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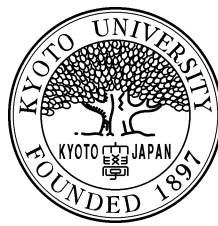
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Correctness of a Higher-Order Removal Transformation through a Relational Reasoning

by

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Abstract. The syntactic logical relations developed by Pitts are applied to show the correctness of a higher-order removal program transformation algorithm. The convenient proof method that resorts to the induction on the structure of programs does not apply because of the circular references to be introduced by the transformation. Using a variant of the syntactic logical relations, in which every pair of the transformation source and target are related, one can break the circularity and make an inductive proof go through. This demonstrates that the syntactic logical relations provide a basis of another general proof method for showing the correctness of program transformations.

1 Introduction

The aim of program transformation is to improve the run-time efficiency, keeping the semantics of the source program. The correctness proof on a program transformation algorithm is usually done by an inductive argument on the program structure, where each induction step is proved by an equational reasoning on the general syntactic pattern of the corresponding local transformation site. This inductive proof principle applies to a large class of program transformation algorithms, but there are certain ones that require a stronger one.

In this paper, we demonstrate that the *syntactic logical relations* developed by Pitts [13] can serve as another powerful device for proving the correctness of program transformations. The logical relations are a type-indexed family of relations $\{\Delta_\tau\}_\tau$ between program expressions, where each Δ_τ is inductively defined on the structure of type τ [9]. Pitts developed an operational technique to construct logical relations over a syntactic domain and called them ‘syntactic’ logical relations. He also showed that the syntactic logical relations coincide with the observational equivalence relation, *i. e.*, $(M, M') \in \Delta_\tau$ for some τ iff M and M' show the same evaluation behavior when they are embedded in any context of a larger program.

The syntactic logical relations provide a firm basis for arguing the observational equivalence between the transformation source and target. Given a transformation algorithm, we alter the original definition of the syntactic logical relations so that they relate every pair of a source program and its transformation

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result. That is, we construct the family of relations satisfying

$$(M, \mathcal{W}[[M]]) \in \Delta_\tau,$$

where M is an arbitrary source expression of type τ and $\mathcal{W}[[M]]$ stands for the transformation result. Then the correctness of the transformation (*i. e.*, the source program and its transformation result behave similarly) follows from the coincidence between the logical relations and the observational equivalence.

There are a few attempts to apply a syntactically formulated relational framework to the correctness proof of program transformation. An example is a boxing transformation on polymorphic values [7, 8]. However, the language considered does not have fixpoint recursion. The proof technique in the present paper has a more powerful ability to reason about the observational equivalence in the presence of fixpoint operators (and hence it is sensitive to termination behavior too). Johann [6] exploited the parametricity result induced from the syntactic logical relations to give a formal justification on the shortcut fusion transformation [4], which is a popular transformation algorithm for removing intermediate data structures that are produced between producer/consumer function pairs. The present paper demonstrates that not only the parametricity but also the framework of the syntactic logical relations itself can be a formal basis for arguing the correctness of program transformations.

We show how the syntactic logical relations can effectively constitute a formal correctness proof, through a non-trivial example of program transformation, namely, a *higher-order removal transformation*, which was introduced by the author as a transformation step for removing higher-order functions in a particular class of programs [11]. The major difficulty in giving a correctness proof for this transformation is raised by a *circularity* to be introduced into the structure of the target program. The presence of circularity makes it difficult to show the total correctness of transformation (*i. e.*, the semantics of the whole program is preserved), since there is no base case to induct on the program structure. Using logical relations, however, we can break the circularity and make the induction go through.

Though we employed Pitts' syntactic logical relations, it would be also possible to give the correctness proof using logical relations that are, usually done as such, defined over semantic domains, as Nielsen [10] did in the correctness proof of the general higher-order removal algorithm (*a.k.a.* defunctionalization [14]). However, we prefer Pitts' syntactic approach, since we can avoid technical complications that arise from the domain theoretic approach.

The rest of the paper is organized as follows. Section 2 informally presents the higher-order removal transformation algorithm mentioned above. Section 3 introduces a relational framework for reasoning about observational equivalence of programs based on the syntactic logical relations. Section 4 gives a formal correctness proof of the higher-order removal transformation. Finally Section 5 concludes the paper with discussions on future research topics.

2 The Higher-Order Removal Transformation by Example

Deforestation [18] is a program transformation which removes intermediate data structures that are produced by a function and are immediately consumed by another function. Though notable refinements and improvements on the deforestation algorithm have been proposed [4, 15, 1, 16], it had been long undiscovered how to deforest functions that are defined by means of *accumulating parameters*, which are function arguments passed around throughout a series of recursive calls, as popularly seen in the tail recursive definition of list reverse function. A solution, which is based on the framework of macro tree transducers [2], to this problem was recently proposed by Voigtländer [17]. The author independently developed another one, which was inspired from the composition method for attribute grammars [3].

The program transformation considered in this paper is a higher-order removal transformation, which is a vital step in the latter deforestation algorithm. Let us explain the deforestation process by applying it to an example given in Figure 1. We use Haskell like syntax [5] extended with record syntax: $(l_1=M_1, \dots, l_n=M_n)$ expresses a record with labels l_1, \dots, l_n ($n \geq 0$) associated with expressions M_1, \dots, M_n , *resp.*, $\#l M$ selects the value associated with the field l of record M . $(l_1::\tau_1, \dots, l_n::\tau_n)$ represents the type of a record whose label l_i is each associated with a value of type τ_i .

The source program to which deforestation process is applied is the function `revflat` given in Figure 1(a). It is a composition of a producer function `flat` and a consumer function `rev`, which compute the preorder traversal list of leaves of a binary tree and the reversal of list elements, respectively. Though the definition may look verbose, the intention is made clear by removing all the record labels. For example, the definition of `flat` is equivalent to the following program:

```
flat :: T a → [a] → [a]
flat (Node(t,t')) x0 = flat t (flat t' x0)
flat (Leaf a)      x0 = a:x0
```

We put distinct record labels as the “tags” to uniquely identify the accumulating parameter and the computation result of each different function; `h` and `l` are used for tagging the accumulating parameter and the computation result of the function `flat`, *resp.*; similarly, `k` and `j` for those of the function `rev`. The named record labels are more useful for the purpose of unique identification than the unlabeled tuples.

Figure 2 illustrates the whole deforestation process, which comprises of four subtransformation steps. First, it applies shortcut fusion [4], which is a standard deforestation technique, in order to remove intermediate data structures and to obtain a single recursive function definition. The result is, however, a higher-order function, and we would like to remove this higher-orderedness. For this, we further apply two transformations, which perform type conversions on the higher-order function. They are intended to translate the program into a form

```

data T a = Node (T a, T a) | Leaf a

flat :: T a → (h::[a]) → (l::[a])
flat (Node(t,t')) x0 = (l=#l (flat t (h=#l (flat t' (h=#h x0)))))
flat (Leaf a)      x0 = (l=a:(#h x0))

rev :: [a] → (k::[a]) → (j::[a])
rev (a:t) x0 = (j=#j (rev t (k=a:(#k x0))))
rev []      x0 = (j=#k x0)

revflat :: T a → [a]
revflat x = #j (rev (#l (flat x (h=[]))) (k=[]))

```

Figure 1(a): Source program

```

rf :: T a → ((hk::[a]) → (hj::[a])) → (lk::[a]) → (lj::[a])
rf (Node(t,t')) x0 = let x2 = rf t' (\y2 -> (hj=#hj (x0 (hk=#hk y2)))) in
                      let x1 = rf t  (\y1 -> (hj=#lj (x2 (lk=#hk y1)))) in
                      \y0 -> (lj=#lj (x1 (lk=#lk y0)))
rf (Leaf a)      x0 = \y0 -> (lj=#hj (x0 (hk=a:(#lk y0))))

revflat :: T a → [a]
revflat x = #lj (rf x (\y -> (hj=#hk y)) (lk=[]))

```

Figure 1(b): Intermediate transformation result

```

rf' :: T a → (hj :: [a], lk :: [a]) → (hk :: [a], lj :: [a])
rf' (Node(t,t')) x0 = let x2 = rf' t' (hj=#hj x0, lk=#hk x1)
                      x1 = rf' t  (hj=#lj x2, lk=#lk x0)
                      in (lj=#lj x1, hk=#hk x2)
rf' (Leaf a)      x0 = (lj=#hj x0, hk=a:(#lk x0))

revflat :: T a → [a]
revflat x = #lj (rf' x (hj=#hk (rf' x (hj=Ω, lk=[])), lk=[]))

```

Figure 1(c): The result of higher-order removal transformation

Fig. 1. Transformation example

```

flat :: T a → (h::[a]) → (l::[a]),  rev :: [a] → (k::[a]) → (j::[a])
      ↓ shortcut fusion
rf :: a T → (h::(k::[a])→(j::[a])) → (l::(k::[a])→(j::[a]))
      ↓
rf :: a T → ((h::(k::[a]))→(h::(j::[a]))) → ((l::(k::[a]))→(l::(j::[a])))
      ↓
rf :: a T → ((hk::[a])→(hj::[a])) → ((lk::[a])→(lj::[a]))
      ↓ higher-order removal
rf' :: a T → (hj::[a],lk::[a]) → (hk::[a],lj::[a])

```

Fig. 2. The whole deforestation process

that is suitable as the input to the final higher-order removal transformation step. The intermediate result by these transformations is given in Figure 1(b). (Since the main concern of this paper is in the application of the syntactic logical relations to the correctness proof of a program transformation, we do not go any further on the details of these preceding transformations. The transformation rules for them can be found in [11].)

We notice that, in Figure 1(b), the result of every recursive call of $\mathbf{rf} \ t \ \dots$ (where t is either the variable \mathbf{t} or \mathbf{t}') is bound by a let construct to a variable \mathbf{x}_i ($i > 0$) and also that every let bound variable \mathbf{x}_i appears, per each constructor case of the definition of \mathbf{rf} , once and only once in the form $\#1j \ (\mathbf{x}_i \ (\mathbf{lk}=M))$; We write $M_{\mathbf{x}_i}$ for such expression M . The occurrence of the formal function argument \mathbf{x}_0 of \mathbf{rf} is also linear and it appears in the form $\#hj \ (\mathbf{x}_0 \ (\mathbf{hk}=M_{\mathbf{x}_0}))$.

