2(y, w'_1) \wedge \mathit{pop}_2(w'_1, w'_2) \wedge \mathit{collapse}(w'_2, c_v)))))) \\ & \wedge \dots \end{aligned}$$

We have only mentioned two of the $6 \times 8 + 2 \times 8 = 64$ elements of the final conjunction in the formula above, but the remainder follow the same pattern. There are 6 different predicates that



A.3 Undecidability for \mathcal{A}_{3_2} -CPDA

We give the full definition of $\mathcal{A}_{3_2}^P$:

Definition 22

The \mathcal{A}_{3_2} -CPDA $\mathcal{A}_{3_2}^P$ behaves as follows:

- It begins by behaving in the same way as $\mathcal{A}_{2^+}^P$, performing only 2-stack operations until it reaches the control-state $u_1u_2v_1v_2^{start}$ or $v_1v_2u_1u_2^{start}$. If it is unable to reach such a state, it goes into a distinguished *fail* state and aborts.
- The automaton then pushes a record of its $\mathcal{A}_{3_2}^P$ control-state on to the stack and performs $push_3; pop_2; pop_2; pop_2; pop_2$. This will return the stack to the original $\mathcal{A}_{2^+}^P$ *guess*-configuration. It then behaves from here as though it were \mathcal{A}_2^P in the *guess* control state (with a stack s) until it reaches an s -verifier-configuration (or finds it is unable to, in which case it aborts).
- The previous step is repeated until an end_s configuration is reached, at which point the CPDA pushes the $\mathcal{A}_{2^+}^P$ control-state onto the stack and enters a distinguished $guess_{3_2}$ control-state.

The following transitions are then added:

- An ϵ -transition going from any configuration to a distinguished control-state *prototest* via a pop_3 operation.
- The *only* transition going from a *prototest* control-state is allowed when the top_1 stack-symbol is one of: $u_1u_2v_1v_2, u_1v_1u_2v_2, u_1v_1v_2u_2, v_1u_1u_2v_2, v_1u_1v_2u_2, v_1v_2u_1u_2$ (in particular when the top symbol does not have a *start* or *end* flag). This transition is given the label *toTest* and moves to control-state *test* with no stack operation.
- We also allow a *toTest*-labelled transition from a configuration with control-state $guess_{3_2}$ to control-state *test* whilst not performing any stack operation.

We further add these transitions:

- A transition *to2⁺* performing a pop_1 and entering control-state *abcd* whenever in control-state *test* with top stack element *abcd* where *abcd* is a control-state of $\mathcal{A}_{2^+}^P$. From this control-state $\mathcal{A}_{3_2}^P$ behaves in the same way as $\mathcal{A}_{2^+}^P$, performing only order-2 operations.
- From any configuration with *test* control-state there exist transitions labelled $push_3$ and pop_3 performing the respective stack operations whilst remaining in control-state *test*.

Lemma 24

There exists a Σ_2 sentence ϕ of **FO** such that for all instances P of Post's Correspondence Problem we have: $\mathcal{G}^\epsilon(\mathcal{A}_{3_2}^P) \models \phi$ iff P has a solution.

Proof. Let us first interpret Lemma 20 in the context of $\mathcal{A}_{3_2}^P$. Since $\mathcal{A}_{3_2}^P$ is designed to generate arbitrary verifiers for some stack s created at the outset, beginning with 0_s and ending with end_s , Lemma 20 implies that there is a solution to P if and only if $\mathcal{A}_{3_2}^P$ can reach a configuration of the form $(guess_{3_2}, s)$ such that for every pair of 2-stacks t, t' occurring in s with t' immediately above t , $t' = t^+$.

We already have a Π_1 formula $\psi(x, y)$ in first-order logic expressing that $y = x^+$ where x and y range over 2-stacks reachable by $\mathcal{A}_{2^+}^P$. This was given in the proof of Lemma 21. Now observe that for any 3-stack s and sequence of 2-stack operations \vec{op} we have $\vec{\theta}(s) = \vec{\theta}(pop_3(push_3(s)))$ if and only if $\vec{\theta}(top_3(s)) = \vec{\theta}(top_3(pop_3(s)))$. We can thus exploit the $\mathcal{A}_{2^+}^P$ -simulation feature of $\mathcal{A}_{3_2}^P$ to

express that some variable x bound to a configuration of \mathcal{A}_{3_2} of the form $(test, s)$ has the property that $top_3(pop_3(s))^+ = top_3(s)$. This can be done by the Π_1 formula $\chi(x)$:

$$\forall y_1 y_2 y. \forall z. (\mathbf{pop}_3(x, y_1) \rightarrow \mathbf{push}_3(y_1, y_2) \rightarrow \mathbf{to2}^+(y_2, y) \rightarrow \mathbf{to2}^+(x, z) \rightarrow \psi(y, z))$$

over both the graph $\mathcal{G}(\mathcal{A}_{3_2}^P)$ and $\mathcal{G}^\epsilon(\mathcal{A}_{3_2}^P)$ ($\mathcal{A}_{3_2}^P$ has no ϵ -transitions reachable from a configuration with control-state $test$).

The construction of $\mathcal{A}_{3_2}^P$ ensures that the configurations we can reach from $(guess_{3_2}, s)$ by a (possibly empty) sequence of ϵ -transitions followed by a $toTest$ -transition are precisely those of the form $(test, s')$ such that s' is a prefix of s whose 2-stacks all occur in s . Hence these stacks are precisely those reachable by a $toTest$ -transition in the ϵ -closure of the configuration graph. Thus combining all of the observations above the required Σ_2 sentence ϕ is:

$$\phi := \exists x. \forall y (\mathbf{guess}_{3_2}(x) \wedge \mathbf{toTest}(x, y) \wedge \chi(y) \vee (\mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_1 \mathbf{v}_2^{start}(y) \vee \mathbf{v}_1 \mathbf{v}_2 \mathbf{u}_1 \mathbf{u}_2^{start}(y)))$$

(disregarding when y is a verifier with the $start$ flag as this is at the bottom and so there is no stack to compare below this). ◀

A.4 The Non-Locality of 3_2 -CPDA

► **Definition 39.** Let P be an instance of Post's Correspondence Problem. The 3_3 -CPDA $\mathcal{A}_{3_3}^P$ has stack alphabet:

$$\begin{aligned} \Sigma \cup [1_u, 2_u, \dots, m_u] \cup [1_v, 2_v, \dots, m_v] \cup \{ \mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_1 \mathbf{v}_2^{start}, \mathbf{v}_1 \mathbf{v}_2 \mathbf{u}_1 \mathbf{u}_2^{start}, \mathbf{u}_1 \mathbf{v}_1^{end}, \mathbf{v}_1 \mathbf{u}_1^{end} \} \\ \cup \{ \mathbf{abcd} : \{a, b, c, d\} = \{u_1, u_2, v_1, v_2\} \} \cup \{ \bullet \} \end{aligned}$$

It initially behaves by non-deterministically choosing one of the following:

- Push any member of Σ onto the stack.
- If the Σ symbols in the stack since the last symbol of the form i_u in the top 1-stack (or the bottom of the 1-stack if there is no such symbol) form the word u_j , then it may perform $push_3; push_1^{j_u, 3}$.
- If the Σ symbols in the stack since the last symbol of the form i_v in the top 1-stack (or the bottom of the 1-stack if there is no such symbol) form the word v_j , then it may perform $push_3; push_1^{j_v, 3}$.

Finite control-states enforce the precondition on the second and third options.

Once the top two elements of the stack are of the form i_u, i_v for some i (in either order), the automaton enters the next phase and generate the first element of the verification chain:

- Perform $push_2; push_2$
- Perform $pop_1; push_2; push_2$
- Either push $\mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_1 \mathbf{v}_2^{start}$ or $\mathbf{v}_1 \mathbf{v}_2 \mathbf{u}_1 \mathbf{u}_2^{start}$ onto the stack depending on whether the top two elements were in the order $i_u i_v$ or $i_v i_u$.

The automaton then iteratively produces further candidates for elements in the verification chain:

- Perform $push_3$.
- Perform $pop_2; pop_2 pop_2 pop_2$
- Perform $push_1^{\bullet, 3}$
- Perform $push_2$ followed by iterated pop_1 until the top element of the stack is no longer a \bullet .
- Generate a further four 2-stacks representing a u_1, u_2, v_1, v_2 in exactly the same way as for $\mathcal{A}_{3_2}^P$, recording the ordering (possibly with an end flag) on top.
- The automaton breaks from this iteration at this point iff an element with an end flag was just deployed.

After this phase the automaton enters a distinguished control-state $candidate$. It then leaves this control-state to perform $push_3; pop_2; pop_2; pop_2; pop_2$ and enters control-state $chainpos$. It then repeatedly performs the following:

- pop_1 entering a non-distinguished control-state.
 - If the top element is a \bullet it enters control-state *chainpos* and goes back to the item above.
- We additionally add transitions from all configurations labelled by pop_1 , pop_2 , pop_3 and *collapse* performing the respective stack operations whilst transitioning to a distinguished control-state *test*.

Lemma 25

Let P be an instance of Post's Correspondence Problem. Then there exists a Σ_2 sentence ϕ of *FO* such that:

$$\mathcal{G}(\mathcal{A}_{3_3}^P) \models \phi$$

(note *no* ϵ -closure) if and only if P has a solution.

Proof. For the same reasons as with $\mathcal{A}_{3_2}^P$ it is the case that P has a solution if and only if $\mathcal{A}_{3_3}^P$ can reach a configuration (*candidate*, t) such that, for every pair of 2-stacks s, s' occurring in t with s' is the 2-stack immediately above s , it is the case that $s' = s^+$.

Assuming that the variable x is bound to a configuration (*test*, t') where t' is an initial segment of a stack t such that (t , *candidate*) is reachable, we can assert that the top two 2-stacks of t' form a pair with the credentials above using the following Π_1 formula $\psi(x)$ over $\mathcal{G}(\mathcal{A}_{3_3})$:

$$\begin{aligned} & \forall s'. \forall u_2 v_2 u_1 v_1. \forall w w'. \forall c_u c_v. (\mathbf{pop}_3(x, s') \rightarrow \mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_1 \mathbf{v}_2(x) \rightarrow \mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_1 \mathbf{v}_2(s')) \\ & \rightarrow \mathbf{pop}_2(x, v_1) \rightarrow \mathbf{pop}_2(v_1, w) \rightarrow \mathbf{pop}_2(w, u_1) \rightarrow \mathbf{pop}_1(s', v_2) \\ & \rightarrow \mathbf{pop}_2(s', w') \rightarrow \mathbf{pop}_2(w', u_2) \rightarrow \mathbf{collapse}(u_1, c_u) \rightarrow \mathbf{collapse}(v_1, c_v) \\ & \rightarrow (\mathbf{collapse}(u_2, c_u) \wedge \mathbf{collapse}(v_2, c_v)) \end{aligned}$$

$\wedge \dots$

where as with the proof of Lemma 21 we have illustrated just one of 64 conjuncts that go through all possible orderings of the u_1, u_2, v_1, v_2 in the top and penultimate 2-stacks. The correctness of this formula follows from the fact that every element constituting the guess of a solution of P is equipped with a 3-link pointing to a distinct 2-stack.

The design of $\mathcal{A}_{3_3}^P$ ensures that the elements in the verification-chain contained in t (*i.e.* all candidates for the pairing s, s' in t) are precisely those that can be reached by performing a *collapse* operation on a (*chainpos*, t') configuration reached from (*candidate*, t). Assuming that x is again bound to a (*candidate*, t) configuration, we can thus assert that x represents a solution to P with the following Π_1 formula $\chi(x)$ over $\mathcal{G}(\mathcal{A}_{3_3}^P)$:

$$\begin{aligned} \chi(x) := & \forall y. \forall z. (\mathbf{chainpos}(y) \rightarrow \mathbf{pop}_3(y, x) \rightarrow \mathbf{collapse}(y, z) \\ & \rightarrow \neg(\mathbf{u}_1 \mathbf{u}_2 \mathbf{v}_1 \mathbf{v}_2^{start}(z) \vee \mathbf{v}_1 \mathbf{v}_2 \mathbf{u}_1 \mathbf{u}_2^{start}(z)) \rightarrow \psi(z)) \end{aligned}$$

We can thus take the required Σ_2 formula ϕ (asserting the existence of such a solution witnessing configuration x) to be:

$$\phi := \exists x. (\mathbf{candidate}(x) \wedge \chi(x))$$

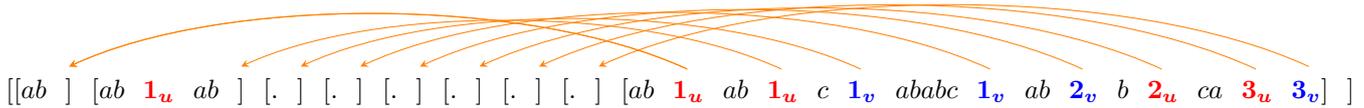
◀

A.5 Σ_1 Undecidability for 4_2 -CPDA

A.5.1 The modification

We modify the verification chain so that only one pair of collapses needs to be compared for equality rather than previously where two comparisons were required (for the u and the v). This allows us to avoid the problem above.