The result of applying the higher-order removal transformation is given in Figure 1(c). At the type level, this transformation is understood as a type conversion

$$\begin{aligned} \text{from } \sigma_1 &= ((\mathbf{hk} :: [\mathbf{a}]) \rightarrow (\mathbf{hj} :: [\mathbf{a}])) \rightarrow ((\mathbf{lk} :: [\mathbf{a}]) \rightarrow (\mathbf{lj} :: [\mathbf{a}])) \\ \text{to } \sigma_2 &= (\mathbf{hj} :: [\mathbf{a}], \mathbf{lk} :: [\mathbf{a}]) \rightarrow (\mathbf{hk} :: [\mathbf{a}], \mathbf{lj} :: [\mathbf{a}]). \end{aligned}$$

Notice that \mathbf{hj} and \mathbf{lk} , which are the labels of record types occurring at negative positions in the higher-order function type σ_1 , constitute the argument type $(\mathbf{hj} :: [\mathbf{a}], \mathbf{lk} :: [\mathbf{a}])$ of the first-order function type σ_2 and also that \mathbf{hk} and \mathbf{lj} , which are the labels of records occurring at positive positions in σ_1 , constitute the result type $(\mathbf{hk} :: [\mathbf{a}], \mathbf{lj} :: [\mathbf{a}])$ of σ_2 .

$$\begin{aligned} \mathcal{W}'[[H :: T]] &= \mathcal{W}'[[H]] :: \mathcal{W}'[[T]] \\ \mathcal{W}'[[\#lk \ y_0]] &= \#lk \ x_0 \\ \mathcal{W}'[[\#hk \ y_i]] &= \#hk \ x_i & (1 \leq i \leq n) \\ \mathcal{W}'[[\#hj \ (x_0 \ (\mathbf{hk} = M_{\mathbf{x}_0}))]] &= \#hj \ x_0 \\ \mathcal{W}'[[\#lj \ (x_i \ (\mathbf{lk} = M_{\mathbf{x}_i}))]] &= \#lj \ x_i & (1 \leq i \leq n) \\ \mathcal{W}'[[M]] &= M & (\text{otherwise}) \end{aligned}$$

Fig. 3. Transformation rules for higher-order removal

The higher-order removal transformation on the function \mathbf{rf} that respects the above type conversion is formulated as follows. (The transformation on $\mathbf{revflat}$ is a bit technical, and is discussed later in Section 4.2.) Every \mathbf{let} binding site $\mathbf{x}_i = \mathbf{rf} \ t \ (\backslash y_i \rightarrow (\mathbf{hj}=N_i))$ is rewritten to

$$\mathbf{x}_i = \mathbf{rf}' \ t \ (\mathbf{hj}=\mathcal{W}'[[N_i]], \mathbf{lk}=\mathcal{W}'[[M_{\mathbf{x}_i}]]) \quad (1)$$

where $\mathcal{W}'[[M]]$ denotes a transformation on M , which is inductively defined on the structure of M by the rules given in Figure 3. (We only consider a special class of expressions and hence the rules in the figure are sufficient for the transformation.) The linearity in the use of each variable \mathbf{x}_i is crucial here for uniquely identifying the expression $M_{\mathbf{x}_i}$. The function value $\backslash y_0 \rightarrow (\mathbf{lj}=N_0)$ returned

by the function \mathbf{rf} in Figure 1(b) is transformed similarly but to $(\mathbf{lj}=\mathcal{W}'[[N_0]], \mathbf{hk}=\mathcal{W}'[[M_{x_0}]])$. To complete the transformation, the sequential let bindings are replaced with a single circular let. The final transformation result is given in Figure 1(c).

The above transformation process (1) is explained as follows. Every recursive call $\mathbf{rf} \ t \ \dots$, whose result is denoted by a variable x_i ($i > 0$), is transformed into $\mathbf{rf}' \ t \ R$, where R is a record of type $(\mathbf{hj}::[\mathbf{a}], \mathbf{lk}::[\mathbf{a}])$ and the value of R at each record label is drawn from the source program as follows: \mathbf{hj} value is set to N_i , which is taken from the \mathbf{hj} field of the record expression returned by the function $\backslash y_i \rightarrow (\mathbf{hj}=N_i)$ (*i. e.*, the second argument to the recursive call); Since every variable x_i is bound to the result of a recursive call $\mathbf{rf}' \ t \ \dots$ (of type $(\mathbf{hk}::[\mathbf{a}], \mathbf{lj}::[\mathbf{a}])$) in the target program, every application site $\#\mathbf{lj} \ (x_i \ (\mathbf{lk}=M))$ is rewritten to $\#\mathbf{lj} \ x_i$, which just refers to the \mathbf{lj} value returned by the recursive call. Also, every occurrence of expression $\#\mathbf{hk} \ y_i$ is rewritten to $\#\mathbf{hk} \ x_i$, which just takes the \mathbf{hk} value returned by the recursive call. The transformation for the case $i = 0$ is similarly explained.

The above explanation only alludes to the validity of the transformation from the viewpoint of the type correctness and it tells little about the semantic correctness. It is indeed difficult to give a complete justification on the transformation in a descriptive way. The source of difficulty is that the transformation we consider is a *non-local transformation*, where the result of transformation on a program expression depends on that of another transformation site (*e. g.*, in the transformation rule (1), the transformation result refers to that of another site, namely $\mathcal{W}'[[M_{x_i}]]$). Even worse, the target program involves a *circularity*, which is introduced by the circular let construct, in its program structure. Due to this circularity, it is even not obvious if the transformation preserves the termination behavior of the source program.

In order to obtain a complete justification, we would need to resort to a formal argument based upon a firm mathematical basis. We notice that the usual inductive argument on the program structure does not work effectively, since there is no base case to induct on the circular structure. In [17], Voigtländer faced this problem in the correctness proof of his deforestation algorithm too. He argued the correctness of each local transformation step only, leaving that of the entire transformation not formally proved.

In the present paper, we employ the syntactic logical relations [13] as the mathematical basis for reasoning about the correctness of the higher-order removal program transformation. For this, we reformulate the syntactic logical relations $\{\Delta_\tau\}_\tau$ so that, every transformation source M and its transformation result, denoted by $\mathcal{W}[[M]]$, are related, *i. e.*, $(M, \mathcal{W}[[M]]) \in \Delta_\tau$. This enables a simultaneous reasoning on different transformation sites: we can induce the relation between the pair of a transformation source and its result (which includes references to the results of transformation on other sites) from the type structure, not resorting to the induction hypothesis on the program structure.

We note that, unlike the usual logical relations, the logical relations formulated as above induce relations between expressions of different types. That is,

Δ_τ is a relation between expressions of type τ and $\mathcal{T}[\tau]$, where $\mathcal{T}[\cdot]$ is a type conversion function that replaces every type subexpression σ_1 in τ with σ_2 . We will discuss the observational equivalence of expressions of different types up to certain contexts that subsume this type mismatch. (See Section 4.2 for the details.)

3 Relational Framework for a Functional Language

This section constructs a relational framework for reasoning about observational equivalence of programs, following the technique developed in [13]. The considered programming language is a simply typed call-by-name functional language.¹ In order to avoid syntactic verbosity, we assume the only recursive data structure is lists. However, the following results are easily generalized to include other data structures such as binary trees.

3.1 The simply typed functional language

The set of types and language expressions are defined as follows.

$$\begin{array}{ll}
 \text{Types} & \tau ::= \tau \rightarrow \tau \mid (l_1 : \tau_1, \dots, l_n : \tau_n) \mid \tau \text{ list} \\
 \text{Expressions} & M ::= x \mid \lambda x : \tau. M \mid MM \mid \mathbf{fix} M \\
 & \mid (l_1 = M_1, \dots, l_n = M_n) \\
 & \mid \mathbf{match} M \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M \\
 & \mid \mathbf{nil}_\tau \mid M :: M \mid \mathbf{case} M \mathbf{of} \mathbf{nil} \Rightarrow M, x :: y \Rightarrow M
 \end{array}$$

Types are either a function type, a record type, or a list type. The set of type expressions are defined inductively, with *unit type* $()$ (the record type which has no record labels) being the base case of induction. We say a type τ is τ' -free, if τ has no occurrence of τ' as a type subexpression.

The syntax of the language is an extension of the simply typed λ -calculus with fixpoint operator $\mathbf{fix} M$, records $(l_1 = M_1, \dots, l_n = M_n)$ ($n \geq 0$), **match**-expression on records, empty list \mathbf{nil}_τ , list constructor $M :: M$, and **case**-branch on lists. Records are labeled products, where the order of labels is insignificant. Expression $\mathbf{match} M \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M'$ matches a record M against a pattern $(l_1 = x_1, \dots, l_n = x_n)$ and evaluates M' with binding each x_i to the corresponding element identified by the label l_i (the set of labels l_1, \dots, l_n is a subset of the labels of the record M).

As usual, a variable occurrence of x in an expression M is said to be *free*, if x is not bound by any binding of λ -, **match**-, and **case**-constructs in M . We write $fv(M)$ to denote the set of free variables in M . An expression M is called *closed* if $fv(M) = \emptyset$. We write $M[x_1/N_1, \dots, x_n/N_n]$ to represent a *substitution* to expression M whose free occurrences of variables x_1, \dots, x_n are simultaneously replaced with N_1, \dots, N_n , *resp.* We assume any substitution is capture-free, *i. e.*, any free variable in N_i 's is not bound by the substitution.

¹ We consider a monomorphically typed language since parametricity is not the concern of the present paper. The results in the paper can be easily generalized to a polymorphically typed language, however.

$$\frac{
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\frac{
F \Downarrow \lambda x : \tau.M \quad M[x/A] \Downarrow V \quad F(\mathbf{fix} F) \Downarrow V
}{V \Downarrow V}
}{FA \Downarrow V}
}{\mathbf{fix} F \Downarrow V}
}{M \Downarrow (l_1 = M_1, \dots, l_n = M_n, \dots)} \quad M'[x_1/M_1, \dots, x_n/M_n] \Downarrow V
}{\mathbf{match} M \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M' \Downarrow V}
}{M \Downarrow \mathbf{nil}_\tau \quad M_1 \Downarrow V} \quad \frac{
M \Downarrow H :: T \quad M_2[x/H, y/T] \Downarrow V
}{\mathbf{case} M \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2 \Downarrow V}
}{\mathbf{case} M \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2 \Downarrow V}$$

Fig. 4. Operational Semantics

$$\frac{
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\Gamma(x) = \tau \quad \Gamma, x : \tau \vdash M : \tau' \quad \Gamma \vdash F : \tau \rightarrow \tau' \quad \Gamma \vdash A : \tau
}{\Gamma \vdash x : \tau}
}{\Gamma \vdash \lambda x : \tau.M : \tau \rightarrow \tau'}
}{\Gamma \vdash F : \tau \rightarrow \tau}
}{\Gamma \vdash \mathbf{fix} F : \tau}
}{\Gamma \vdash (l_1 = M_1, \dots, l_n = M_n) : (l_1 : \tau_1, \dots, l_n : \tau_n)}
}{\Gamma \vdash M : (l_1 : \tau_1, \dots, l_n : \tau_n, \dots)} \quad \Gamma, x_1 : \tau_1, \dots, x_n : \tau_n \vdash M' : \tau
}{\Gamma \vdash \mathbf{match} M \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M' : \tau}
}{\Gamma \vdash \mathbf{nil}_\tau : \tau \text{ list} \quad \Gamma \vdash M : \tau \quad \Gamma \vdash M' : \tau \text{ list}}
}{\Gamma \vdash M : \tau \text{ list} \quad \Gamma \vdash M_1 : \tau' \quad \Gamma, x : \tau, y : \tau \text{ list} \vdash M_2 : \tau'}
}{\Gamma \vdash \mathbf{case} M \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2 : \tau'}$$

Fig. 5. Typing Rules

The formal (call-by-name) operational semantics is given in Figure 4. The *evaluation relation* is expressed by a binary relation $M \Downarrow V$, which reads the expression M is evaluated to V , where V is a *value* that belongs to a subset of expressions defined below.

$$V ::= \lambda x : \tau.M \mid (l_1 = M_1, \dots, l_n = M_n) \mid \mathbf{nil}_\tau \mid M :: M.$$

The typing rules are defined in the usual way, as given in Figure 5. A *typing judgment* is a ternary relation $\Gamma \vdash M : \tau$, where Γ is a finite map from variables to types, called *type environment*, M is an expression, and τ is a type. We conventionally write a type environment as $x_1 : \tau_1, \dots, x_n : \tau_n$ ($n \geq 0$). We write $\text{Exp}(\tau)$ for the set of closed expressions of type τ , that is, $\text{Exp}(\tau) = \{M \mid \Gamma \vdash M : \tau\}$.

In what follows, we assume a few syntactic conventions for brevity.

We write Ω_τ for $\mathbf{fix}(\lambda x : \tau.x)$, which is an expression of type τ that diverges under any context. The subscript may be omitted occasionally.

The *field selection operator* $\#l M$ is a shorthand for

$$\#l M = \mathbf{match} M \mathbf{of} (l = z) \Rightarrow z \quad (z \text{ is a fresh variable}).$$

Circular let definitions are expressed by combining fixpoint and record operators:

$$\begin{aligned}
& \mathbf{let} x_1 = M_1; \dots; x_n = M_n \mathbf{in} M \\
= & \mathbf{match} (\mathbf{fix} (\lambda r : (\overline{x}_1 : \tau_1, \dots, \overline{x}_n : \tau_n)). \\
& \quad \mathbf{match} r \mathbf{of} (\overline{x}_1 = x_1, \dots, \overline{x}_n = x_n) \Rightarrow (\overline{x}_1 = M_1, \dots, \overline{x}_n = M_n))) \\
& \mathbf{of} (\overline{x}_1 = x_1, \dots, \overline{x}_n = x_n) \Rightarrow M
\end{aligned}$$

where each τ_i is the type of M_i and the variable r and the labels $\overline{x_i}'$ s are fresh.

3.2 The syntactic logical relation

We construct the syntactic logical relations for the simply typed functional language defined above. Most of the proofs, which can be found in Pitts' original paper [13], are omitted.

Frame stacks and termination relation We represent evaluation contexts by *frame stacks*.

Definition 1 (Frame stacks). *The grammar of frame stacks, ranged over by S , is given by*

$$S ::= Id \mid S \circ F,$$

where F ranges over frames:

$$F ::= (- M) \mid (\mathbf{match} - \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M) \\ \mid (\mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2).$$

A frame stack is essentially a finite list of frames, with Id being the empty list representing a null context. We refer to the length of S meaning the number of frames in S .

$$\frac{\frac{\frac{}{\Gamma \vdash Id : \tau \multimap \tau}}{\Gamma \vdash S : \tau \multimap \tau'} \quad \frac{\frac{\Gamma \vdash S : \tau' \multimap \tau'' \quad \Gamma \vdash A : \tau}{\Gamma \vdash S \circ (- A) : \tau \multimap \tau' \multimap \tau''}}{\Gamma, x_1 : \tau_1, \dots, x_n : \tau_n \vdash M' : \tau}}{\Gamma \vdash S \circ (\mathbf{match} - \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M') : (l_1 : \tau_1, \dots, l_n : \tau_n, \dots) \multimap \tau'} \quad \frac{\frac{\Gamma \vdash S : \tau'' \multimap \tau' \quad \Gamma \vdash M_1 : \tau'' \quad \Gamma, x : \tau, y : \tau \mathit{list} \vdash M_2 : \tau''}{\Gamma \vdash S \circ (\mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2) : \tau \mathit{list} \multimap \tau'}}$$

Fig. 6. Typing rules for frame stacks

We are only interested in well-typed frame stacks. A typing judgment on a frame stack S is written $\Gamma \vdash S : \tau \multimap \tau'$, which reads: S represents a context which yields, under a type environment Γ , a value of type τ' when its hole is filled with any expression of type τ . A frame stack is well-typed if it has a typing judgment derived from the rules given in Figure 6.

In the following, we write $Stack(\tau, \tau')$ to denote the set of well-typed frame stacks $\{S \mid \emptyset \vdash S : \tau \multimap \tau'\}$. We also write $Stack(\tau)$ when $\tau' = \tau'' \mathit{list}$ for some τ'' .

The operation of applying a frame stack $S \in Stack(\tau, \tau')$ to an expression $M \in Exp(\tau)$, written SM , is defined as follows, by induction on the length of S :

$$Id M = M \\ (S \circ F)M = S(F[M]),$$

$$\begin{array}{c}
\frac{S \top M[x/A]}{S \circ (-A) \top \lambda x : \tau.M} \quad \frac{S \circ (-A) \top F}{S \top FA} \quad \frac{S \circ (-\mathbf{fix} F) \top F}{S \top \mathbf{fix} F} \\
\frac{Id \top \mathbf{nil}_\tau}{S \circ (\mathbf{match} - \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M') \top M} \quad \frac{S \top \mathbf{match} M \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M'}{S \top M'[x_1/M_1, \dots, x_n/M_n]} \\
\frac{S \circ (\mathbf{match} - \mathbf{of} (l_1 = x_1, \dots, l_n = x_n) \Rightarrow M') \top (l_1 = M_1, \dots, l_n = M_n, \dots)}{S \top \mathbf{case} M \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2} \quad \frac{S \circ (\mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2) \top M}{S \top M_1} \\
\frac{Id \top \mathbf{nil}_\tau}{S \circ (\mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2) \top \mathbf{nil}_\tau} \quad \frac{S \top M_2[x/H, y/T]}{S \circ (\mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow M_1, x :: y \Rightarrow M_2) \top H :: T}
\end{array}$$

Fig. 7. Rules for termination relation

where $F[M]$ represents the syntactic replacement of ‘-’ in F with M .

A binary relation $S \top M$ is defined inductively, for every $S \in \text{Stack}(\tau)$ and $M \in \text{Exp}(\tau)$, by the rules given in Figure 7. The relation $S \top M$ reads: the evaluation of M under context S terminates and yields $\mathbf{nil}_{\tau'}$ for some τ' .

Proposition 1. *For all types τ, τ' , frame stack $S \in \text{Stack}(\tau)$, and expression $M \in \text{Exp}(\tau)$, it holds that*

$$S M \Downarrow \mathbf{nil}_{\tau'} \quad \text{iff} \quad S \top M.$$

$\top\top$ -closed relations Let us write $\text{Rel}(\tau, \tau')$ to denote the set of all relations between well-typed expressions that are subsets of $\text{Exp}(\tau) \times \text{Exp}(\tau')$. Similarly, we write $\text{StRel}(\tau, \tau')$ to denote the set of all relations between stack frames that are subsets of $\text{Stack}(\tau) \times \text{Stack}(\tau')$.

The duality between expressions and stack frames induces a pair of complement operators $(-)^{\top}$ between $\text{Rel}(\tau, \tau')$ and $\text{StRel}(\tau, \tau')$.

Definition 2. *For any $r \in \text{Rel}(\tau, \tau')$, we define*

$$r^{\top} = \{(S, S') \mid \forall (M, M') \in r (S \top M \Leftrightarrow S' \top M')\}.$$

Also, for any $s \in \text{StRel}(\tau, \tau')$, we define

$$s^{\top} = \{(M, M') \mid \forall (S, S') \in s (S \top M \Leftrightarrow S' \top M')\}.$$

The two $(-)^{\top}$ operators together define a Galois connection [12] with respect to inclusion (i. e., $r \subseteq s^{\top} \Leftrightarrow s \subseteq r^{\top}$). An important property derived from Galois connections is that the double-negation operators $(-)^{\top\top}$ are a closure operator. That is, they are monotone ($r \subseteq r' \Rightarrow r^{\top\top} \subseteq r'^{\top\top}$), inflationary ($r \subseteq r^{\top\top}$), and idempotent ($r^{\top\top} = (r^{\top\top})^{\top\top}$).

Definition 3. *A relation r is called $\top\top$ -closed, if $r = r^{\top\top}$.*

Defining logical relation For each type constructor, we define a relation constructor, called *action*.