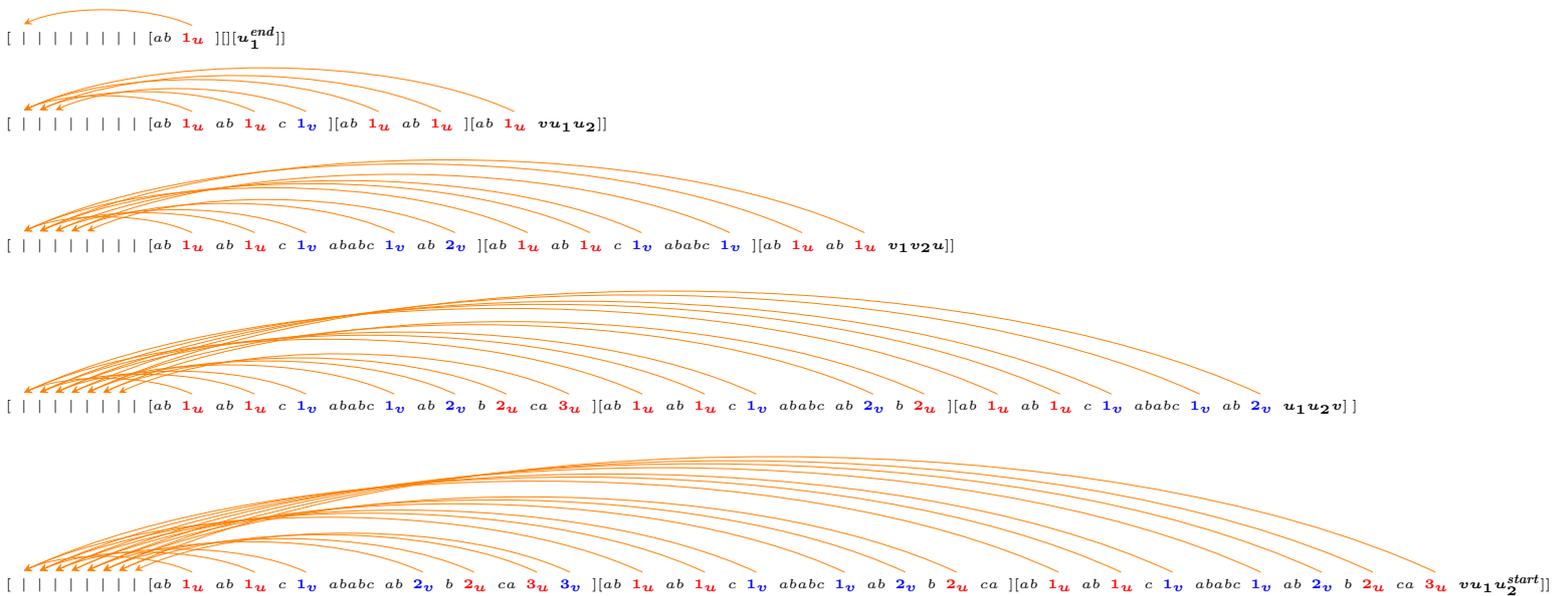
Proceeding with our running example, a solution to a PCP instance will be represented using a 2-stack in exactly the same manner as before:



The difference is the manner in which the ‘verification chain’ used to check the correctness of an alleged representation is constructed and represented in a 3-stack. In this modified chain of 2-stacks it is the top three 1-stacks that are significant. Each element in the stack will possess either ‘ u v_1 and v_2 ’ 1-stacks (in some order) or v , u_1 and u_2 1-stacks. This contrasts with the original verification chain where each point possessed a u_1 , u_2 , v_1 and v_2 1-stack.

We refer to the u or v 1-stack in a chain position as *guaranteed* and the u_2 or v_2 stack as *tentative* with the associated u_1 or v_1 as the *condition stack*. If the condition stack represents the same position in either the u or v subsequence from the previous member in the chain, then the tentative stack correctly represents the next position in the u or v subsequence. This is the same idea as before. The guaranteed stack, however, will always *unconditionally* represent the next position in the v or u subsequence.

The following shows this new kind of a verification chain as a 3-stack:



As before, a token describing the ordering of the stacks is added to the top of each element in the chain.

Let us formally define a 3_2 -CPDA that generates verification chains in the manner illustrated in the example above.

► **Definition 40.** Let P be an instance of PCP. The 3_2 -CPDA $\mathcal{A}_{3_2^{alt}}^P$ shares stack alphabet with \mathcal{A}_2^P but with extra symbols: $vu_1u_2, u_1vu_2, u_1u_2v, vu_1u_2^{start}, u_1^{end}, uv_1v_2, v_1uv_2, v_1v_2u, uv_1v_2^{start}, v_1^{end}$.

$\mathcal{A}_{3_2^{alt}}^P$ initially behaves the same way as \mathcal{A}_2^P in order to generate a 2-stack representing a postulated solution to P . At this point the top two elements of the stack will either be $i_u i_v$ or $i_v i_u$ for some $i \in [1..m]$. We then perform $push_2; push_2; pop_1; push_2$ followed by $push_1^{uv_1v_2^{start}}$ if the top two symbols are $i_v i_u$ and $push_1^{vu_1u_2^{start}}$ if $i_u i_v$. The automaton then performs $push_3$ and behaves as follows, examining the token on top of the stack to ascertain which option should be taken:

- If the current guaranteed stack of the top_3 element (which has just been copied) is below both the condition and tentative stacks, then we should perform pop_2 until the guaranteed stack is the top_2 stack—*i.e.* perform $pop_2; pop_2$. Then:
 - If the guaranteed stack is a u stack (rather than a v stack) then perform pop_1 until another j_u or j_v is found for some $j \in [1..m]$.
 - * At the *first new* j_u to be discovered, we deem the resulting top_2 to be the new u stack. If v_1 and v_2 are still to be produced we perform $push_2$ and continue with the pop_1 s.
 - * At all *subsequent* j_u discovered, we just perform pop_1 and continue with the pop_1 s.
 - * If a j_v is found and we have not yet created a new v_1 , then we non-deterministically choose whether to deem this stack to be the new v_1 . If we choose not to we just proceed with more pop_1 s. If we choose to do so, then we perform $push_2$.
 - * The *first new* j_v to be found *since creating* v_1 should become the new v_2 stack. If the new u stack has not yet been created then we perform $push_2$ and continue with the popping.
 - * All *subsequent* j_v found *since creating* the new v_2 should just be popped and the pop_1 s continued.
 - * If the empty 1-stack is produced, then abort (and fail) if either u_1 has not yet been generated or either u_2 or v have been generated. Otherwise perform $push_2; push_1^{u_1^{end}}$.
 - * If the new v, u_1 and u_2 have all been created, then cease the pop_1 s and perform $push_1^{token}$ where *token* is the token (without a start or end flag) denoting the order in which the stacks were produced.
 - If the guaranteed stack is a v stack (rather than a u stack) then do the same as above interchanging u and v .
- If the condition stack of the top_3 element in the chain is below both the guaranteed and tentative stacks, then we should perform pop_2 until the condition stack is the top_2 stack—*i.e.* perform $pop_2; pop_2$. Then:
 - If the condition stack is a u_1 stack (rather than a v_1 stack) then perform pop_1 until another j_u or j_v is found for some $j \in [1..m]$.
 - * At the *first new* j_u to be discovered we just perform pop_1 and continue with the pop_1 operations. At the *second new* j_u to be discovered, we deem the current top_2 stack to be the new u stack. If the new v_1 and v_2 have not yet been created we perform $push_2$ and continue with the pop_1 operations.
 - * At all *subsequent* j_u discovered, we just perform pop_1 and continue with the pop_1 s.
 - * If a j_v is discovered then we behave in the same way as in the case when the guaranteed stack u is below the condition stack v_1 (see above). This creates the v_1 and v_2 stacks.
 - * If an empty 1-stack is produced or we have just finished creating all of the new u, v_1 and v_2 then again we behave in the same manner as when the guaranteed stack is below the condition stack.
 - Note that the condition stack will always be below the tentative stack, so we have already exhausted the possibilities.

- If it is not the case that $top_1(u) = i_u$ and $top_1(v_2) = i_v$ or $top_1(u_2) = i_u$ and $top_1(v) = i_v$ (depending on which combination of stacks the recently produced chain element uses) for some $i \in [1..m]$ then the automaton aborts into a fail state.
- If we have deployed a token with an *end* marker, then we halt and move into a distinguished control-state $guess_{3_2}$. Otherwise we perform a $push_3$ operation and repeat.

► **Remark.** Suppose that an element in a chain generated by $\mathcal{A}_{3_2}^P$ consists of a v and u_1, u_2 stacks. If v is the first (lowest) of these, then the next element in the chain will consist of a v, u_1 and u_2 . If u_1 is the lowest, then the next element in the chain will consist of a u, v_1 and v_2 .

We formalise what it means to be a correct verification chain in this new style using a revised successor operation \oplus to be to $\mathcal{A}_{3_2}^P$ what $+$ is to $\mathcal{A}_{3_2}^P$.

► **Definition 41.** Let s be a 2-stack over the alphabet of \mathcal{A}_2^P . The *successor* s^\oplus of s is the unique stack such that:

- $pop_2; pop_2; pop_2(s^\oplus) = pop_2; pop_2; pop_2(s)$
- Where a, b, c are (in order) the top three 1-stacks of s^\oplus : $c \sqsubseteq_1 b \sqsubseteq_1 a$.
- If the bottom of the top three 1-stacks in s is a u or u_1 stack, then s^\oplus should consist of a u, v_1 and v_2 stack, if its a v or v_1 stack then, s^\oplus should consist of a v, u_1 and u_2 stack.
- Let s_u be either the u_2 or u stack in s (whichever s possesses). Let s_v be either the v_2 or v stack in s (whichever s possesses).
 - If s^\oplus possesses u_1 , then this $u_1 = s_u$ and its u_2 has as its top_1 element the highest element of the form i_u below $top_1(s_u)$. If such an element does not exist, u_2 should be empty. Moreover the v of s^\oplus should have as its top_1 element the highest element of the form i_v below $top_1(s_v)$. If such an element does not exist, v should be empty.
 - If s^\oplus possesses v_1 , then this $v_1 = s_v$ and its v_2 has as its top_1 element the highest element of the form i_v below $top_1(s_v)$. If such an element does not exist, v_2 should be empty. Moreover the u of s^\oplus should have as its top_1 element the highest element of the form i_u below $top_1(s_u)$. If such an element does not exist, u should be empty.

The following Lemma is almost an immediate consequence of the definitions and Lemma 16.

► **Lemma 42.** Let P be an instance of Post's Correspondence Problem and let s be a 2-stack generated by \mathcal{A}_2^P . The 2-stack s represents a solution to P in the sense of Lemma 16 iff there is a 'verification chain' of 2-stacks s_1, s_2, \dots, s_k for some k such that:

- $s_1 = push_2; push_2; pop_1; push_2(s)$ (with top three stacks defined to be v, u_1, u_2 or u, v_1, v_2 if the top two elements of s are respectively of the form $i_v i_u$ or $i_u i_v$)
- s_k has empty stacks as its top two 1-stacks
- $s_{i+1} = s_i^\oplus$ for every $1 \leq i < k$.
- For each element s_i in the chain we have $top_1(v) = j_v$ and $top_1(u_2) = j_u$ or $top_1(u) = j_u$ and $top_1(v_2) = j_v$ for some $j \in [1..m]$ (depending on what selection of stacks s_i has).

Proof. We establish the result by arguing that such a sequence exists iff s satisfies the conditions set out in Lemma 16.

Argue by induction on l that an initial segment of such a chain s_1, s_2, \dots, s_l exists with j_1, j_2, \dots, j_l the associated indices mentioned in the fourth condition iff the top-most l elements of s of the form i_u are $(j_1)_u, (j_2)_u, \dots, (j_l)_u$, and the topmost l elements of s of the form i_v are $(j_1)_v, (j_2)_v, \dots, (j_l)_v$ (ordered top down).