Definition 4 (Actions). Let r, r', r_1, \dots, r_n be relations such that $r \in \text{Rel}(\tau, \tau')$, $r' \in \text{Rel}(\sigma, \sigma')$, $r_i \in \text{Rel}(\tau_i, \tau'_i)$ ($i = 1, \dots, n$).

We define actions $(-) \rightarrow (-) : \text{Rel}(\tau, \tau') \times \text{Rel}(\sigma, \sigma') \rightarrow \text{Rel}(\tau \rightarrow \sigma, \tau' \rightarrow \sigma')$, $(l_1 : (-), \dots, l_n : (-)) : \text{Rel}(\tau_1, \tau'_1) \times \dots \times \text{Rel}(\tau_n, \tau'_n) \rightarrow \text{Rel}((l_1 : \tau_1, \dots, l_n : \tau_n), (l_1 : \tau'_1, \dots, l_n : \tau'_n))$, and $(-)list : \text{Rel}(\tau, \tau') \rightarrow \text{Rel}(\tau \text{ list}, \tau' \text{ list})$ as follows.

$$\begin{aligned} r \rightarrow r' &= \{(F, F') \mid (FA, F'A') \in r' \text{ for all } (A, A') \in r\} \\ (l_1 : r_1, \dots, l_n : r_n) &= \{((l_1 = M_1, \dots, l_n = M_n), (l_1 = M'_1, \dots, l_n = M'_n)) \mid \\ &\quad (M_1, M'_1) \in r_1, \dots, (M_n, M'_n) \in r_n\}^{\top\top} \\ (r)list &= \nu\gamma.\Phi_r(\gamma) \end{aligned}$$

In the definition of $(r)list$, $\Phi_r : \text{Rel}(\tau \text{ list}, \tau' \text{ list}) \rightarrow \text{Rel}(\tau \text{ list}, \tau' \text{ list})$ is a function such that $\Phi_r(\gamma) = (\{\mathbf{nil}_\tau, \mathbf{nil}_{\tau'}\} \cup \{(H, T), (H', T') \mid (H, H') \in r \text{ and } (T, T') \in \gamma\})^{\top\top}$, and $\nu\gamma.F(\gamma)$ denotes a greatest fixpoint of a function F .

The action for list types is well-defined (i. e., the greatest fixpoint exists), since $\top\top$ -closure is monotone and hence so is Φ_r .

Definition 5. The syntactic logical relations $\{\Delta_\tau\}_\tau$ are inductively defined on the structure of type τ by the following construction rules:

$$\begin{aligned} \Delta_{\tau \rightarrow \tau'} &= \Delta_\tau \rightarrow \Delta_{\tau'} \\ \Delta_{(l_1 : \tau_1, \dots, l_n : \tau_n)} &= (l_1 : \Delta_{\tau_1}, \dots, l_n : \Delta_{\tau_n}) \\ \Delta_{\tau \text{ list}} &= (\Delta_\tau)list \end{aligned}$$

The above definition is carefully designed so that each relation Δ_τ is $\top\top$ -closed at any type index τ . This, together with the following theorem, justifies the application of the fixpoint operator to expression M of any type $\tau \rightarrow \tau$.

Theorem 1. [13, Theorem 3.11] Let $r \in \text{Rel}(\tau, \tau')$ be a $\top\top$ -closed relation, and let $F \in \text{Exp}(\tau \rightarrow \tau)$ and $F' \in \text{Exp}(\tau' \rightarrow \tau')$ be expressions such that $(FA, F'A') \in r$ for all $(A, A') \in r$. Then, it holds that $(\mathbf{fix} F, \mathbf{fix} F') \in r$.

This theorem also gives a justification on the relational reasoning of programs that involve circular let expressions and recursive function definitions, which are a derivative of fixpoint operator.

The next proposition, which is drawn from [13], shows a bisimilarity property of the relation on list types.

Proposition 2. The relation $\Delta_{\tau \text{ list}}$ is the greatest bisimulation, i. e., $\Delta_{\tau \text{ list}}$ is a greatest relation r that satisfies, whenever $(L, L') \in \Delta_{\tau \text{ list}}$,

(i) $L \Downarrow \mathbf{nil}_\tau$ iff $L' \Downarrow \mathbf{nil}_\tau$, and

- (ii) if $L \Downarrow H :: T$ then $L' \Downarrow H' :: T'$ for some H' and T' such that $(H, H') \in \Delta_\tau$ and $(T, T') \in \Delta_{\tau \text{ list}}$.
- (iii) if $L' \Downarrow H' :: T'$ then $L \Downarrow H :: T$ for some H and T such that $(H, H') \in \Delta_\tau$ and $(T, T') \in \Delta_{\tau \text{ list}}$.

3.3 Equational congruence relation and its properties

Let us write $M \sim M'$ to indicate that closed expressions M and M' are related w.r.t. the above logical relations, *i. e.*, $(M, M') \in \Delta_\tau$ for some type τ . The next proposition holds for \sim -relation.

Proposition 3. [13, Proposition 4.6] *The relation \sim is a congruence relation, i. e., it is reflexive, symmetric, transitive, and substitutive (i. e., if $fv(M) = \{x_1, \dots, x_n\}$ and $M_1 \sim M'_1, \dots, M_n \sim M'_n$ then $M[x_1/M_1, \dots, x_n/M_n] \sim M[x_1/M'_1, \dots, x_n/M'_n]$).*

In order for this proposition to hold for the present language, we need to verify some properties concerning record types. The proof is given in Appendix.

In addition to the congruence, several equational properties on \sim can be derived from the so-called *Kleene equivalence*.

Proposition 4. [13, Corollary 3.15] *Let $M, M' \in \text{Exp}(\tau)$. M and M' are called Kleene equivalent, written $M =_{\text{kl}} M'$, if it holds that $\forall V.(M \Downarrow V \Leftrightarrow M' \Downarrow V)$.*

Kleene equivalence respects \sim relation, that is, if $M_1 =_{\text{kl}} M'_1, M_2 =_{\text{kl}} M'_2$, and $M_1 \sim M_2$, then $M'_1 \sim M'_2$.

$$\begin{aligned}
& (\lambda x : \tau.M)N \sim M[x/N] & \text{fix } F \sim F(\text{fix } F) & \text{let } \mathcal{B} \text{ in } M \sim M\theta \\
& \#l(l = M, \dots) \sim M & \text{case nil}_\tau \text{ of nil} \Rightarrow M_1, h :: t \Rightarrow M_2 \sim M_1 \\
& & \text{case } H :: T \text{ of nil} \Rightarrow M_1, h :: t \Rightarrow M_2 \sim M_2[h/H, t/T] \\
& \text{let } \mathcal{B} \text{ in } M \sim M\theta & \text{let } \mathcal{B} \text{ in } (\lambda x : \tau.M) \sim \lambda x : \tau.(\text{let } \mathcal{B} \text{ in } M) \\
& \text{let } \mathcal{B} \text{ in } MN \sim (\text{let } \mathcal{B} \text{ in } M)(\text{let } \mathcal{B} \text{ in } N) & \text{let } \mathcal{B} \text{ in } \#l M \sim \#l(\text{let } \mathcal{B} \text{ in } M) \\
& \text{let } \mathcal{B} \text{ in } (l_1 = N_1, \dots, l_m = N_m) \sim (l_1 = \text{let } \mathcal{B} \text{ in } N_1, \dots, l_m = \text{let } \mathcal{B} \text{ in } N_m) \\
& \text{let } \mathcal{B} \text{ in } H :: T \sim (\text{let } \mathcal{B} \text{ in } H) :: (\text{let } \mathcal{B} \text{ in } T)
\end{aligned}$$

where $\mathcal{B} = x_1 = M_1; \dots; x_n = M_n$ and $\theta = [x_1/\text{let } \mathcal{B} \text{ in } M_1, \dots, x_n/\text{let } \mathcal{B} \text{ in } M_n]$.

Fig. 8. Derived \sim -relations

Figure 8 gives several \sim -relations derived from Kleene equivalence; \sim -relation is stable up to β -reductions, fixpoint unfoldings (and therefore circular let unfoldings), and destructor/constructor pair cancellations (for records and lists); Also, the circular let constructs commute with several other constructs.

Since it has been proved that the syntactic logical relations coincide with the observational equivalence [13, Theorem 4.15], we hitherto reason about observational equivalence of expressions up to \sim , using the laws in Proposition 3 and Figure 8.

We notice that, though the present formalization considers list types only, the above results are easily generalized to any polynomial data types, *e. g.* binary trees. The relations for any polynomial data types can be defined as a greatest fixpoint of a monotone function, likewise in the definition for list types.

4 The Correctness of Higher-Order Removal Transformation

Throughout this section, we write U, X, Y to denote disjoint sets of variables $U = \{u_1, \dots, u_m\}$, $X = \{x_0, \dots, x_n\}$, and $Y = \{y_0, \dots, y_n\}$ ($m, n \geq 0$). We also fix a list type τ *list*.

4.1 Definition of the higher-order removal transformation

Our transformation algorithm applies to a class of expressions of the following form (which is referred to as I , in the rest of the paper):

$$\begin{aligned}
 I = & \lambda x_0 : (hk : \tau \text{ list}) \rightarrow (hj : \tau \text{ list}). \\
 & \text{let } x_n = f_n (\lambda y_n : (hk : \tau \text{ list}).(hj = N_n)) \text{ in} \\
 & \quad \dots \\
 & \text{let } x_1 = f_1 (\lambda y_1 : (hk : \tau \text{ list}).(hj = N_1)) \text{ in} \\
 & \lambda y_0 : (lk : \tau \text{ list}).(lj = N_0)
 \end{aligned} \tag{2}$$

where f_1, \dots, f_n ($n \geq 0$) are variables of type $((hk : \tau \text{ list}) \rightarrow (hj : \tau \text{ list})) \rightarrow ((lk : \tau \text{ list}) \rightarrow (lj : \tau \text{ list}))$, and N_1, \dots, N_n are expressions that belong to a particular syntactic class. That is, $N_0 \in \text{Exp}_i^{\Gamma_U, X, Y, \pi}((lj : \tau \text{ list}))$ and $N_i \in \text{Exp}_i^{\Gamma_U, X, Y, \pi}(hj : \tau \text{ list})$ ($1 \leq i \leq n$), where the syntactic class designated by $\text{Exp}_i^{\Gamma_U, X, Y, \pi}(\tau)$ is defined as below.