First the \Rightarrow direction. The base case ($l = 1$) is immediate since all stacks generated by \mathcal{A}_2^P must have top two elements of the form $j_u j_v$ or $j_v j_u$ for some j . Suppose now that an initial segment of such a chain $s_1, s_2, \dots, s_l, s_{l+1}$ exists with fourth-condition indices $j_1, j_2, \dots, j_l, j_{l+1}$. By the induction hypothesis, we just need to check that if the top elements of either v or v_2 in s_l and either

u or u_2 in s_l are respectively the l th j_v and j_u elements from the top of s , then the top elements of either v or v_2 in $(s_l)^\oplus$ and either u or u_2 in $(s_l)^\oplus$ are respectively the $(l+1)$ th elements of the form j_v and j_u from the top of s . But this is ensured directly by the fourth point in the definition of $^\oplus$.

Now consider the \Leftarrow direction. Again the base case ($l = 1$) is straightforward since s_1 is explicitly defined to meet the criteria. Suppose that the topmost $l+1$ elements of the form j_u of s are: $(j_1)_u, (j_2)_u, \dots, (j_l)_u, (j_{l+1})_u$ and the topmost $l+1$ elements of the form j_v of s are: $(j_1)_v, (j_2)_v, \dots, (j_l)_v, (j_{l+1})_v$. By the induction hypothesis we already have a chain s_1, s_2, \dots, s_l and so we just need to show that $(s_l)^\oplus$ both exists and satisfies the requisite criteria. If it does exist, then as above the fourth clause in the definition of $^\oplus$ ensures that the fourth requirement of the Lemma is satisfied, which is the only one that would need to be established (the first applies only to s_1 , the second is not relevant to initial prefixes and the third is by assumption). Thus it is only existence that we need to establish. But the $^\oplus$ successor always exists. The top three stacks are all initial segments of s (exhaustively defined—they are defined to be the empty stack if an appropriate element in s does not exist) and so can be linearly ordered with respect to \sqsubseteq_1 . \blacktriangleleft

The following Lemma is critical—it tells us that $\mathcal{A}_{3_2^{alt}}^P$ is able to construct an appropriate chain of successors if one exists and moreover provides a sufficient (and necessary) condition for a stack it generates representing such a chain.

► **Lemma 43.** *Let P be an instance of Post's Correspondence Problem. For any 2-stack s generated by $\mathcal{A}_{3_2^{alt}}^P$ there exists a sequence of 2-stacks s_1, s_2, \dots, s_k satisfying the condition in Lemma 42 iff $\mathcal{A}_{3_2^{alt}}^P$ can reach a configuration ($\mathbf{guess}_{3_2}, [s'_1, s'_2, \dots, s'_k]$) such that:*

- $s'_i = \mathit{push}_1^{\mathit{token}}(s_i)$ for each $1 \leq i \leq k$ where *token* is a token indicating the ordering of the top three stacks with a *start* flag for s'_1 and a *end* flag for s'_k .
 - For every $1 \leq i < k$:
 - If s'_{i+1} contains a u_1 then this is equal to u_2 or u in s'_i (depending on which one s'_i contains)
 - or if s'_{i+1} contains a v_1 then this is equal to v_2 or v in s'_i (depending on which one s'_i contains).
- Note that for each i only one of the above will hold.

Proof. First let us argue in the \Rightarrow direction. First argue by induction on l that if we have an initial prefix s_1, s_2, \dots, s_l of such a sequence s_1, s_2, \dots, s_k , then $\mathcal{A}_{3_2^{alt}}^P$ can generate a stack $[s'_1, s'_2, \dots, s'_l]$ without aborting, during the phase after generating the 2-stack s , such that:

- $s'_i = \mathit{push}_1^{\mathit{token}}(s_i)$ for each $1 \leq i \leq l$ where *token* is a token indicating the ordering of the top three stacks with a *start* flag for s'_1 and a *end* flag for s'_k .
 - For every $1 \leq i < l$:
 - If s'_{i+1} contains a u_1 then this is equal to u_2 or u in s'_i (depending on which one s'_i contains)
 - or if s'_{i+1} contains a v_1 then this is equal to v_2 or v in s'_i (depending on which one s'_i contains).
- Note that for each i only one of the above will hold.

For the base case ($l = 1$) the result is immediate as $\mathcal{A}_{3_2^{alt}}^P$ will construct s'_1 from s in exactly the way that s_1 is defined in Lemma 42 (adding a token on top).

For the inductive step, suppose that $\mathcal{A}_{3_2^{alt}}^P$ has already generated $[s'_1, s'_2, \dots, s'_l]$ corresponding to a sequence s_1, s_2, \dots, s_l . Suppose now that this sequence extends to $s_1, s_2, \dots, s_l, s_{l+1}$. The automaton will perform $\mathit{push}_3; \mathit{pop}_2 \mathit{pop}_2$ in preparation to generate s'_{l+1} . We consider two cases:

Case when the guaranteed stack of s'_l (or by induction hypothesis equivalently s_l) is below both the condition and tentative stacks: W.l.o.g. assume that the guaranteed stack of s'_l is a u stack (the case when it is a v stack is similar). Due to the position of v we must have in s_l : $v \sqsupseteq_1 u_1 \sqsupseteq_1 u_2$. Thus the u_1 of $s_{l+1} = s_l^\oplus$, which is the u_1 of s_l can indeed be produced by performing pop_1 operations on the v of s_l (s'_l). The automaton is free to pick anything to be the u_1 of s_{l+1} and so in

particular can choose the correct value. The new v of s_{l+1} is restricted to be correct with respect to the v of s_l and similarly the restriction on u_2 is precisely what is required with respect to u_1 in s_{l+1} .

Case when the condition stack of s'_l (or by induction hypothesis equivalently s_l) is below both the guaranteed and tentative stacks: Again w.l.o.g. assume that the condition stack of s'_l is a u_1 stack (the case when it is a v_1 stack is similar). Due to the position of u_1 we must have in s_l : $u_1 \sqsupseteq_1 v$ and $u_1 \sqsupseteq_1 u_2$. Since the new v_1 in s_{l+1} should be equal to v in s_l and the new u in s_{l+1} an initial prefix of u_2 in s_l , it must be possible to form both of these from performing pop_1 operations on the u_1 in s_l . The automaton is unconstrained in picking the v_1 , so in particular it is able to guess the correct position—again the constraint on picking the new v_2 relative to v_1 is precisely the correct one. Note also that the constraint on picking the new u relative to the old u_1 is precisely the correct one—popping to the next j_u will yield the old u_2 and so popping from that to the second j_u will yield the correct new u .

Either way since the sequence $s_1, s_2, \dots, s_l, s_{l+1}$ by assumption exhibits equality of the top elements of the u_2 and v or v_2 and u in each element in the chain, it will carry out the above without aborting. Furthermore the second condition on the s'_i is satisfied since the s_i form a \oplus -successor chain.

This establishes the induction hypothesis is true for all $l \leq k$. In particular when $l = k$ the top two 1-stacks of s_k (or s'_k ignoring the token on top) will be empty and so the automaton will halt in control-state $guess_{3_2}$ as required.

Now let us consider the \Leftarrow direction. We argue by induction on the converse hypothesis to what we had before. Suppose that $\mathcal{A}_{3_2}^P$ generates a stack $[s'_1 s'_2 \dots s'_l]$ (in the phase following the construction of the 2-stack s) that corresponds to a correct initial segment of a verification chain s_1, s_2, \dots, s_l . Suppose now that $\mathcal{A}_{3_2}^P$ proceeds to generate $[s'_1 s'_2 \dots s'_l s'_{l+1}]$ that satisfies the conditions in the converse of the induction hypothesis used previously. This stack must have been produced from $[s'_1 s'_2 \dots s'_l]$ by beginning with a $push_3; pop_2; pop_2$. Again we should consider the same two cases as before, noting that the additional assumed constraint on s'_{l+1} relative to s'_l ensures that the guessed new u_1/v_1 for s'_{l+1} must indeed be the u_1/v_1 for s'_l (i.e. the u_2/v_2 of s'_l or equivalently s_l). The new u_2/v_2 and v/u will be correctly created by the automaton, as discussed before when arguing in the \Rightarrow direction.

The fact that the automaton does not fail means that it must have successfully found that the u/u_2 and v_2/v stacks in s_{l+1} share top_1 elements. Thus $s_{l+1} = s'_l \oplus$ as required and also satisfy the top_1 equality requirement.

The automaton will only halt in control-state $guess_{3_2}$ if it detects two empty 1-stacks (modulo the token), constituting the final s_k in the chain. \blacktriangleleft

A.5.2 Exploiting $\mathcal{A}_{3_2}^P$ in a 4-CPDA

Since only one comparison needs to be made between adjacent elements, the problem illustrated in Figure 2 is no longer an issue. The same idea that took us from $\mathcal{A}_{3_2}^P$ to $\mathcal{A}_{5_2}^P$ can thus be used to go from $\mathcal{A}_{3_2}^P$ to a 4₂-CPDA $\mathcal{A}_{4_2}^P$.

► **Definition 44.** Let P be an instance of Post's Correspondence Problem. The 4₂-CPDA $\mathcal{A}_{4_2}^P$ shares the same stack-alphabet as $\mathcal{A}_{3_2}^P$. It begins by behaving as $\mathcal{A}_{3_2}^P$ until this automaton halts in control-state $guess_{3_2}$. It then performs a $push_4$ operation and non-deterministically decides whether to operate in 'A-mode' or 'B-mode'. If it decides to operate in A-mode:

- Perform *collapse* on the conditional stack (either u_2 or v_2 depending on which it has) of the top_3 element of the verification chain.
- Perform $push_4; pop_3$ —this reveals the previous member of the verification chain as the top_3 stack.

- Repeat until *collapse* has been performed on the second member of the verification chain (we do not do this to the first member). Once this stage is reached, enter distinguished control state *A*.

If it decides to operate in *B*-mode, it proceeds as follows:

- First examines the token on top of the top_3 stack to determine whether the condition stack of the top_3 element in the chain is u_1 or v_1 . If it is u_1 set $w := u$ and if it is v_1 set $w := v$.
- Performs $pop_3; push_3$ so that a copy of the previous element in the chain is now the top_3 stack. The automaton then performs *collapse* on either the guaranteed stack w or the tentative stack w_2 depending on which this previous element in the chain possesses.
- Perform $push_4; pop_3$.
- Repeat until *collapse* has been performed on copies of all but the last members of the verification chain (including the first represented by the bottom 3-stack). Once done enter distinguished control-state *B*.

We add an additional transition labelled *toCandidate* from both *A* and *B* to a distinguished control-state *candidate*.

Lemma 26

There exists a Σ_1 -sentence ϕ such that for every instance P of Post's Correspondence Problem we have $\mathcal{G}(\mathcal{A}_{4_2}^P) \models \phi$ iff P has a solution.

Proof. Combine Lemmas 42 and 43. Thus P has a solution if and only if $\mathcal{A}_{3_2}^{P,alt}$ can reach a configuration $(guess_{3_2}, [s_1, s_2, \dots, s_k])$ such that: For every $1 \leq i < k$:

- If s_{i+1} contains a u_1 then this is equal to u_2 or u in s_i (depending on which one s_i contains)
- or if s_{i+1} contains a v_1 then this is equal to v_2 or v in s_i (depending on which one s_i contains).

We claim that this is the case iff $\mathcal{A}_{4_2}^P$ can both reach a configuration (A, t) and a configuration (B, t) for some stack t .

Suppose first that such a pair of configurations is indeed reachable for $\mathcal{A}_{4_2}^P$. Since a stack produced by either an *A*-mode run or a *B*-mode run from a $\mathcal{A}_{3_2}^{P,alt}$ stack $[s_1, s_2, \dots, s_k]$ will have this 3-stack as its bottom most 3-stack we may conclude that the configuration (A, t) as well as the configuration (B, t) must be produced beginning with the same $\mathcal{A}_{3_2}^{P,alt}$ stack. Since a *collapse* on two elements in copies of some 2-stack s_i will yield the same result iff they are the same, the construction of the *A* and *B* modes ensures that the equalities required to relate each s_i to s_{i+1} (for $1 \leq i < k$) must hold. After all, the i th *collapse* performed in *B*-mode will be on the appropriate component of s_i for $1 \leq i < k$ whilst the i th *collapse* performed in *A*-mode will be on the correspondingly appropriate component of s_{i+1} . The results of these *collapses* are directly compared since *collapse* is performed on a copy of the relevant 2-stack that has precisely the same set of 2-stacks below it in each case.

It follows from the above that P does indeed have a solution.

Conversely begin by assuming that P has a solution. It follows that $\mathcal{A}_{3_2}^{P,alt}$ must be able to reach a configuration $(guess_{3_2}, [s_1 \ s_2 \ \dots \ s_k])$ satisfying the conditions above. By the converse considerations to before (in terms of comparing *collapses*) these conditions must ensure that the *A*-mode and the *B*-mode both generate the same stack from this starting point, as required.

We can therefore take as the required Σ_1 -sentence the following:

$$\exists x. \exists y. \exists z. (A(x) \wedge B(y) \wedge toCandidate(x, z) \wedge toCandidate(y, z))$$



B Decidability on n_n -CPDA

μ CPDA

B.0.3 The Extended Model

An n_S - μ CPDA is a device that has an n_S -CPDA at its disposal but may intervene and manipulate it beyond its normal course depending on whether the original n_S -CPDA satisfies various μ -calculus sentences in its current configuration.

► **Definition 45.** An n_S - μ CPDA \mathcal{B} is a tuple:

$$\left\langle \Sigma, \Pi, Q, q_0, \Gamma, R'_{a_1}, R'_{a_2}, \dots, R'_{a_r}, P'_{b_1}, P'_{b_2}, \dots, P'_{b_{r'}} \right\rangle$$

where $\left\langle \Sigma, \Pi, Q, q_0, \Gamma, R'_{a_1}, R'_{a_2}, \dots, R'_{a_r}, P'_{b_1}, P'_{b_2}, \dots, P'_{b_{r'}} \right\rangle$ is an n_S -CPDA called *the underlying n_S -CPDA*; $R'_{a_i} \subseteq L_\mu^0 \times \Theta_{n_S} \times Q$ and $P'_{b_j} \in L^0\mu$ for each $1 \leq i \leq r$ and $1 \leq j \leq r'$.

As with CPDA configurations are elements of $Q \times \text{stack}_{n_S}^C(\Gamma)$ but the only transitions allowed are specified by the R'_{a_i} with reference to the R_{b_j} rather than by the R_{b_j} themselves. Likewise P'_{b_i} are the only unary predicates it has.

► **Definition 46.** Let \mathcal{B} be an n_S - μ CPDA with underlying n_S -CPDA \mathcal{A} . Let $(q, s), (q', s')$ be configurations of \mathcal{B} (and hence also of \mathcal{A}). There is an a_i labelled transition from (q, s) to (q', s') in \mathcal{B} just in case $\mathcal{G}(\mathcal{A}), (q, s) \models \phi$ where $(\phi, \theta, q') \in R'_{a_i}$ and $s' = \theta(s)$. Likewise we have (q, s) satisfying the predicate b_i just in case $\mathcal{G}(\mathcal{A}), (q, s) \models P'_{b_i}$.

Given these transition edges and predicates of \mathcal{B} the graphs $\mathcal{G}(\mathcal{B})$ and $\mathcal{G}^\epsilon(\mathcal{B})$ are defined in the same way as with conventional CPDA.

► **Example 47.** Consider a standard order-1 pushdown automaton that has control-states $\{q_0, q_1\}$ and stack alphabet $\{a, b\}$. Give it has a transition relation $R_c := \{(q_0, \text{pop}_1, q_0)\}$ and predicates $P_a := \{(q_0, a)\}$, $P_b := \{(q_0, b)\}$.

Suppose that we extend this to a 1- μ PDA with a sole μ PDA transition relation $R'_c := \{((\mu X.(\mathbf{a} \vee [c]X) \wedge \mathbf{b}), \text{push}_1^a, q_1)\}$. Then this μ PDA will have a c -labelled transition from the configuration $(q_0, [bbaaabbbbb])$ to the configuration $(q_1, [bbaaabbbbb])$ but *no other* transitions from this configuration.

The μ -calculus sentence asserts that the current configuration has b on top of the stack but that repeated popping will yield a on top.

B.0.4 Strong Isomorphisms

Two graphs are said to be isomorphic if *qua* graphs they are essentially the same. As expected the formal definition is as follows:

► **Definition 48.** Let \mathcal{G} and \mathcal{G}' be graphs sharing a signature \mathfrak{S} with respective node sets N and N' . We say that \mathcal{G} and \mathcal{G}' are *isomorphic*, written $\mathcal{G} \cong \mathcal{G}'$ just in case there is a bijection $f : N \rightarrow N'$ (called an isomorphism) such that for every $u \in N$ and unary predicate \mathbf{b} of \mathfrak{S} interpreted as $\mathbf{b}_{\mathcal{G}}$ in \mathcal{G} and $\mathbf{b}_{\mathcal{G}'}$ in \mathcal{G}' we have $u \in \mathbf{b}_{\mathcal{G}}$ iff $f(u) \in \mathbf{b}_{\mathcal{G}'}$ and for every edge \mathbf{a} we have $u\mathbf{a}u'$ in \mathcal{G} iff $f(u)\mathbf{a}f(u')$ in \mathcal{G}' .

It is well known that the theories in all logics we have introduced are invariant under isomorphism—a sentence will hold in a graph \mathcal{G} just in case it holds in all isomorphic graphs \mathcal{G}' .

Note that every CPDA \mathcal{A} can be viewed as a μ CPDA \mathcal{B} . We simply take \mathcal{B} to have underlying CPDA \mathcal{A} and give it a predicate for every control-state/stack-alphabet pair in $Q \times \Gamma$ to facilitate a μ -calculus sentence asserting that we are currently in a particular control-state with a particular symbol on top of the stack. This allows us to reconstruct the original transition relation of \mathcal{A} in \mathcal{B} . It thus follows that for every CPDA \mathcal{A} there exists a μ CPDA \mathcal{B} such that $\mathcal{G}^\epsilon(\mathcal{B}) \cong \mathcal{G}^\epsilon(\mathcal{A})$.

For CPDA there is a stronger notion of isomorphism where stack structure and control-states are preserved as well. This will be the form of isomorphism to which we usually appeal. In particular the definition makes sense when comparing μ CPDA and CPDA.

► **Definition 49.** Let \mathcal{A} and \mathcal{A}' be n_S - μ CPDA (and in particular either or both may be an n_S -CPDA). We say that $\mathcal{G}(\mathcal{A})$ and $\mathcal{G}(\mathcal{A}')$ (resp. $\mathcal{G}^\epsilon(\mathcal{A})$ and $\mathcal{G}^\epsilon(\mathcal{A}')$) are *strongly isomorphic* just in case there is an isomorphism L between the graphs where for any configuration (q, s) of \mathcal{A} we can define L by an expression of the form $L(q, s) := (L(q), L(s))$ where $L(\text{pop}_k(s)) = \text{pop}_k(L(s))$ for every $1 \leq k \leq n$; $L(\text{collapse}(s)) = \text{collapse}(L(s))$ and $L(\perp_n) = \perp_n$, overloading L to additionally denote a map on both control-states and constructible stacks.

We write $\mathcal{G}(\mathcal{A}) \hat{\cong} \mathcal{G}(\mathcal{A}')$ (resp. $\mathcal{G}^\epsilon(\mathcal{A}) \hat{\cong} \mathcal{G}^\epsilon(\mathcal{A}')$) to indicate this.

Note that whilst L is a bijection between the domains of each graphs, in the ϵ -transition there may be intermediate control-states accessed during the course of ϵ -transitions that do not appear in nodes of the ϵ -closure of the graph. Therefore L may not be a bijection between control-states. Nevertheless, for control states belonging to the ϵ -closure (on which L is a bijection) we adopt the convention ' $L(q) := q$ '. The corresponding convention for stacks ' $L(s) := s$ ' is not used as it would be highly misleading; two occurrences of a symbol a in s may map to different symbols in $L(s)$.

B.0.5 Representing as Conventional CPDA

Just as every n_S -CPDA can be viewed as an n_S - μ CPDA it turns out that the converse holds as well. Indeed we can view the main result of [2] as saying precisely this.

► **Theorem 50.** *Given any n_S - μ CPDA \mathcal{B} there exists an n_S -CPDA \mathcal{A} such that $\mathcal{G}(\mathcal{B}) \hat{\cong} \mathcal{G}(\mathcal{A})$ and so also $\mathcal{G}^\epsilon(\mathcal{B}) \hat{\cong} \mathcal{G}^\epsilon(\mathcal{A})$.*

Proof. Let \mathcal{A}^- be the n_S -CPDA underlying \mathcal{B} with control-states $Q_{\mathcal{A}^-}$. Extend $Q_{\mathcal{A}^-}$ with a fresh distinguished control-state \star . Add fresh distinguished edges \hat{q} for every $q \in Q_{\mathcal{A}^-}$ from the configuration (\star, s) to the configuration (q, s) for every stack s and have a transition θ for every n_S -stack operation connecting (\star, s) to $(\star, \theta(s))$. Making \star the initial state call the resulting automaton \mathcal{A}^* .

Now let $\phi_1, \phi_2, \dots, \phi_m$ be a list of all of the μ -calculus sentences occurring in transition relations of \mathcal{B} . Let ϕ_i^q be the μ -calculus sentence $[\hat{q}]\phi_i$ for every $q \in Q_{\mathcal{A}^-}$ and $1 \leq i \leq m$. Logical reflection for CPDA, as established in [2], allows us to construct an automaton \mathcal{A}_{LR}^* such that there exists an isomorphism $f : \mathcal{G}^\epsilon(\mathcal{A}^*) \cong \mathcal{G}^\epsilon(\mathcal{A}_{LR}^*)$ and additionally there is a set $S_{[\hat{q}]\phi_i} \subseteq Q_{\mathcal{A}_{LR}^*} \times \Gamma_{\mathcal{A}_{LR}^*}$ such that a configuration (p, t) of \mathcal{A}_{LR}^* satisfies $\mathcal{G}^\epsilon(\mathcal{A}_{LR}^*), (p, t) \models [\hat{q}]\phi_i$ just in case $(p, \text{top}_1(t)) \in S_{[\hat{q}]\phi_i}$. That is \mathcal{A}_{LR}^* generates the same ϵ -closure as \mathcal{A}^* but is also 'aware' of what μ -calculus properties are satisfied at each configuration.

Note that we do not quite have a strong isomorphism here. Whilst [2] tells us the stacks either side of the isomorphism satisfy the required structural similarity, the control-state in the image of the isomorphism depends on the stack in the input configuration as well as the control-state. That said, the converse does hold: the control-state in the image determines the control-state in the input of the isomorphism. In particular it is well-defined to delete all control-states from \mathcal{A}_{LR}^* that are not

associated with \star in \mathcal{A}^* . We also remove all edges other than those of the form θ for $\theta \in \Theta_n$. Call the resulting automaton \mathcal{A}_{LR}^{**} .

Now we construct the n -CPDA \mathcal{B} to have the same control-states $Q_{\mathcal{A}}$ as \mathcal{A} and the stack-alphabet of \mathcal{A}_{LR}^{**} . In order to simulate \mathcal{A} when in control-state q it may do the following:

- Pick a \mathcal{A} -transition dependent on μ -calculus sentence ϕ that performs stack-operation θ whilst moving to control-state q' .
- Check that the top element of the stack belongs to $S_{[q]\phi}$ in which case we are indeed in a configuration corresponding to a \mathcal{A} -configuration in control-state q at which ϕ holds.
- Transition into control-state q' whilst performing the stack-operation dictated by the \mathcal{A}_{LR}^{**} -transition θ .

Then $g : \mathcal{G}(\mathcal{B}) \cong \mathcal{G}(\mathcal{A})$ with $g(q, s) := g(q, t)$ where $f(\star, s) = (_, t)$.

◀

B.1 Monotonic CPDA

We will without loss of generality make the assumption that $push_n$, pop_n and collapse on n -links is only performed during ϵ -transitions. This avoids the need for case separation when monotising automata—we can just focus on ϵ -edges. Generality is not lost since ϵ -closure allows us to decompose an a -labelled $push_n$ edge (for example) into an ϵ -transition with $push_n$ followed by an a -edge with nop .

We will also use Σ to denote the set of *non- ϵ* transition labels and view ϵ as lying outside of Σ .

B.1.0.1 Lemma 29

Let \mathcal{A} be an n -CPDA with edge alphabet Σ and unary predicates Π . Then there exists an n -CPDA \mathcal{A}^\uparrow such that $\mathcal{G}^\epsilon(\mathcal{A}) \cong \mathcal{G}^\epsilon(\mathcal{A}^\uparrow \upharpoonright_{\Sigma, \Pi})$ but whose additional distinguished edge labels include $r_\epsilon \notin \Sigma$ such that \mathcal{A}^\uparrow is monotonic via r_ϵ and $(q, s)r_{r_\epsilon}^\uparrow a(q', s')$ just in case $(q, s)r_{r_\epsilon}^* a(q', s')$.