Definition 6. Let $\Gamma_U = u_1 : \tau_1, \dots, u_m : \tau_m$ be a type environment and π be a function $\{0, \dots, n\} \mapsto \{0, \dots, n\}$ such that $i > \pi(i)$ for every $i = 1, \dots, n$.

We define a family of set of expressions $\{\text{Exp}_i^{\Gamma_U, X, Y, \pi}(\tau)\}_{0 \leq i \leq n}$ inductively by the following rules (for brevity, we write $\text{Exp}_i(\tau)$ for $\text{Exp}_i^{\Gamma_U, X, Y, \pi}(\tau)$):

- h1** $M \in \text{Exp}_i(\tau)$ whenever $\Gamma_U \vdash M : \tau$,
- h2** $H :: T \in \text{Exp}_i(\tau \text{ list})$ if $H \in \text{Exp}_i(\tau)$ and $T \in \text{Exp}_i(\tau \text{ list})$,
- h3** $\#lk y_0 \in \text{Exp}_0(\tau \text{ list})$,
- h4** $\#hk y_i \in \text{Exp}_i(\tau \text{ list})$ ($1 \leq i \leq n$),
- h5** $\#hj (x_0 (hk = M_{x_0})) \in \text{Exp}_{\pi(0)}(\tau \text{ list})$, where $\text{fv}(M_{x_0}) \cap X = \emptyset$ and $M_{x_0} \in \text{Exp}_{\pi(0)}(\tau \text{ list})$, and
- h6** $\#lj (x_i (lk = M_{x_i})) \in \text{Exp}_{\pi(i)}(\tau \text{ list})$ ($1 \leq i \leq n$), where $\text{fv}(M_{x_i}) \cap X = \emptyset$ and $M_{x_i} \in \text{Exp}_{\pi(i)}(\tau \text{ list})$.

For each i , $Exp_i(\tau)$ represents a syntactically restricted set of expressions of type τ , which possibly contains free variables from U , X , and Y . Each variable $x_i \in X$ has to appear in a function application form (Rules **h5** and **h6**. $\pi(i)$ refers to the index j of expression N_j from which the variable x_i is referenced); Each variable $y_i \in Y$ must appear with a field selection operator (**h3** and **h4**). The above expressions can be combined by the list constructor (**h2**).

The expression I is further assumed to meet a *linearity condition*: Each variable $x_i \in X$ occurs once and only once throughout the expressions N_0, \dots, N_n . (The side condition $i > \pi(i)$ ($i = 1, \dots, n$) guarantees that every use of x_i is preceded by the corresponding let binding **let** $x_i = \dots$.) We intendedly excluded λ -abstractions from the above rules, in order to prevent each unique occurrence of a variable x_i from being applied to the argument that receives varying denotations. This may happen when a λ -expression that abstracts the x_i 's application is used in different contexts, *e. g.*, $(\lambda f. \dots f A_1 \dots f A_2)(\lambda z. \#lj(x_i(lk = \#lkz)))$.

$$\begin{aligned}
& \mathcal{W}[\lambda x_0 : (hk : \tau \text{ list}) \rightarrow (hj : \tau \text{ list}). \\
& \quad \mathbf{let} \ x_n = f_n \ (\lambda y_n : (hk : \tau \text{ list}).(hj = N_n)) \ \mathbf{in} \\
& \quad \dots \\
& \quad \mathbf{let} \ x_1 = f_1 \ (\lambda y_1 : (hk : \tau \text{ list}).(hj = N_1)) \ \mathbf{in} \ \lambda y_0 : (lk : \tau \text{ list}).(lj = N_0)] \\
& = \lambda x_0 : (hj : \tau \text{ list}, lk : \tau \text{ list}). \\
& \quad \mathbf{let} \ x_n = f'_n \ (hj = \mathcal{W}'[[N_n]], lk = \mathcal{W}'[[M_{x_n}]]); \\
& \quad \dots \\
& \quad x_1 = f'_1 \ (hj = \mathcal{W}'[[N_1]], lk = \mathcal{W}'[[M_{x_1}]]) \\
& \quad \mathbf{in} \ (lj = \mathcal{W}'[[N_0]], hk = \mathcal{W}'[[M_{x_0}]])
\end{aligned}$$

where \mathcal{W}' is the transformation defined in Figure 3, and variables f_1, \dots, f_n and f'_1, \dots, f'_n denote recursive function calls to a substructure of the input data type.

Fig. 9. The higher-order removal transformation

The formal definition of the higher-order removal transformation \mathcal{W} is given in Figure 9. It is easy to verify that this transformation is type correct.

Theorem 2. *Let us write $\sigma_1 = ((hk : \tau \text{ list}) \rightarrow (hj : \tau \text{ list})) \rightarrow ((lk : \tau \text{ list}) \rightarrow (lj : \tau \text{ list}))$ and $\sigma_2 = (hj : \tau \text{ list}, lk : \tau \text{ list}) \rightarrow (hk : \tau \text{ list}, lj : \tau \text{ list})$. If $\Gamma_U, f_1 : \sigma_1, \dots, f_n : \sigma_1 \vdash I : \sigma_1$, then $\Gamma_U, f'_1 : \sigma_2, \dots, f'_n : \sigma_2 \vdash \mathcal{W}[[I]] : \sigma_2$.*

4.2 Correctness of higher-order removal transformation

For the purpose of proving the correctness of the transformation, we reformulate the syntactic logical relations $\{\Delta_\tau\}_\tau$, as we discussed in Section 2. We replace only the relation indexed by $\sigma_1 = ((hk : \tau \text{ list}) \rightarrow (hj : \tau \text{ list})) \rightarrow ((lk : \tau \text{ list}) \rightarrow (lj : \tau \text{ list}))$ with the relation Θ defined below.

Definition 7. $\Theta \in \text{Rel}(((hk : \tau \text{ list}) \rightarrow (hj : \tau \text{ list})) \rightarrow ((lk : \tau \text{ list}) \rightarrow (lj : \tau \text{ list})), (hj : \tau \text{ list}, lk : \tau \text{ list}) \rightarrow (hk : \tau \text{ list}, lj : \tau \text{ list}))$ is a relation defined by:

$$(I, J) \in \Theta \quad \text{iff}$$

$$(a) \quad (\#hk (J (hj = H, lk = L)), \#hk (J (hj = H', lk = L'))) \in \Delta_{\tau \text{ list}} \text{ for all } (L, L') \in \Delta_{\tau \text{ list}} \text{ and } H, H' \in \text{Exp}(\tau \text{ list}), \text{ and}$$

$$(b) \quad \left(\begin{array}{l} \#lj (I G (lk = L)), \\ \#lj (J (hj = \#hj (G' (hk = \#hk (J (hj = \Omega_{\tau \text{ list}}, lk = L'))))), \end{array} \right) \in \Delta_{\tau \text{ list}}$$

for all $(G, G') \in (hk : \Delta_{\tau \text{ list}}) \rightarrow (hj : \Delta_{\tau \text{ list}})$ and $(L, L') \in \Delta_{\tau \text{ list}}$.

We note that the above modification does retain the original relation Δ_{τ} whenever τ is σ_1 -free, i. e., τ is free from occurrences of σ_1 . This implies that the observational equivalence of programs of σ_1 -free types can be safely reasoned up to \sim -relation introduced in Section 3.3. In what follows, we assume τ ranges over the set of σ_1 -free types.

We prove that Θ relates the transformation source I and the target $\mathcal{W}[[I]]$.

Proposition 5. For every expression I of the form (2), it holds that

$$(I\theta_0, \mathcal{W}[[I]\theta'_0]) \in \Theta$$

for any $\theta_0 = [u_1/U_1, \dots, u_m/U_m, f_1/I_1, \dots, f_n/I_n]$ and $\theta'_0 = [u_1/U'_1, \dots, u_m/U'_m, f'_1/J_1, \dots, f'_n/J_n]$ satisfying $(U_k, U'_k) \in \Delta_{\Gamma_U(u_k)}$ ($1 \leq k \leq m$) and $(I_i, J_i) \in \Theta$ ($1 \leq i \leq n$).

Before giving the proof, let us explain what are the intentions behind the definition of Θ and how they contribute to establishing the formal proof.

The property (a) of the definition of Θ indicates that the hk value of the record computed by the transformed program $J = \mathcal{W}[[I]]$ depends only on the lk value of the input record and is not affected at all by the input hj value. This means the expression H' for the hj field can be substituted with any other well-typed expression. This property is crucially exploited in the proof in order to break the circularity introduced by the circular let construct: We can suppress the circular references in the transformed program by virtually replacing certain variable references with expressions that do not cause circularity.

The property (b) implies that the lj value, which carries the final answer computed by the original producer/consumer function pair, of the record computed by a single call to I is obtained by using J twice. Computing an lj value by a call to I with G being the initial accumulating parameter is equal to computing an lj value by first calling J to obtain the hk value from the input lk value L' , and then by applying J to the pair of the hj value and the input lk value L' , where the hj value is obtained by applying G' (an observationally equivalent copy of G) to the hk value computed by the first call of J . This justifies the transformation on $\#lj(x_i(lk = M_{x_i}))$ by \mathcal{W}' .

To show the proposition, we need the following lemma, which shows that the subtransformation \mathcal{W}' also preserves the observational equivalence of programs under certain contexts.

Lemma 1. Let $I_1, J_1, \dots, I_n, J_n, U_1, U'_1, \dots, U_m, U'_m$ be expressions as in Proposition 5. Let us write $\mathcal{B}, \mathcal{B}'$ for

$$\begin{aligned} \mathcal{B} &= x_n = I_n(\lambda y_n : (hk : \tau \text{ list}).(hj = N_n)) \mathbf{in} \\ &\quad \dots \mathbf{in let } x_1 = I_1(\lambda y_1 : (hk : \tau \text{ list}).(hj = N_1)) \\ \mathcal{B}' &= x_n = J_n(hj = \mathcal{W}'[[N_n]], lk = \mathcal{W}'[[M_{x_n}]]); \\ &\quad \dots ; x_1 = J_1(hj = \mathcal{W}'[[N_1]], lk = \mathcal{W}'[[M_{x_1}]]) \end{aligned}$$

Then, for any i ($1 \leq i \leq n$), $(G, G') \in (hk : \Delta_\tau \text{ list}) \rightarrow (hj : \Delta_\tau \text{ list})$ and $(L, L') \in \Delta_\tau$, it holds that

- (a) $(M\theta\eta_i, \mathbf{let } \mathcal{B}'\theta'_H \mathbf{in } \mathcal{W}'[[M]]\theta'_H) \in \Delta_\tau$ for every $H \in \text{Exp}(\tau \text{ list})$ and $M \in \text{Exp}_i(\tau)$ such that $\text{fv}(M) \cap X = \emptyset$, and
- (b) $(\mathbf{let } \mathcal{B}\theta \mathbf{in } M\theta\eta_i, \mathbf{let } \mathcal{B}'\theta' \mathbf{in } \mathcal{W}'[[M]]\theta') \in \Delta_\tau$ for every $M \in \text{Exp}_i(\tau)$.

where

$$\begin{aligned} \theta &= [x_0/G, y_0/(lk = L), u_1/U_1, \dots, u_m/U_m], \\ \theta' &= [x_0/\mathbf{let } x_0 = (hj = \#hj (G'(hk = \#hk (\mathbf{let } \mathcal{B}' \mathbf{in } \mathcal{W}'[[M_{x_0}]])), \\ &\quad lk = L') \mathbf{in } x_0, \quad u_1/U'_1, \dots, u_m/U'_m] \\ \theta'_H &= [x_0/(hj = H, lk = L'), u_0/U'_0, \dots, u_m/U'_m], \\ \eta_0 &= [], \\ \eta_i &= [y_i/(hk = \#hk (J_i(\mathbf{let } \mathcal{B}'\theta' \mathbf{in } (hj = \mathcal{W}'[[N_i]]\theta', lk = \mathcal{W}'[[M_{x_i}]]\theta')))]. \end{aligned}$$

Proof. We first show property (a) by induction on i and the structure of M . We only prove the cases where M is an expression corresponding to the cases **h3** and **h4** in Definition 6. (The cases **h5** and **h6** do not matter, since $\text{fv}(M) \cap X = \emptyset$.)

$$\begin{aligned} \text{Case } M &= \#lk y_0. \quad M\theta\eta_i = \#lk (lk = L) \sim \#lk (lk = L') \\ &\sim \mathbf{let } \mathcal{B}'\theta'_H \mathbf{in } \#lk x_0\theta'_H = \mathbf{let } \mathcal{B}'\theta'_H \mathbf{in } \mathcal{W}'[[M]]\theta'_H \end{aligned}$$

Case $M = \#hk y_i$.

$$\begin{aligned} M\theta\eta_i &= \#hk (hk = \#hk \\ &\quad (J_i(\mathbf{let } \mathcal{B}'\theta' \mathbf{in } (hj = \#hj \mathcal{W}'[[N_i]]\theta', lk = \#lk \mathcal{W}'[[M_{x_i}]]\theta')))) \\ &\sim \mathbf{let } \mathcal{B}'\theta' \mathbf{in } \#hk (J_i(hj = \Omega_\tau \text{ list}, lk = \#lk \mathcal{W}'[[M_{x_i}]]\theta')) \quad \text{by Def.7(a)} \\ &\sim \#hk (J_i(hj = \Omega_\tau \text{ list}, lk = \#lk M_{x_i}\theta\eta_{\pi(i)})) \quad \text{by I.H.} \\ &\sim \#hk (J_i(hj = \Omega_\tau \text{ list}, lk = \#lk (\mathbf{let } \mathcal{B}'\theta'_H \mathbf{in } \mathcal{W}'[[M_{x_i}]]\theta'_H))) \quad \text{by I.H.} \\ &\sim \#hk (\mathbf{let } \mathcal{B}'\theta'_H \mathbf{in } (J_i(hj = \#hj \mathcal{W}'[[N_i]]\theta'_H, lk = \#lk \mathcal{W}'[[M_{x_i}]]\theta'_H))) \\ &\quad \text{by Def.7(a)} \\ &\sim \mathbf{let } \mathcal{B}'\theta'_H \mathbf{in } \#hk x_i = \mathbf{let } \mathcal{B}'\theta'_H \mathbf{in } \mathcal{W}'[[M]] \end{aligned}$$

The proof of property (b) is by induction on i and the structure of M , where we take the order on i as $n \prec n-1 \prec \dots \prec 0$, with n being the base case of induction. We only prove the cases where M is an expression corresponding to **h3–h6** in Definition 6.

Case $M = \#lk\ y_0$. $\mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } \#lk\ y_0\theta\eta_i = \#lk\ (lk = L) \sim \#lk\ (lk = L')$
 $\sim \#lk\ x_0\theta' \sim \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \#lk\ x_0\theta' = \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \mathcal{W}'\llbracket M \rrbracket\theta'$

Case $M = \#hk\ y_i$.

$\mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } M\theta\eta_i$
 $= \#hk(hk = \#hk(J_i(\mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } (hj = \#hj\ \mathcal{W}'\llbracket N_i \rrbracket\theta', lk = \#lk\ \mathcal{W}'\llbracket M_{x_i} \rrbracket\theta'))))$
 $\sim \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \#hk\ x_i = \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \mathcal{W}'\llbracket M \rrbracket\theta'$

Case $M = \#hj\ (x_0\ (hk = M_{x_0}))$.

$\mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } M\theta\eta_i = \mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } \#hj\ (G\ (hk = M_{x_0}\theta\eta_i))$
 $\sim \#hj\ (G\ (hk = \mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } M_{x_0}\theta\eta_i))$
 $\sim \#hj\ (G'\ (hk = \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \mathcal{W}'\llbracket M_{x_0} \rrbracket\theta'))$ by I.H.
 $\sim \#hj\ (hj = \#hj\ (G'\ (hk = \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \mathcal{W}'\llbracket M_{x_0} \rrbracket\theta')), lk = L')$
 $\sim \#hj\ x_0\theta' = \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \mathcal{W}'\llbracket M \rrbracket\theta'$

Case $M = \#lj\ (x_j\ (lk = M_{x_j}))$ where $i = \pi(j)$.

$\mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } M\theta\eta_i = \mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } \#lj\ (x_j\ (lk = M_{x_j}\theta\eta_i))$
 $\sim \mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } \#lj\ (I_j\ (\lambda y_j : (hk : \tau\ list).(hj = N_j\theta))\ (lk = M_{x_j}\theta\eta_i))$
 $\sim \mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } \#lj\ (J_j\ (hj = \#hj$
 $\quad ((\lambda y_j : (hk : \tau\ list).(hj = N_j\theta))$
 $\quad \quad (hk = \#hk\ (J_j\ (hj = \Omega_{\tau\ list}, lk = M_{x_j}\theta\eta_i)),$
 $\quad \quad lk = M_{x_j}\theta\eta_i)))$ by Def.7(b)
 $\sim \mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } \#lj\ (J_j\ (hj = \#hj$
 $\quad ((\lambda y_j : (hk : \tau\ list).(hj = N_j\theta))$
 $\quad \quad (hk = \#hk\ (J_j\ (\mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } (hj = \mathcal{W}'\llbracket N_j \rrbracket\theta',$
 $\quad \quad \quad lk = \mathcal{W}'\llbracket M_{x_j} \rrbracket\theta'))),$
 $\quad \quad lk = M_{x_j}\theta\eta_i)))$ by Def.7(a) and I.H.
 $\sim \mathbf{let\ } \mathcal{B}\theta \mathbf{ in\ } \#lj\ (J_j\ (hj = N_j\theta\eta_j, lk = M_{x_j}\theta\eta_i))$
 $\sim \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \#lj\ (J_j\ (hj = \mathcal{W}'\llbracket N_j \rrbracket\theta', lk = \mathcal{W}'\llbracket M_{x_j} \rrbracket\theta'))$ by I.H.
 $\sim \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \#lj\ x_j = \mathbf{let\ } \mathcal{B}'\theta' \mathbf{ in\ } \mathcal{W}'\llbracket M \rrbracket\theta'$ \square

Proof. (of Proposition 5) Let $(G, G') \in (hk : \Delta_{\tau\ list}) \rightarrow (hj : \Delta_{\tau\ list})$ and $(L, L') \in \Delta_{\tau\ list}$. We write J for $\mathcal{W}\llbracket I \rrbracket$.

First we show property (a) of Definition 7. For any $H, H' \in \text{Exp}(\tau\ list)$ we have

$\#hk\ (J\theta'_0(hj = H, lk = L)) \sim \#hk\ (J\theta'_0(hj = H, lk = L'))$
 $\sim \mathbf{let\ } \mathcal{B}'\theta'_H \mathbf{ in\ } \#hk\ \mathcal{W}'\llbracket M_{x_0} \rrbracket\theta'_H$
 $\sim \#hk\ M_{x_0}\theta\eta_{\pi(0)} \sim \mathbf{let\ } \mathcal{B}'\theta'_{H'} \mathbf{ in\ } \#hk\ \mathcal{W}'\llbracket M_{x_0} \rrbracket\theta'_{H'}$ by lemma 1(a), twice
 $\sim \#hk\ (J\theta'_0(hj = H', lk = L')).$

We derive the property (b) as follows.