Proof. Due to Theorem 50 it is sufficient to define an order- n μ CPDA $\mathcal{A}^{\uparrow\mu}$ that satisfies the requirements. Conversely it is easy to construct an order- n μ CPDA \mathcal{A}^μ that shares the same configuration graph as \mathcal{A} since the current control-state and top stack symbol can trivially be detected with a μ -calculus sentence. Extend this to a μ CPDA $\mathcal{A}^{\uparrow\mu}$ as follows:

- Add a unary predicate q for each control-state q of \mathcal{A} .
- Add a marker **marker** $[\gamma]$ to the stack-alphabet for each γ in the stack alphabet of Γ . The automaton ensures that at most one of these is on the stack at any one time. Extend the Σ transitions to treat **marker** $[\gamma]$ as γ and add a single unary predicate **marker** asserting that the marker is on top of the stack.
- We add edges labelled **deployMarker** that simply rewrites the top element of the stack γ to **marker** $[\gamma]$ without changing the control-state.
- Add edges labelled **removeMarker** that rewrite a **marker** $[\gamma]$ on top of the stack to γ without altering the control-state.
- Add edges $\epsilon_{<n}$ for each ϵ -transition in \mathcal{A} not performing a *collapse* on an n -link; a pop_n nor a $push_n$.
- Add edges ϵ_{push_n} for each ϵ -transition in \mathcal{A} that performs a $push_n$ operation.

Now let ϕ_q be the μ -calculus assertion: ‘We can perform **deployMarker** and then perform arbitrary ϵ transitions, beginning with a $push_n$ and immediately removing the marker from the copy, ending up back with the stack at which we started, and indeed stopping precisely when we end up back where we started, with the marker on top and in control-state q .’

This can be expressed in the μ -calculus by the following:

$$\phi_q := \langle \mathbf{deployMarker} \rangle \langle \epsilon_{push_n} \rangle \langle \mathbf{removeMarker} \rangle \mu X.((q \wedge \mathbf{marker}) \vee (\langle \epsilon \rangle X \wedge \neg \mathbf{marker}))$$

We define an r_ϵ -edge to occur whenever we have an $\epsilon_{<n}$ -edge or an ϵ_{push_n} -edge. We additionally add an r_ϵ -edge to control-state q' via nop whenever $\phi_{q'}$ holds in the current configuration (possible since it is a μ CPDA).

Observe that reachability via r_ϵ -edges preserves the original stack alphabet—markers are only implicitly deployed in the definition of each ϕ_q , they are never introduced by an actual transition of $\mathcal{A}^{\uparrow\mu}$.

Now we argue for correctness. We disregard the single $a \in \Sigma$ -transition at the end of the path since by our w.l.o.g. assumption this is an order $(n - 1)$ -operation and so not pertinent to the definition of a climb.

First suppose that $(q, s)r_{\epsilon^*}^\uparrow(q', s')$ (derived from \mathcal{A}). All operations featuring in this path other than a pop_n or a $collapse$ on an n -link can be replaced directly by an r_ϵ -edge. So we just need to show that pop_n and $collapse$ on n -links can also be replaced. The fact that we are considering a climb rather than an arbitrary run tells us that for every stack t occurring in the run witnessing $(q, s)r_{\epsilon^*}^\uparrow(q', s')$ we must have $pop_n(s) \sqsubset_n t$. It must thus be that for every instance of $collapse$ on an n -link or pop_n resulting in a configuration (p', t) there must be an earlier configuration of the form (p, t) in the run that is followed by a $push_n$ operation. But then $\phi_{p'}$ holds at this configuration and so there is an r_ϵ -transition from (p, t) to (p', t) , as required.

Conversely suppose that there is an r_ϵ^* path from (q, s) to (q', s') . Argue by induction on the length of the path. If $pop_n(s) \sqsubset_n t$, then $t' = push_n(t)$ and $t' = \theta(t)$ for any $\theta \in \Theta_{n-1}$ must satisfy $pop_n(s) \sqsubset_n t'$. Moreover these operations for r_ϵ -edges are directly inherited from the original ϵ -edges and so the path is as required for these operations. It just remains to consider r_ϵ resulting from a $\phi_{p'}$ -test at a configuration (p, t) with $s \sqsubset_n t$, resulting in (p', t) . But $\phi_{p'}$ asserts the existence of precisely such an ϵ -path. ◀

► **Remark.** Since the initial configuration has the empty stack \perp_n and we can w.l.o.g. view ' $pop_n(\perp_n)$ ' $\sqsubset_n t$ as holding for any stack t (for example by treating the initial stack as $push_n(\perp_n)$) and ensuring the automaton never pops down below this) we get that all reachable configurations are *monotonically reachable* from the initial configuration via $\{r_\epsilon \cup \Sigma\}$ -labelled paths.

Lemma 31

Let \mathcal{A} be an n -CPDA with unary predicates Π . Then there exists an n -CPDA \mathcal{A}^\downarrow with stack-alphabet Γ^\downarrow and control-state space Q^\downarrow such that $\mathcal{G}(\mathcal{A}) \cong \mathcal{G}(\mathcal{A} \upharpoonright_{\Pi^\downarrow})$ and that also has a predicate P^\downarrow for each $P \in \Pi$ such that P holds of precisely those configurations c from which \mathcal{A} has an ϵ -fall to a configuration c' satisfying P .

Proof. As with the proof of Lemma 29 we work with n - μ CPDA instead of n -CPDA, as permitted by Theorem 50. In fact we begin the construction of $\mathcal{A}^{\downarrow\mu}$ (the μ CPDA meeting the requirements that can then be translated to the CPDA \mathcal{A}^\downarrow) in exactly the same way as $\mathcal{A}^{\uparrow\mu}$ from Lemma 29. We further add an edge q for each $q \in Q$ that transitions to control-state q without altering the stack; a pop_n edge performing a pop_n operation without altering the control-state; and a $\mathbf{destroy}_n$ edge for every ϵ -edge performing a $collapse$ on an n -link or a pop_n operation, making the same transition as the ϵ -edge.

We can define the property $\mathbf{marker}^\downarrow$ asserting that a marker has already been deployed to the top of some $(n-1)$ -stack below in L_μ :

$$\mathbf{marker}^\downarrow := \mu X.(\mathbf{marker} \vee \langle \mathbf{pop}_n \rangle X)$$

For each predicate $P \in \Pi$ the following μ -calculus ψ_{P^\downarrow} sentence defines the required predicate P^\downarrow . It asserts reachability whilst making sure the final result is an ϵ -fall by deploying the marker every time we make a \mathbf{push}_n operation, thereby enforcing that we should eventually descend below the marker:

$$\begin{aligned} \psi_{P^\downarrow} := & \mu X.(((P \wedge \neg \mathbf{marker}^\downarrow) \\ & \vee \langle \mathbf{destroy}_n \cup \langle \epsilon_{<n} \rangle X \\ & \vee (\neg \mathbf{marker}^\downarrow \wedge \langle \mathbf{deployMarker} \rangle \langle \epsilon_{\mathbf{push}_n} \rangle X) \\ & \vee (\mathbf{marker}^\downarrow \wedge \langle \epsilon_{\mathbf{push}_n} \rangle X))) \end{aligned}$$

Note that some stacks during the run asserted to exist by ψ_{P^\downarrow} may contain multiple markers at one time (unlike with \mathcal{A}^\uparrow). With \mathcal{A}^\uparrow we were concerned about knowing when we return to exactly the same stack, whereas here we just want to make sure that we do not stop until we have returned to the last stack at which we performed a \mathbf{push}_n (in order to get an ϵ -fall). ◀

Lemma 33

Let (q, s) and (q', s') be two configurations of a CPDA \mathcal{A} and let $(q, L(s))$ and $(q', L(s'))$ be the corresponding configurations in $\mathcal{A}^{\uparrow\downarrow}$ via the strong isomorphism. Then $(q, s) \mathbf{r}_{\epsilon^* a}(q', s')$ just in case $(q, L(s)) \mathbf{b}_a L(q', L(s'))$.

Proof. Suppose first that $(q, L(s)) \mathbf{b}_a(q', L(s'))$. Then by definition there must be an ϵ -fall from $(q, L(s))$ to some configuration $(q'', L(s''))$ in $\mathcal{A}^{\uparrow\downarrow}$ such that $(q'', L(s'')) \mathbf{r}_{r_\epsilon^* a}^\uparrow(q', L(s'))$. But the latter implies $(q'', L(s'')) \mathbf{r}_{\epsilon^* a}^\uparrow(q', L(s'))$ and so there is an $\epsilon^* a$ path in $\mathcal{A}^{\uparrow\downarrow}$ from $(q, L(s))$ to $(q', L(s'))$. But this uses edges inherited from the original \mathcal{A} and so $(q, s) \mathbf{r}_{\epsilon^* a}(q', s')$ in \mathcal{A} .

Conversely suppose that $(q, s) \mathbf{r}_{\epsilon^* a}(q', s')$ in \mathcal{A} . This must be witnessed by a run and we may take the right-most element (q'', s'') in the run such that $\mathbf{pop}_n(s'') \sqsubseteq_n \mathbf{pop}_n(t)$ for stacks t to the left of s'' in the run. This is the ‘lowest point’ the n -stack reaches in the run. By definition of ϵ -fall we have an ϵ -fall from (q, s) to (q'', s'') . By Lemma 29 we must also have $(q'', L(s'')) \mathbf{r}_{r_\epsilon^* a}^\uparrow(q', L(s'))$ in $\mathcal{A}^{\uparrow\downarrow}$ since $\mathbf{pop}_n(s'') \sqsubseteq_n \mathbf{pop}_n(s')$ (due to it being the lowest point in the run). We thus have the required bounce. ◀

B.2 Link Trails: Towards Link Elimination for n_n -CPDA

Lemma 36

Consider two *constructible* n -stacks s and s' with $\mathbf{stripln}(s) = \mathbf{stripln}(s')$. Assume for every stack or atomic element a contained within s and corresponding element a' in s' we have $\mathbf{col}(a) = \mathbf{col}(a')$. Then $s = s'$.

Proof. Suppose for contradiction that despite the conditions holding we have $s \neq s'$. Since $\mathbf{stripln}(s) = \mathbf{stripln}(s')$ the difference must be entirely down to a discrepancy in n -links. Since colouring determines which atomic elements are the source of a link (those not coloured \perp) it must, more specifically, be down to a discrepancy in the target of a link emanating from a particular atomic element. Let a be the lowest atomic element in s (with corresponding element a' in s') such that the

n -link from a and the n -link from a' have different targets. By assumption of a being the lowest such element we must have $s_{<a} = s'_{<a'}$.

Suppose for contradiction that neither a nor a' were produced by a $push_1^{a,n}$ or $push_1^{a',n}$ operation. Since s and s' are both constructible, there must be a sequence of stack operations constructing s and s' . Let i be the order of the last $push_i$ operation that occurs in this sequence for s that creates the position a and after which the position a is never discarded. Let i' be similar for s' and a' . So $i \geq 2$ and $i' \geq 2$. Note that since $s_{<a} = s'_{<a'}$ it must in particular be the case $top_i(pop_i(s_{<a})) = top_i(pop_i(s'_{<a'}))$ and indeed that $top_{i'}(pop_{i'}(s_{<a})) = top_{i'}(pop_{i'}(s'_{<a'}))$. Thus the $push_i$ and $push_{i'}$ operations must both create an a and a' that is a copy of an element with the same link. This is a contradiction since we are assuming a and a' have different targets.

So w.l.o.g. assume that a is produced by a $push_i$ operation whilst a' is produced by a $push_1^{a',n}$ operation. Let t_j be the j -stack containing position a (in s) and t'_j be the j -stack containing a' (in s') for $1 \leq j \leq i - 1$. By assumption we have $\mathbf{col}(t_j) = \mathbf{col}(t'_j)$ for each j . It will be helpful to further define $t_0 := a$ and $t'_0 = a'$.

We now argue by induction that for all $0 \leq j < n - 1$ it is the case that $\mathbf{col}(t_j) = \mathbf{col}(t'_j) = c_>$ and that there is no freshly created n -link (i.e. n -link from an element b such that $l_r(b) = 1$) in t_{j+1} .