$$\begin{aligned}
& \#lj (I\theta_0 G (lk = L)) \\
\sim & \#lj (\mathbf{let} \mathcal{B}\theta \mathbf{in} (lj = N_0\theta\eta_0)) \sim \mathbf{let} \mathcal{B}\theta \mathbf{in} N_0\theta\eta_0 \\
\sim & \mathbf{let} \mathcal{B}'\theta' \mathbf{in} \mathcal{W}'\llbracket N_0 \rrbracket\theta' && \text{by lemma 1(b)} \\
\sim & \#lj (J\theta'_0 x_0\theta') \\
\sim & \#lj (J\theta'_0 (hj = \#hj (G'(hk = \mathbf{let} \mathcal{B}'\theta' \mathbf{in} \mathcal{W}'\llbracket M_{x_0} \rrbracket\theta')), lk = L')) \\
\sim & \#lj (J\theta'_0 (hj = \#hj (G'(hk = M_{x_0}\theta\eta_i)), lk = L')) && \text{by lemma 1(a)} \\
\sim & \#lj (J\theta'_0 (hj = \#hj (G'(hk = \mathbf{let} \mathcal{B}'\theta'_{\Omega_\tau \text{ list}} \mathbf{in} \mathcal{W}'\llbracket M_{x_0} \rrbracket\theta'_{\Omega_\tau \text{ list}})), \\
& \quad lk = L')) && \text{by lemma 1(a)} \\
\sim & \#lj (J\theta'_0 (hj = \#hj (G'(hk = \#hk (J\theta'_0 (hj = \Omega_\tau \text{ list}, lk = L')), \\
& \quad lk = L')))) \quad \square
\end{aligned}$$

The total correctness of the higher-order removal transformations is derived from the Proposition 5. Suppose we are given the following expressions \mathcal{I} and \mathcal{J} :

$$\begin{aligned}
\mathcal{I} &= \lambda f : \tau \text{ list} \rightarrow ((hk : \tau \text{ list}) \rightarrow (hj : \tau \text{ list})) \rightarrow ((lk : \tau \text{ list}) \rightarrow (lj : \tau \text{ list})). \\
& \quad (\lambda x : \tau \text{ list}. \mathbf{case} x \mathbf{of} \mathbf{nil} \Rightarrow I_{\mathbf{nil}}, h :: t \Rightarrow I_{h::t}[f_1/f t, \dots, f_n/f t]) \\
\mathcal{J} &= \lambda f' : \tau \text{ list} \rightarrow (hj : \tau \text{ list}, lk : \tau \text{ list}) \rightarrow (hk : \tau \text{ list}, lj : \tau \text{ list}) \\
& \quad (\lambda x : \tau \text{ list}. \mathbf{case} x \mathbf{of} \mathbf{nil} \Rightarrow \mathcal{W}\llbracket I_{\mathbf{nil}} \rrbracket, \\
& \quad \quad h :: t \Rightarrow \mathcal{W}\llbracket I_{h::t} \rrbracket[f'_1/f' t, \dots, f'_n/f' t])
\end{aligned}$$

where

- $I_{\mathbf{nil}}$ is an expression of the form (2) with $U = \emptyset$ and $n = 0$ (i. e., no **let**-bindings), and
- $I_{h::t}$ is an expression of the form (2) with $U = \{h\}$.

In the above, $f t$ and $f' t$ express recursive calls to the list substructure t . This is generalized to any polynomial data types: *E. g.*, for the case of binary trees instead of lists, the variables f_i 's (f'_i 's, *resp.*) would be substituted with either $f t$ or $f' t$ ($f' t$ or $f' t'$, *resp.*), where t and t' are variables representing the two different subtrees of a tree node.

In the present paper, we only prove the observational equivalence between **fix** \mathcal{I} and **fix** \mathcal{J} , when they are applied to lists of finite length. We notice that the observationally equivalent pairs of expressions of lists of length less than n is characterized by the relation $\Phi_{\Delta_\tau}^n(\emptyset)$, where Φ_r is the function given in Definition 4. This characterization can be also generalized to any polynomial data types, with an appropriate definition of Φ_r .

Theorem 3 (Correctness of transformation). *Let \mathcal{I} and \mathcal{J} be expressions defined as above. It holds that*

$$((\mathbf{fix} \mathcal{I})L, (\mathbf{fix} \mathcal{J})L') \in \Theta \quad \text{for every } (L, L') \in \Phi_{\Delta_\tau}^n(\emptyset) \ (n \geq 1).$$

We prove this theorem by induction on the length of lists, where the induction principle is justified by the following lemma.

Lemma 2. *If $(L, L') \in \Phi_{\Delta_\tau}^n(\emptyset)$ ($n \geq 1$), then the following properties hold.*

- (i) $L \Downarrow \mathbf{nil}_\tau$ iff $L' \Downarrow \mathbf{nil}_\tau$, and
- (ii) if $L \Downarrow H :: T$ then $L' \Downarrow H' :: T'$ for some H' and T' such that $(H, H') \in \Delta_\tau$ and $(T, T') \in \Phi_{\Delta_\tau}^{n-1}(\emptyset)$.
- (iii) if $L' \Downarrow H' :: T'$ then $L \Downarrow H :: T$ for some H and T such that $(H, H') \in \Delta_\tau$ and $(T, T') \in \Phi_{\Delta_\tau}^{n-1}(\emptyset)$.

In particular when $n = 1$, if $L \Downarrow V$ and $L' \Downarrow V'$ then $V = V' = \mathbf{nil}_\tau$.

Proof. The proof is by induction on n . Since $\Phi_{\Delta_\tau}^n(\emptyset)$ is smaller than the least fixpoint of Φ_{Δ_τ} , it is included by $\Delta_{\tau \text{ list}}$, the greatest fixpoint of Φ_{Δ_τ} . So, the properties in proposition 2 hold for any $(L, L') \in \Phi_{\Delta_\tau}^n(\emptyset)$ and therefore property (i) immediately follows.

Now we show property (ii) and (iii). If $n = 1$, $\Phi_{\Delta_\tau}^n(\emptyset) = \{(\mathbf{nil}_\tau, \mathbf{nil}_\tau)\}^{\top\top}$. Suppose $L \Downarrow H :: T$. By proposition 2, we have $L' \Downarrow H' :: T'$ for some H' and T' . Letting $S = \mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow \mathbf{nil}_{\tau'}, h :: t \Rightarrow \mathbf{nil}_{\tau'}$ and $S' = \mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow \mathbf{nil}_{\tau'}, h :: t \Rightarrow \Omega_{\tau'}$, we have $S \top L$ and $S' \not\top L'$ but on the other hand $S \top \mathbf{nil}_\tau$ iff $S' \top \mathbf{nil}_\tau$ implies $(S, S') \in \{(\mathbf{nil}_\tau, \mathbf{nil}_\tau)\}^{\top} = (\Phi_{\Delta_\tau}^n(\emptyset))^{\top}$, which contradicts to $(L, L') \in \Phi_{\Delta_\tau}^n(\emptyset)$. Hence we have $L \Downarrow H :: T$ and similarly for L' . Since L and L' never evaluate to a non-empty list, property (ii) and (iii) hold vacuously.

Suppose $n > 1$. We only show property (ii). The proof for (iii) is similar.

If $L \Downarrow H :: T$, by proposition 2, we have $L' \Downarrow H' :: T'$ for some H' and T' such that $(H, H') \in \Delta_\tau$ and $(T, T') \in \Delta_{\tau \text{ list}}$. To show $(T, T') \in \Phi_{\Delta_\tau}^{n-1}(\emptyset)$, suppose $(S_0, S'_0) \in (\Phi_{\Delta_\tau}^{n-1}(\emptyset))^{\top}$. Defining $S_1 = \mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow \mathbf{nil}_{\tau'}, h :: t \Rightarrow S_0 t$ and $S'_1 = \mathbf{case} - \mathbf{of} \mathbf{nil} \Rightarrow \mathbf{nil}_{\tau'}, h :: t \Rightarrow S'_0 t$, we will show $(S_1, S'_1) \in (\Phi_{\Delta_\tau}^n(\emptyset))^{\top}$. Since $(\Phi_{\Delta_\tau}^n(\emptyset))^{\top} = (\{(\mathbf{nil}_\tau, \mathbf{nil}_\tau)\} \cup \{(H_1 :: T_1, H'_1 :: T'_1) \mid (H_1, H'_1) \in \Delta_\tau, (T_1, T'_1) \in \Phi_{\Delta_\tau}^{n-1}(\emptyset)\})^{\top}$, it is enough to show $S_1 \top L_1$ iff $S'_1 \top L'_1$ for every $(L_1, L'_1) \in \{(\mathbf{nil}_\tau, \mathbf{nil}_\tau)\} \cup \{(H_1 :: T_1, H'_1 :: T'_1) \mid (H_1, H'_1) \in \Delta_\tau, (T_1, T'_1) \in \Phi_{\Delta_\tau}^{n-1}(\emptyset)\}$. For the case $L_1 = L'_1 = \mathbf{nil}_\tau$, since $S_1 \top L_1 \Downarrow \mathbf{nil}_\tau$ and $S'_1 \top L'_1 \Downarrow \mathbf{nil}_\tau$ hold by the definition of S_1 and S'_1 , this property follows from proposition 1. If $L_1 = H_1 :: T_1$ and $L'_1 = H'_1 :: T'_1$, then we have $S_1 \top L_1 \Leftrightarrow Id \top S_0 T_1 \Leftrightarrow S_0 T_1 \Downarrow \mathbf{nil}_{\tau'} \Leftrightarrow S_0 \top T_1 \Leftrightarrow S'_0 \top T'_1 \Leftrightarrow S'_0 T'_1 \Downarrow \mathbf{nil}_{\tau'} \Leftrightarrow Id \top S'_0 T'_1 \Leftrightarrow S'_1 \top L'_1$ by proposition 1. Now it follows that $S_0 \top T \Leftrightarrow S_0 T \Downarrow \mathbf{nil}_{\tau'} \Leftrightarrow Id \top S_0 T \Leftrightarrow S_1 \top L \Leftrightarrow S'_1 \top L' \Leftrightarrow Id \top S'_0 T' \Leftrightarrow S'_0 T' \Downarrow \mathbf{nil}_{\tau'} \Leftrightarrow S'_0 \top T'$ by proposition 1. Since S_0 and S'_0 are arbitrary, this proves $(T, T') \in \Phi_{\Delta_\tau}^{n-1}(\emptyset)$. \square

The proof of Theorem 3 follows below.

Proof. (of Theorem 3) Proof is by induction on n . If both L and L' diverge, then so do both $(\mathbf{fix} \mathcal{I})L$ and $(\mathbf{fix} \mathcal{J})L'$. Hence $((\mathbf{fix} \mathcal{I})L, (\mathbf{fix} \mathcal{J})L') \in \Theta$.