For the base case take $j = 0$. It must be the case that $\mathbf{col}(a) = \mathbf{col}(a') = c_>$ since the only other option is $c_=-$ which is impossible since $l_a(a) \neq l_a(a')$. Since any n -link above a' in t'_1 must share the target of a' (as it would be another freshly created link in the same n -stack) it follows that these would also have colour $c_=-$. This means that there can be no freshly created n -links above a in t_1 since these would have colour $c_>$ which would not match the corresponding colour in t'_1 . There can be no freshly created n -links below a in t_1 as a is not freshly created and so any stack containing such an n -link below a would not be constructible.

For the induction step consider $j > 0$. We have $\mathbf{col}(t_j) = \mathbf{col}(t'_j)$ by assumption. We also assume as part of the induction hypothesis that t_j contains no freshly created n -link. Suppose that there is a freshly created n -link in a j -stack below t_j in t_{j+1} . Then there must be a corresponding freshly created n -link in t'_{j+1} below t'_j (from the assumption that a and a' form the lowest n -link discrepancy in s and s'). It follows that $\mathbf{col}(t'_j) = c_=-$ (since t'_j also contains a fresh n -link) and so by equality of colouring $\mathbf{col}(t_j) = c_=-$. But due to the fact that t_j contains no freshly-created n -link we would also have $\mathbf{col}(t_j) = c_<$, a contradiction. Thus there is no freshly created n -link below t_j in t_{j+1} . If there is a freshly created n -link in t_{j+1} above t_j then there must be a lowest j -stack u_j containing such a link. But then $\mathbf{col}(u_j) = c_>$ since there are no freshly created n -links below it in t_{j+1} . So the corresponding j -stack u'_j in t'_j must also have $\mathbf{col}(u'_j) = c_>$. But this is impossible since there is a freshly created n -link in t'_j and so $\mathbf{col}(u'_j) \in \{c_<, c_=-\}$. It follows that there is no freshly created n -link in t_{j+1} .

Now observe that $\mathbf{col}(t'_j) = c_>$ since from the paragraph above no fresh n -links can occur below it in t'_{j+1} . Thus we also have $\mathbf{col}(t_j) = c_>$. We have thus established the induction hypothesis.

Recall that the position a was produced by a $push_i$ operation for $2 \leq i \leq n$. Suppose first that $2 \leq i < n$. The result above tells us that $\mathbf{col}(t_{i-1}) = c_>$ but also that t_{i-1} contains no fresh n -links. This is a contradiction since the only way an $(i - 1)$ -stack derived from a copy of the $(i - 1)$ -stack below it could contain a link with a higher target is if it creates a fresh link.

Now suppose that $i = n$. We know from the induction hypothesis that t_{n-1} contains no fresh n -link. Thus we have $\mathbf{col}(t_{n-1}) \in \{c_=-, c_<\}$. But since t'_{n-1} does contain a fresh n -link we must have $\mathbf{col}(t'_{n-1}) = c_>$. Thus $\mathbf{col}(t_{n-1}) \neq \mathbf{col}(t'_{n-1})$, which is the required contradiction. ◀

The next step is to show how a CPDA can dynamically assign colours to its stacks correctly. We restrict ourselves to automata that *only* have n -links so that the only way to destroy internal stacks is using a higher-order *pop* operation. Let s be an n_n -CPD stack over the alphabet Γ . We define the

colour tracking stack $\mathbf{colTr}(s)$ to be the stack over the alphabet:

$$\Gamma \times \{ \perp, c_-, c_+ \} \times \prod_{i=0}^{n-2} \{ c_-, c_+, c_+ \}^{n-1-i} \cup [1..(n-1)] \times \{ c_-, c_+, c_+ \}$$

We construct $\mathbf{colTr}(s)$ from s by first replacing each atomic element a in s with an element

$$(a, c_0, (b_1^0, \dots, b_{n-1}^0), (b_2^1, \dots, b_{n-1}^1), \dots, (b_{n-1}^{n-2}))$$

where:

- $c_0 := \mathbf{col}(a)$
- $b_j^0 \in \{ c_-, c_+ \}$ for $1 \leq j \leq n-1$ just in case a sources an n -link and one of the following holds:
 - $\mathbf{col}(top_{j+1}(s_{\leq a})) = c_+$ but $\mathbf{col}(top_{j+1}(s_{< a})) \neq c_+$ in which case $b_j^0 = \mathbf{col}(top_{j+1}(s_{< a}))$.
 - There is another atomic element a' anywhere below a in $top_{j+1}(s_{\leq a})$ also sourcing an n -link such that $l_a(a') = l_a(a)$ and such that $\mathbf{col}(top_{j+1}(s_{\leq a})) = c_+$ but $\mathbf{col}(top_{j+1}(s_{< a})) = b_j^0 \neq c_+$.
- $b_j^0 = c_+$ otherwise.
- For each $1 \leq i \leq n-2$ let $s_i := top_{i+1}(s_{\leq a})$. Then for each $i < j \leq n-1$ we have $b_j^i \in \{ c_-, c_+ \}$ just in case one of the following holds:
 - $\mathbf{col}(s_i) = c_+$ but $\mathbf{col}(top_{j+1}(s_{< s_i})) = b_j^i \neq c_+$
 - There is another i -stack s'_i occurring anywhere below s_i in $top_{j+1}(s_{< s_i})$ such that $l_a(s'_i) = l_a(s_i)$ and $\mathbf{col}(s'_i) = c_+$ but $\mathbf{col}(top_{j+1}(s_{< s'_i})) = b_j^i \neq c_+$.
- $b_j^i = c_+$ otherwise.

We finish the construction of $\mathbf{colTr}(s)$ by adding a decoration $(i, \mathbf{col}(s_i))$ on top of each i -stack s_i in s for $1 \leq i \leq n-1$.

The idea is that each component stack of s is annotated with its colour and the additional decorations provide the necessary information to determine how a stack operation affects the colours.

► **Lemma 51.** *Let s be an n_n -stack over an alphabet Γ . Suppose that for $0 \leq k < k' \leq n-1$ we have $\mathbf{col}(top_{i+1}(s)) = c_+$ for every i with $k \leq i < k'$. Then there is no k -stack s_k strictly below $top_{k+1}(s)$ in $top_{k'+1}(s)$ such that $l_a(s_k) \geq l_a(top_{k+1}(s))$.*

Proof. First we claim that $l_a(top_{i+1}(s)) = l_a(top_{k+1}(s))$ for $k \leq i \leq k'$. To see this argue by induction on i (for $k \leq i \leq k'$). The base case is trivial (since $i = k$). For the induction step note that since $\mathbf{col}(top_{i+1}(s)) = c_+$ it must be that $l_a(top_{i+1}(s))$ is greater than $l_a(s_i)$ for any i -stack s_i below $top_{i+1}(s)$ in $top_{i+2}(s)$. It then follows by definition that $l_a(top_{i+2}(s)) = l_a(top_{i+1}(s)) = l_a(top_{k+1}(s))$.

It follows that for any given $k \leq i < k'$ we cannot have a k -stack s_k with $l_a(s_k) \geq l_a(top_{k+1}(s))$ below $top_{i+1}(s)$ in $top_{i+2}(s)$ since that would contradict the assumption that $top_{i+1}(s) = c_+$. This in turn implies that there is no k -stack s_k strictly below $top_{k+1}(s)$ in $top_{k'+1}(s)$ such that $l_a(s_k) \geq l_a(top_{k+1}(s))$. ◀

Hence we can use the decorations according to the following lemma:

► **Lemma 52.** *Let s be an n_n -stack over an alphabet Γ . Suppose that for $0 \leq k < k' \leq n-1$ we have $\mathbf{col}(top_{i+1}(s)) = c_+$ for every $k \leq i < k'$. Suppose further that s' is an n_n -stack such that $pop_{k+1}(\mathbf{colTr}(s)) = pop_{k+1}(\mathbf{colTr}(s'))$ but where $top_{k+1}(s') \neq c_+$. Then where*

$$top_1(\mathbf{colTr}(s)) = (a, c_0, (b_1^0, \dots, b_{n-1}^0), (b_2^1, \dots, b_{n-1}^1), \dots, (b_{n-1}^{n-2}))$$

we have:

$$\mathbf{col}(top_{k'+1}(s')) = \begin{cases} b_{k'}^k & \text{if } \mathbf{col}(top_{k'+1}(s)) = c_{>} \\ c_{<} & \text{otherwise} \end{cases}$$

Proof. We may appeal to Lemma 51 in order to get that there is no k -stack s_k below $top_{k+1}(s)$ in $top_{k'+1}(s)$ such that $l_a(s_k) = l_a(top_{k+1}(s))$. Moreover we must have $l_a(top_{k'+1}(s')) = l_a(s_{<top_{k+1}(s)})$ due to the fact that $\mathbf{col}(top_{k'+1}(s')) \neq c_{>}$ but s and s' are equal everywhere below $top_{k'+1}(s')$. In the case when $\mathbf{col}(top_{k'+1}(s')) = c_{>}$ the definition of $b_{k'}^k$ thus implies that $\mathbf{col}(top_{k'+1}(s')) = b_{k'}^k$.

Consider now the only other case when $\mathbf{col}(top_{k'+1}(s)) \in \{c_{=}, c_{<}\}$. Again by Lemma 52 we know that $l_a(top_{k+1}(s))$ is strictly greater than $l_a(s_k)$ for any k -stack below it in $top_{k'+1}(s)$. We also know that $l_a(top_{k+1}(s')) < l_a(top_{k+1}(s))$ due to colouring. Thus we can conclude that $l_a(top_{k'+1}(s')) < l_a(top_{k'+1}(s))$ meaning that $\mathbf{col}(top_{k'+1}(s')) = c_{<}$. ◀

It is also helpful to be able to use colour annotations to recover which stacks contain fresh links.

► **Lemma 53.** *Let s be an n_n -stack. Then for each $2 \leq i \leq n$, the stack $top_i(s)$ contains an n -link from an atom a with $l_r(a) = 1$ iff $\mathbf{col}(top_n(s)) = c_{>}$ and additionally for each j such that $i \leq j < n$ we have $\mathbf{col}(top_j(s)) \in \{c_{=}, c_{>}\}$.*

Proof. First suppose that $top_i(s)$ contains an n -link from an atom a with $l_r(a) = 1$. Since no link in the $(n-1)$ -stack below can source a link with the same target, we must have $\mathbf{col}(top_n(s)) = c_{>}$. Moreover, no link in the $top_n(s)$ stack can have a target above that of a . Since $top_i(s)$ contains a , $top_j(s)$ must contain a for $i \leq j < n$ and so $\mathbf{col}(top_j(s)) \in \{c_{=}, c_{>}\}$, as required.

Now suppose that the right-hand-side of the ‘iff’ holds. Since $\mathbf{col}(top_n(s)) = c_{>}$ the top_n stack must contain a fresh n -link as all other n -links in the top_n stack would have been created and so exist in an n -stack below it. Suppose for contradiction that $top_i(s)$ does not contain a fresh n -link. Then there must be a maximum j with $i < j \leq n-1$ such that $top_j(s)$ does not contain a fresh n -link. But since top_n does contain a fresh n -link there must exist an n -link below $top_j(s)$ in $top_{j+1}(s)$ whence we would have $\mathbf{col}(top_j(s)) = c_{<}$, a contradiction. ◀

The following Lemma tells us that we can preserve the correct annotations whilst manipulating an n_n -stack. Unfortunately we do not have a version of this Lemma for n -stacks containing links of other orders.

► **Lemma 54.** *Let s be an n_n -stack over an alphabet Γ and let θ be an n -stack operation. There then exists a compound stack operation θ' such that $\mathbf{colTr}(\theta(s)) = \theta'(\mathbf{colTr}(s))$ —i.e. θ' could be implemented by an n_n -CPDA. Moreover the number of operations in θ' is bounded.*

Proof. Consider each possible θ in turn.

If it is a $push_1$ operation, then if no link is attached, no colour is affected. We can thus just pop off the colour annotations on top of the stack (which are bounded in number), and push

$$(a, \perp, (b_1^0, \dots, b_{n-1}^0), (b_2^1, \dots, b_{n-1}^1), \dots, (b_{n-1}^{n-2}))$$

on the stack with colour \perp where $b_j^0 := c_{>}$ for all $1 \leq j \leq n-1$ and for each $1 \leq i < j \leq n-1$ we set b_j^i to be the b_j^i from the previous top_1 element on the stack (since this new element has no affect on any colour).