Now we suppose that both L and L' do not diverge. (Non-divergence of one implies that of the other, by lemma 2.) If $n = 1$, then by lemma 2 both L and L'

evaluate to \mathbf{nil}_τ . Then we have $(\mathbf{fix} \mathcal{I})L \sim I_{\mathbf{nil}}$ and $(\mathbf{fix} \mathcal{J})L' \sim \mathcal{W}[[I_{\mathbf{nil}}]]$. Since $(I_{\mathbf{nil}}, \mathcal{W}[[I_{\mathbf{nil}}]]) \in \Theta$ by proposition 5, it follows that $(\mathbf{fix} \mathcal{I})L \sim (\mathbf{fix} \mathcal{J})L'$.

Suppose $n > 1$. By lemma 2, we have $L \Downarrow H :: T$ and $L' \Downarrow H' :: T'$ for some $(H, H') \in \Delta_\tau$ and $(T, T') \in \Phi_{\Delta_\tau}^{n-1}(\emptyset)$. Then, it holds that

$$\begin{aligned} (\mathbf{fix} \mathcal{I})L &\sim I_{h::t}[h/H, f_1/(\mathbf{fix} \mathcal{I})T, \dots, f_n/(\mathbf{fix} \mathcal{I})T] \quad \text{and} \\ (\mathbf{fix} \mathcal{J})L' &\sim \mathcal{W}[[I_{h::t}]] [h/H', f'_1/(\mathbf{fix} \mathcal{J})T', \dots, f'_n/(\mathbf{fix} \mathcal{J})T']. \end{aligned}$$

Since $((\mathbf{fix} \mathcal{I})T, (\mathbf{fix} \mathcal{J})T') \in \Theta$, by induction hypothesis and proposition 5, we have $(\mathbf{fix} \mathcal{I})L \sim (\mathbf{fix} \mathcal{J})L'$. \square

Now we show the total correctness of the higher-order removal transformation using the results in this section. Suppose we are given a recursive definition of function $\mathbf{fix} \mathcal{I}$, a function G of type $((hk : \tau \text{ list}) \rightarrow (hj : \tau \text{ list})) \rightarrow ((lk : \tau \text{ list}) \rightarrow (lj : \tau \text{ list}))$, and lists L and L' of type $\tau \text{ list}$ where L is of finite length. Then, it follows from the property (b) of the relation Θ (Definition 7) that

$$\#lj ((\mathbf{fix} \mathcal{I}) L G (lk = L'))$$

is observationally equivalent to

$$\#lj ((\mathbf{fix} \mathcal{J})(hj = \#hj (G ((\mathbf{fix} \mathcal{J})(hj = \Omega, lk = L'))), lk = L')).$$

Since the two expressions are related up to $\Delta_{\tau \text{ list}}$, they can substitute for each other under any context.

Applying this to the example in Figure 1 (with regarding $\mathbf{fix} \mathcal{I}$ as the recursive function definition of \mathbf{rf} and also $\mathbf{fix} \mathcal{J}$ as that of \mathbf{rf}'), we obtain

$$\begin{aligned} \text{revflat } x = \#lj (\mathbf{rf}' \ x \ (hj=\#hj \ ((\backslash y \rightarrow (hj=\#hk \ y)) \\ (\mathbf{rf}' \ x \ (hj=\Omega, \ lk=[])), \ lk=[]))) \end{aligned}$$

The final result in Figure 1(c) follows by a simple calculation. Note that the diverging expression Ω can be substituted with any well-typed list expression, since it does not affect the computation at all (as indicated by the property (a) of Definition 7).

5 Conclusion

We have shown that the framework of syntactic logical relations developed by Pitts [13] can be a powerful device in proving the correctness of program transformation. This was evidenced through a concrete example, a higher-order removal transformation, which is a part of a deforestation algorithm for functions with accumulating parameters.

We believe that the general proof method presented in this paper can apply to the correctness proof of other program transformations. In fact, the two auxiliary transformation processes between the shortcut fusion and the higher-order removal transformation (in Figure 2) can be justified by a similar proof

technique. This fact constitutes the complete correctness proof for the deforestation algorithm that was proposed by the author [11], together with a few more technical elaborations on the syntactic condition to be met by the two transformations. The author would like to report this result in a near future.

In Theorem 3, we assumed that the inputs are only finite lists (or finite polynomial data structures, in general). We leave the proof for the inputs of infinite lists open, as we were not able to prove the relation Θ is $\top\top$ -closed: If Θ were proved $\top\top$ -closed, we would have it as a direct consequence of Theorem 1 without resorting to the induction principle on finite lists. This implies that the $\top\top$ -closedness is a key to the question if the composition algorithms for functions with accumulating parameters are valid for infinite data structures. It is folklore in the community of macro tree transducers and attribute grammars that the answer is positive, but there is no formal justification.

The open problem mentioned above raises some technical issues which may be worth investigating. For the relation Θ to be $\top\top$ -closed, so must be both of the two properties in Definition 7. Though each property has its own difficulty in showing its $\top\top$ -closedness, that of the property (b) seems more fundamental: The problem amounts to showing the $\top\top$ -closedness of a relation $\Delta_{\tau \rightarrow \tau}$, which is defined for some particular type τ by $\Delta_{\tau \rightarrow \tau} = \{(F, F') \mid (FA, F'(F'A')) \in \Delta_{\tau} \text{ for all } (A, A') \in \Delta_{\tau}\}$. An attempt to show this $\top\top$ -closedness would be stuck, since we only consider contexts with a single hole whereas in this case we need to reason about contexts with two different holes. It would be interesting to investigate a refinement of Pitts' proof technique for proving (or disproving) this $\top\top$ -closedness.

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Appendix

A Relational Properties of Records

Lemma 3. *Let r_1, \dots, r_n be relations such that $r_i \in \text{Rel}(\tau_i, \tau'_i)$ ($i = 1, \dots, n$).*

The following properties hold for the action $(l_1 : r_1, \dots, l_n : r_n)$.

- (i) *If $(M_1, M'_1) \in r_1, \dots, (M_n, M'_n) \in r_n$, then $((l_1 = M_1, \dots, l_n = M_n), (l_1 = M'_1, \dots, l_n = M'_n)) \in (l_1 : r_1, \dots, l_n : r_n)$.*
- (ii) *$(l_1 : r_1, \dots, l_n : r_n)$ is $\top\top$ -closed.*
- (iii) *Suppose we are given a relation $r \in \text{Rel}(\tau, \tau')$, and open expressions N and N' satisfying:*

$$\begin{aligned}
 &x_1 : \tau_1, \dots, x_k : \tau_k \vdash N : \tau, \quad x_1 : \tau'_1, \dots, x_k : \tau'_k \vdash N' : \tau', \quad \text{and} \\
 &\forall (M_1, M'_1) \in r_1, \dots, (M_k, M'_k) \in r_k. \\
 &\quad ((N[x_1/M_1, \dots, x_k/M_k], N'[x_1/M'_1, \dots, x_k/M'_k]) \in r),
 \end{aligned}$$

- for some k ($0 \leq k \leq n$).
- If $(S, S') \in r^\top$ then $(S \circ (\mathbf{match} - \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N), S' \circ (\mathbf{match} - \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N')) \in (l_1 : r_1, \dots, l_n : r_n)^\top$.
- (iv) Let r , N , and N' be defined as above. If r is a $\top\top$ -closed relation and $(M, M') \in (l_1 : r_1, \dots, l_n : r_n)$, then we have $(\mathbf{match} M \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N, \mathbf{match} M' \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N') \in r$.
- (v) If $(M, M') \in (l_1 : r_1, \dots, l_n : r_n)$ and r_i 's are all $\top\top$ -closed, then $((l_1 = \#l_1 M, \dots, l_n = \#l_n M), (l_1 = \#l_1 M', \dots, l_n = \#l_n M')) \in (l_1 : r_1, \dots, l_n : r_n)$.

Proof. Property (i) and (ii) follow immediately from the definition of the action for record types and the monotonicity of the $\top\top$ -closure.

To show (iii), take any $(M_1, M'_1) \in r_1, \dots, (M_n, M'_n) \in r_n$. Writing $\rho = (l_1 = x_1, \dots, l_k = x_k)$, we have

$$\begin{aligned} & S \circ (\mathbf{match} - \mathbf{of} \rho \Rightarrow N) \top (l_1 = M_1, \dots, l_n = M_n) \\ \Leftrightarrow & S \top N[x_1/M_1, \dots, x_k/M_k] \\ \Leftrightarrow & S' \top N'[x_1/M'_1, \dots, x_k/M'_k] \quad \text{since } (S, S') \in r \\ \Leftrightarrow & S' \circ (\mathbf{match} - \mathbf{of} \rho \Rightarrow N') \top (l_1 = M'_1, \dots, l_n = M'_n) \end{aligned}$$

Hence it holds that $(S \circ (\mathbf{match} - \mathbf{of} \rho \Rightarrow N), S' \circ (\mathbf{match} - \mathbf{of} \rho \Rightarrow N')) \in \{((l_1 = M_1, \dots, l_n = M_n), (l_1 = M'_1, \dots, l_n = M'_n)) \mid (M_1, M'_1) \in r_1, \dots, (M_n, M'_n) \in r_n\}^\top = (l_1 : r_1, \dots, l_n : r_n)^\top$

Let us show property (iv). For any $(M, M') \in (l_1 : r_1, \dots, l_n : r_n)$ and $(S, S') \in r^\top$, we have

$$\begin{aligned} & S \top \mathbf{match} M \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N \\ \Leftrightarrow & S \circ (\mathbf{match} - \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N) \top M \\ \Leftrightarrow & S' \circ (\mathbf{match} - \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N') \top M' \quad \text{by (iii)} \\ \Leftrightarrow & S' \top \mathbf{match} M' \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N' \end{aligned}$$

Since S and S' are arbitrary, it holds that

$$\begin{aligned} & (\mathbf{match} M \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N, \\ & \mathbf{match} M' \mathbf{of} (l_1 = x_1, \dots, l_k = x_k) \Rightarrow N') \in r^{\top\top} = r. \end{aligned}$$

Property (v) follows immediately from (iv) and (i).