If it is a $push_1^{a,n}$ operation, then again we first pop off the colour annotations on top of the stack. In the light of Lemma 53 these colour annotations allow us to deduce the set $F \subseteq [2..n]$ of elements i such that $top_i(s)$ contains a fresh n -link. The colour of any top_i -stack with $i \in F$ is unchanged

since they already contain a link with the highest possible target. The colour of top_i -stacks with $i \notin F$ (with $i \in [1..n]$) are set as follows (which do not necessarily but may result in a change of colour):

- if $i + 1 \in F$ then a stack below $top_i(s)$ in $top_{i+1}(s)$ already contains a link and so the new colour of the new top_i stack is $c_=_$.
- otherwise this is the first fresh link and so the new top_i stack has colour $c_>$.

Note that this ensures the colour c_0 of the new atomic element to be created is either $c_=_$ or $c_>$ depending on whether there already exists a fresh link below it in the top_2 stack. The actual element being pushed onto the stack has the form:

$$(a, c_0, (b_1^0, \dots, b_{n-1}^0), (b_2^1, \dots, b_{n-1}^1), \dots, (b_{n-1}^{n-2}))$$

For all $i \in F$ and all j with $i < j \leq n$ we have b_{j-1}^{i-1} set to the b_{j-1}^{i-1} from the previous top_1 element (as discarding the top_i ($i-1$)-stack is no different to before if it already contained a fresh link). For all $i, j \notin F$ and j with $1 \leq i < j \leq n$ we set b_{j-1}^{i-1} to be the colour of the top_j ($j-1$)-stack prior to pushing the new element on the stack. This is correct since discarding top_i for $i \in F$ will eliminate the newly added fresh n -link, which is the only fresh n -link in both the top_j stack thereby returning the top_j colour to that which it was before it was added. Note that it is impossible for $j \notin F$ but $i \in F$ since $i < j$ and so all cases are covered.

If it is a $push_k$ operation for $2 \leq k \leq n$, then we discard all colour annotations (i, c_i) on top of the top_{i+1} stack for $i \geq k$, perform a $push_k$ operation changing the colour annotation on top of the resulting top-most $k-1$ stack to $(k-1, c_=_)$ and replacing all of the previously discarded decorations unchanged. The colour annotations on i -stacks for $i > k-1$ will remain correct as no new links are created and those on i -stacks for $i < k-1$ will remain correct as they depend only on what was copied in its entirety by the $push_k$ operation.

Observe how none of the b_j^i values of atomic elements in the copied stack need changing. Overloading the notation a consider an atom

$$a := (a, c_0, (b_1^0, \dots, b_{n-1}^0), (b_2^1, \dots, b_{n-1}^1), \dots, (b_{n-1}^{n-2}))$$

occurring in the newly created $(k-1)$ -stack. For each i, j with $i < j < k-1$ note that $top_{j+2}(push_k(\mathbf{colTr}(s))_{\leq a})$ is a copy of a $(j+1)$ -stack in the $(k-1)$ -stack below. Since the meaning of b_j^i is completely determined by the $(j+1)$ -stack in which it resides, this remains correct. For $i < j = k-1$ we have it that s_i is a copy of some stack s'_i below it in the $top_{j+2}(push_k(\mathbf{colTr}(s))_{\leq a}) = top_{k+2}(push_k(\mathbf{colTr}(s))_{\leq a})$ ($j+1$)-stack (so in particular $l_a(s_i) = l_a(s'_i)$). But s'_i would have existed prior to performing $push_k$ and must also contain an atom annotated with b_j^i and so b_j^i must be a correct annotation. For $j > k-1$ (and $i < j$ as usual) we have the case $i \leq k-1$, which implies that $top_{i+1}(push_k(\mathbf{colTr}(s))_{\leq a})$ is a copy of an i -stack below it in its $(j+1)$ -stack, and also the case $i > k-1$ in which case the conditions remain unchanged to before the $push_k$ operation—in particular $push_k$.

If it is a pop_k operation for $k < n$, then first discard all of the decorations from the stack associated with the top_i stack for $k \leq i \leq n$. If $k = 1$ and the top element of the stack is now a linkless element for some a , then we can just pop_1 it off without affecting the colour and restore the decorations unchanged. Otherwise we must be able to see the colour of the top_k stack (even when $k = 1$). If the top_k stack has colour $c_=_$ or $c_<$ then discarding it will not change any other colours and so we simply perform pop_k and restore the previously discarded decorations unchanged. If the top_k stack has colour $c_>$, then again we perform pop_k but we also need to recompute the colours for the top_i stack where $k < i \leq n$ and amend the previously discarded colour decorations accordingly when restoring them. Let $k < l \leq n-1$ be the least $l > k$ such that either $l = n-1$ or else $\mathbf{col}(top_{l+1}(s)) \neq c_>$. We can make use of Lemma 52 to soundly set the colour of

$top_{j+1}(pop_k(\mathbf{colTr}(s)))$ to b_j^{k-1} for $k < j < l$. If $top_{l+1} = c_>$ then Lemma 52 allows us to set its new colour to b_l^{k-1} , if $top_{l+1} \in \{c_<, c_=\}$ then the same lemma tells us to set it to $c_<$.

There is no need to adjust the colour of stacks above l ; either there are no stacks outside of l that have a colour assignment (i.e. when $l = n-1$) or else for $j > l$ we have $\mathbf{col}(top_{j+1}(pop_k(\mathbf{colTr}(s)))) = \mathbf{col}(top_{j+1}(\mathbf{colTr}(s)))$ since $\mathbf{col}(top_{l+1}(\mathbf{colTr}(s))) \in \{c_<, c_=\}$.

If it is a pop_n operation or a *collapse* operation (which must be on an n -link) we do not need to do anything special as all decorations will be accurate. For the *collapse* we just need to pop_1 down to the element on which to collapse. ◀

Lemma 37

Let \mathcal{A} be an n_n -CPDA. Then there exists an n_n -CPDA $\mathbf{lum}(\mathcal{A})$ such that $\mathcal{G}^\epsilon(\mathbf{lum}(\mathcal{A})) \cong \mathcal{G}^\epsilon(\mathcal{A})$ and further such that for any reachable configurations $(q, s), (q, s')$ of $\mathbf{lum}(\mathcal{A})$ we have $s = s'$ iff $\mathbf{stripln}(s) = \mathbf{stripln}(s')$.

Proof. We define $\mathbf{lum}(\mathcal{A})$ to be the n_n -CPDA that replaces all operations of \mathcal{A} generating an a -edge with a compound operation from Lemma 54 where the compound generates a path of the form ϵ^*a . Since $\mathbf{colTr}(s)$ for any stack s includes an annotation of the colour of each constituent stack, Lemma 36 ensures that $s = s'$ iff $\mathbf{stripln}(s) = \mathbf{stripln}(s')$ for any stacks s and s' reachable by $\mathbf{lum}(\mathcal{A})$. The predicates for $\mathbf{lum}(\mathcal{A})$ are induced by those for \mathcal{A} by projecting the stack alphabet and control-states of $\mathbf{lum}(\mathcal{A})$ onto those of \mathcal{A} . ◀

B.3 Meta-Annotations

► **Definition 55.** Fix $k \in \mathbb{N}$ and let \mathcal{A} be an n_n -CPDA with control-states Q and edge-labels in Σ . A k -meta-annotation for \mathcal{A} is a $|\Sigma|.k$ -tuple $((Q_1^a)_{a \in \Sigma}, \dots, (Q_k^a)_{a \in \Sigma})$ where each component is a subset of Q .

Given an n_n -CPDA \mathcal{A} and $k \in \mathbb{N}$ the n -PDA $\mathbf{GrStripln}_k(\mathcal{A})$ is formed using the following recipe:

- Take the n_n -CPDA $\mathbf{lum}(\mathcal{A})$ and modify it so that a single k -meta-annotation $((Q_1^a)_{a \in \Sigma}, \dots, (Q_k^a)_{a \in \Sigma})$ is kept at the top of every $(n-1)$ -stack. No restriction is placed on what this may be (it is non-deterministically chosen from amongst all k -meta-annotations). We add a predicate $\mathbf{Met}(((Q_1^a)_{a \in \Sigma}, \dots, (Q_k^a)_{a \in \Sigma}))$ holding at all configurations with the corresponding meta-annotation on top together with a predicate $\mathbf{Met}(q, ((Q_1^a)_{a \in \Sigma}, \dots, (Q_k^a)_{a \in \Sigma}))$ additionally asserting that the automaton is in control-state q . Unary predicates are inherited directly from \mathcal{A} on the basis of control-state and stack symbol immediately below the meta-annotation. Call this n_n -CPDA $\mathbf{lum}(\mathcal{A})_k^+$.
- Let $\mathbf{GrStripln}_k(\mathcal{A})^-$ be the automaton $\mathbf{lum}(\mathcal{A})_k^{+\uparrow\downarrow}$.
- Finally $\mathbf{GrStripln}_k(\mathcal{A})$ is $\mathbf{GrStripln}_k(\mathcal{A})^-$ restricted to edges that do not perform a *collapse* or a pop_n operation, and we remove all links. Thus $\mathbf{GrStripln}_k(\mathcal{A})$ is an n -PDA. We further add an edge **stackComp** from each configuration (q, s) to a configuration $(s?, s)$ for a distinguished control-state $s?$. This allows stacks from different configurations to be manipulated and compared without prejudice to their control-states. Also add an edge labelled p for every $p \in Q$ such that for any control-state \hat{q} of $\mathbf{GrStripln}_k(\mathcal{A})$ and control-state \hat{p} corresponding to p we have $(\hat{q}, s)p(\hat{p}, s)$. Add an edge pop_n from each (q, s) to $(q, pop_n(s))$.

Let us break down each stage of this construction. We need to classify the stacks for which the k -meta-annotations are considered ‘correct’—something that $\mathbf{lum}(\mathcal{A})_k^+$ has no control over itself—it is a constraint imposed from the outside. Indeed correctness is only defined for k -tuples of configurations since every meta-annotation references reachability to each of k different configurations. This correctness property is known as *consistency*.

► **Definition 56.** Let $(q_1, s_1), \dots, (q_k, s_k)$ be reachable configurations of $\mathbf{lum}(\mathcal{A})_k^+$. Then we say that this k -tuple of configurations is *consistent* just in case the following conditions are met:

- For each i with $1 \leq i \leq k$ it is the case that each $(n-1)$ -stack in s_i contains precisely one meta-annotation, which must occur on top of it.
- Suppose that $t \sqsubseteq_n s_i$ for some $1 \leq i \leq k$. Then the meta-annotation on top of $\mathit{top}_n(t)$ must be $((Q_1^a)_{a \in \Sigma}, \dots, (Q_k^a)_{a \in \Sigma})$ where for each $1 \leq j \leq k$:

$$Q_j^a := \{ q \in Q : (q, t) \mathbf{r}_{\epsilon^* a}^\dagger (q_j, s_j) \}$$

Note that $Q_j^a = \emptyset$ if there is no $\epsilon^* a$ -climb from any configuration (q, t) to (q_j, s_j) , which in particular is the case if $\mathit{pop}_n(t) \not\sqsubseteq_n s_j$.

Now let L be the map from $\mathbf{lum}(\mathcal{A})^+$ -stacks to $\mathbf{GrStripln}_k(\mathcal{A})^-$ -stacks witnessing the strong isomorphism $\mathcal{G}^\epsilon(\mathbf{lum}(\mathcal{A})^+) \cong \mathcal{G}^\epsilon(\mathbf{GrStripln}_k(\mathcal{A})^-) \upharpoonright_{\Pi, \Sigma}$, where Π and Σ are the unary predicates and edge labels from $\mathbf{lum}(\mathcal{A})^+$. So if (q, s) is a node of $\mathcal{G}^\epsilon(\mathbf{lum}(\mathcal{A})^+)$, the corresponding node in $\mathcal{G}^\epsilon(\mathbf{GrStripln}_k(\mathcal{A})^-)$ is $(q, L(s))$. Note further that since $\mathbf{GrStripln}_k(\mathcal{A})^-$ is monotonic, deleting destructive transitions will not change the set of reachable configurations. Thus $(q, \mathbf{stripln}(L(s)))$ is also a reachable configuration of $\mathcal{G}^\epsilon(\mathbf{GrStripln}_k(\mathcal{A}))$. By Lemma 37 $L(s)$ is completely determined by $\mathbf{stripln}(L(s))$, and so for notational convenience we drop the $\mathbf{stripln}()$ and view $(q, L(s))$ as the ‘configuration of $\mathcal{G}^\epsilon(\mathbf{GrStripln}_k(\mathcal{A}))$ corresponding to (q, s) ’.

► **Lemma 57.** For each $k \in \mathbb{N}$ and n_n -CPDA \mathcal{A} , there exists an MSO formula $\mathbf{con}(x_1, x_2, \dots, x_k)$ such that reachable configurations $(q_1, s_1), \dots, (q_k, s_k)$ of $\mathbf{lum}(\mathcal{A})^+$ are consistent just in case:

$$\mathbf{GrStripln}_k(\mathcal{A}) \models \mathbf{con}((q_1, L(s_1)), \dots, (q_k, L(s_k)))$$

and such that for every i with $1 \leq i \leq k$, $\mathbf{GrStripln}_k(\mathcal{A}) \models \mathbf{con}(c_1, \dots, c_k)$ implies that $c_i = (q, L(s))$ for some reachable configuration (q, s) of $\mathbf{lum}(\mathcal{A})^+$.

Proof. First observe that for $\mathbf{lum}(\mathcal{A})_k^+$ configurations (q, s) and (q', s') with corresponding $\mathbf{GrStripln}_k(\mathcal{A})$ configurations $x = (q, L(s))$ and $y = (q', L(s'))$ we can MSO-define $s \sqsubseteq_n s'$ in $\mathcal{G}(\mathbf{GrStripln}_k(\mathcal{A}))$ using a standard least fixed-point construction:

$$x \sqsubseteq_n y := \exists X. (\exists x'. x \mathbf{stackComp} x') (\exists y'. y \mathbf{stackComp} y'). \\ (x' \in X \wedge \phi_{\sqsubseteq_n}(X, y') \wedge \forall Y. (\phi_{\sqsubseteq_n}(Y, y') \rightarrow X \subseteq Y))$$

where

$$\phi_{\sqsubseteq_n}(X, x', y') := \forall z. (z \in X \leftrightarrow (z = y' \vee (\exists z' \in X). z' \mathbf{pop}_n z))$$

We do indeed have $s \sqsubseteq_n s'$ iff $L(s) \sqsubseteq_n L(s')$ since strong isomorphisms preserve stack structure.

We additionally need a way of capturing the configurations of $\mathbf{GrStripln}_k(\mathcal{A})$ that correspond to the reachable configurations of $\mathbf{lum}(\mathcal{A})^+$, namely those monotonically generated by $\mathbf{GrStripln}_k(\mathcal{A})^-$:

$$\mathbf{R}(x) := \exists X. \exists x'. (x' \in X \wedge \phi_{\mathbf{R}}(X) \wedge \forall Y. (\phi_{\mathbf{R}}(Y) \rightarrow X \subseteq Y) \wedge \bigvee_{a \in \Sigma} x' a x)$$

where

$$\phi_{\mathbf{R}}(X) := \forall z. (z \in X \leftrightarrow (z = c_0 \vee (\exists z' \in X). (z' \mathbf{r}_{\epsilon} z \vee \bigvee_{a \in \Sigma \cup \{\epsilon\}} z' a z)))$$

where c_0 is the initial configuration. Using a standard least-fixed-point construction, $\mathbf{R}(x)$ defines those configurations of $\mathbf{GrStripln}_k(\mathcal{A})$ reachable via an $(r_\epsilon + \Sigma + \epsilon)^* \Sigma$ -labelled path. By Remark B.1.0.1 these are precisely the configurations of $\mathbf{GrStripln}_k(\mathcal{A})$ corresponding to those in

$\mathbf{lum}(\mathcal{A})^+$, noting that no r_ϵ -edge is deleted in forming $\mathbf{GrStripln}_k(\mathcal{A})$ from $\mathbf{GrStripln}_k(\mathcal{A})^-$ since the latter is monotonic via r_ϵ . Also note that our w.l.o.g. assumption that all Σ -labelled edges perform an order- $(n-1)$ operation prevents any Σ -labelled edge from being deleted.

For $\mathbf{lum}(\mathcal{A})_k^+$ configurations (q, s) and (q', s') with corresponding $\mathbf{GrStripln}_k(\mathcal{A})$ configurations $x = (q, L(s))$ and $y = (q', L(s'))$ we can MSO-define $(q, s)r_{\epsilon^*a}^\dagger(q', s')$ for $a \in \Sigma$ in $\mathcal{G}(\mathbf{GrStripln}_k(\mathcal{A}))$ with the ϵ^*a -climb interpreted over $\mathbf{lum}(\mathcal{A})^+$ by defining $xr_{\epsilon^*a}^\dagger y$ in $\mathcal{G}(\mathbf{GrStripln}_k(\mathcal{A}))$. These two are equivalent due to Lemma 29 together with the w.l.o.g. assumption that all Σ -labelled operations are order- $(n-1)$.

$$xr_{\epsilon^*a}^\dagger y := xr_{r_\epsilon^*a} y := \exists X. (\exists y'. y' a y). (y' \in X \wedge \phi_{r_{r_\epsilon^*}}(X, x) \wedge \forall Y. (\phi_{r_{r_\epsilon^*}}(Y, x) \rightarrow X \subseteq Y))$$

where

$$\phi_{r_{r_\epsilon^*}}(X, x) := \forall z. (z \in X \leftrightarrow (z = x \vee (\exists z' \in X). z' r_\epsilon z))$$

We define a predicate **meta** asserting that a configuration has a meta-annotation on top:

$$\mathbf{meta}(x) := \bigvee_{m \in M} \mathbf{Met}(m)(x)$$

where M is the set of meta-annotations. We also define the following predicates that can be used to express some basic properties about the meta-annotation on top of a stack:

$$[q \in Q_i^a](x) := \bigvee_{\substack{m = ((Q_1^a)_{a \in \Sigma}, \dots, (Q_k^a)_{a \in \Sigma}) \in M \\ q \in Q_i^a}} \mathbf{Met}(m)(x)$$

for each $1 \leq i \leq k$, $a \in \Sigma$ and $q \in Q$. We can now read off the definition of consistency to define:

$$\mathbf{con}(x_1, x_2, \dots, x_k) := \forall x. \left(\bigvee_{i=1}^k x \sqsubseteq_n x_i \right) \rightarrow \mathbf{meta}(x) \wedge \bigwedge_{\substack{1 \leq i \leq k \\ a \in \Sigma, q \in Q}} [q \in Q_i^a](x) \leftrightarrow \exists y. (\mathbf{R}(y) \wedge x q y \wedge y r_{\epsilon^*a}^\dagger x_i)$$

◀

► **Lemma 58.** *Let \mathcal{A} be an n -CPDA with stack-alphabet Γ . For every quantifier free formula $\phi(x_1, \dots, x_k)$ in **FO** and configurations $(q_1, s_1), \dots, (q_k, s_k)$ in $\mathcal{G}^\epsilon(\mathcal{A})$:*

$$\mathcal{G}^\epsilon(\mathcal{A}) \models \phi((q_1, s_1), \dots, (q_k, s_k)) \Leftrightarrow \mathcal{G}^\epsilon(\mathbf{lum}(\mathcal{A})_k^+) \models \phi((q_1, t_1), \dots, (q_k, t_k))$$

whenever $(q_1, t_1), \dots, (q_k, t_k)$ are consistent reachable configurations of $\mathbf{lum}(\mathcal{A})_k^+$ and $\pi_\Gamma(t_i) = s_i$ for each $1 \leq i \leq k$.

Moreover for every set of \mathcal{A} configurations $(q_1, s_1), \dots, (q_k, s_k)$ there exists a consistent set of reachable configurations $(q_1, t_1), \dots, (q_k, t_k)$ of $\mathbf{lum}(\mathcal{A})_k^+$ such that $\pi_\Gamma(t_i) = s_i$ for each $1 \leq i \leq k$.

Proof. For the first part argue by induction on the structure of ϕ . For the base case note that unary predicates are inherited directly from \mathcal{A} and the fact we are considering ϵ -closure ensures that binary relations are also directly inherited, despite the additional steps of maintaining meta-annotations. For

equality we must appeal to consistency. The Q_i^a component of any meta-annotation m contained in one of the t_j is uniquely determined by (q_i, s_i) (or indeed by (q_i, t_i)) and $t_j \leq m$ by definition of consistency. Thus for any $1 \leq i, j \leq k$ we will have $(q_i, t_i) = (q_j, t_j)$ just in case $s_i = s_j$.

Conjunction and negation are straightforward applications of the induction hypothesis.

The second part is immediate from the fact that we just need to choose Q_i^a for each meta-annotation to be the unique set specified by (q_i, s_i) . ◀

► **Lemma 59.** *Let \mathcal{A} be an n -CPDA. For every Σ_1 sentence ϕ in **FO** we can construct an MSO sentence $\hat{\phi}$ such that:*

$$\mathcal{G}^\epsilon(\mathcal{A}) \models \phi \iff \mathcal{G}(\mathbf{GrStripln}_{\mathcal{A}}(k)) \models \hat{\phi}$$

Proof. Without loss of generality (due to prenex normal form) let us assume that $\phi = \exists x_1. \exists x_2. \dots \exists x_k. \phi'(x_1, \dots, x_k)$ where ϕ' is quantifier free. For each reachable configuration (q, s) of $\mathbf{lum}(\mathcal{A})_k^+$ let $(q, L(s))$ be the corresponding reachable configuration of $\mathbf{GrStripln}_{\mathcal{A}}(k)$. By Lemma 58 it suffices to construct a quantifier free MSO formula $\hat{\phi}'(x_1, \dots, x_k)$ such that for *consistent* $(q_1, s_1), \dots, (q_k, s_k)$:

$$\begin{aligned} \mathcal{G}^\epsilon(\mathbf{lum}(\mathcal{A})_k^+) \models \phi'((q_1, s_1), \dots, (q_k, s_k)) &\iff \\ \mathcal{G}(\mathbf{GrStripln}_k(\mathcal{A})) \models \hat{\phi}'((q_1, L(s_1)), \dots, (q_k, L(s_k))) & \end{aligned}$$

We can then take

$$\hat{\phi} := \exists x_1 \dots \exists x_k \left(\bigwedge_{i=1}^k \mathbf{R}(x_i) \wedge \mathbf{con}(x_1, \dots, x_k) \wedge \hat{\phi}'(x_1, \dots, x_k) \right)$$

where \mathbf{con} is the MSO formula taken from Lemma 57 and \mathbf{R} is the reachability predicate taken from the proof of Lemma 57.

We define $\hat{\phi}'$ by induction on the structure of ϕ' . The atomic cases of equality and unary predicates can have $\hat{\phi}' = \phi'$ due to the strong isomorphism between $\mathbf{lum}(\mathcal{A})_k^+$ and $\mathbf{GrStripln}_k(\mathcal{A})^-$ together with the fact that removing links does not affect equality for $\mathbf{lum}(\mathcal{A})_k^+$. Binary relations must be given a more sophisticated translation since some edges are removed in forming $\mathbf{GrStripln}_k(\mathcal{A})$. We therefore appeal to Lemma 33 telling us that $(q, s)\mathbf{a}(q', s')$ in $\mathcal{G}^\epsilon(\mathbf{lum}(\mathcal{A})_k^+)$ just in case $(q, L(s))\mathbf{b}_a(q', L(s'))$ in $\mathbf{GrStripln}_k(\mathcal{A})^-$. When $\phi'(x, y) = x\mathbf{a}x_i$ we thus express the existence of such a bounce by taking:

$$\hat{\phi}'(x, x_i) := \bigvee_{q \in Q} \bigwedge_{m \in M_{q, a}^i} (\mathbf{Met}(q, m)(x))^\downarrow$$

where Q is the set of control-states of \mathcal{A} and $M_{q, a}^i$ is the set of meta-annotations $((Q_1^a)_{a \in \Sigma}, \dots, (Q_k^a)_{a \in \Sigma})$ such that $q \in Q_i^a$.

Negation and conjunction is a trivial application of the induction hypothesis. ◀

► **Remark.** The method behind the proof of Lemma 59 does not generalise to sentences with quantifier alternation since consistency requires a k -tuple of stacks to be fixed. If one fixes a stack with an existential quantification and then endeavours to add a universal quantification, there may be some stack over which the universal quantifier ranges that does not honour the information in the meta-annotations embedded in the fixed (existentially quantified) stack.

Since $\mathbf{GrStripln}_k(\mathcal{A})$ is an n -PDA it must be the case that $\mathcal{G}^\epsilon(\mathbf{GrStripln}_{\mathcal{A}}(k))$ has decidable MSO theory [5]. Lemma 59 therefore implies:

Theorem 38

Let \mathcal{A} be an n_n -CPDA. Then the Σ_1 theory of $\mathcal{G}^\epsilon(\mathcal{A})$ is decidable.