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# Witnessing (Co)datatypes

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**Abstract.** Datatypes and codatatypes are useful for specifying and reasoning about (possibly infinite) computational processes. The Isabelle/HOL proof assistant has recently been extended with a definitional package that supports both. We describe a complete procedure for deriving nonemptiness witnesses in the general mutually recursive, nested case—nonemptiness being a proviso for introducing types in higher-order logic.

## 1 Introduction

Proof assistants, or interactive theorem provers, are becoming increasingly popular as vehicles for formalizing the metatheory of logical systems and programming languages. Such developments often involve datatypes and codatatypes in various constellations. For example, Lochbihler’s formalization of the Java memory model represents possibly infinite executions using a codatatype [26]. Codatatypes are also useful for capturing lazy data structures, such as Haskell’s lists.

A popular and expanding family of proof assistants, heavily used in software and hardware verification, are those based on higher-order logic (HOL)—examples include HOL4 [37], HOL Light [16], HOL Zero [3], Isabelle/HOL [30], and ProofPower–HOL [4]. They are traditionally built on top of a trusted inference kernel through which all theorems are generated. Various definitional packages reduce high-level specifications to primitive inferences; characteristic theorems are derived rather than postulated. This reduces the amount of code that must be trusted. We recently extended Isabelle/HOL with a definitional package for mutually recursive, nested (co)datatypes [8, 39]. While some proof assistants support codatatypes (notably, Agda, Coq, Matita, and PVS), Isabelle is the first to provide a *definitional* implementation.

In this paper, we focus on a fundamental problem posed by any HOL development that extends the type infrastructure: proofs of, or “witnesses” for, the nonemptiness of newly introduced types. Besides its importance to formal logic engineering, the problem also enjoys theoretical relevance, since it essentially amounts to the decision problem for the nonemptiness of open-ended, mutual, nested (co)datatypes. Furthermore, our modular witness generation algorithm is relevant outside the proof assistant world, in areas such as program synthesis [15].

Our starting point is the nonemptiness requirement on HOL types. This is a well-known design decision connected to the presence of Hilbert choice in HOL [13, 31]. In all HOL-based provers, the following inductive specification of “finite streams” must be rejected because it would lead to an empty datatype:

`datatype  $\alpha$  fstream = FCons  $\alpha$  ( $\alpha$  fstream)`

While checking nonemptiness appears to be an easy reachability test, nested recursion complicates the picture, as shown by this attempt to define infinitely branching trees with finite branches by nested recursion via a codatatype of (infinite) streams:

`codatatype  $\alpha$  stream = SCons  $\alpha$  ( $\alpha$  stream)`  
`datatype  $\alpha$  tree = Node  $\alpha$  (( $\alpha$  tree) stream)`

The second definition should fail: To get a witness for  $\alpha$  tree, we would need a witness for ( $\alpha$  tree) stream, and vice versa. Replacing streams with finite lists should make the definition acceptable, because the empty list stops the recursion. Even though final coalgebras are never empty (except in trivial cases), here the datatype provides a better witness (the empty list) than the codatatype (which requires an  $\alpha$  tree to build an ( $\alpha$  tree) stream). Mutual, nested datatype specifications can be arbitrarily complex:

`datatype ( $\alpha, \beta$ ) tree = Leaf  $\beta$  | Branch (( $\alpha + (\alpha, \beta)$  tree) stream)`  
`codatatype ( $\alpha, \beta$ ) ltree = LNode  $\beta$  (( $\alpha + (\alpha, \beta)$  ltree) stream)`  
`datatype  $t_1 = T_{11}$  ((( $t_1, t_2$ ) ltree) stream) |  $T_{12}$  ( $t_1 \times (t_2 + t_3)$  stream)`  
`and  $t_2 = T_2$  (( $t_1 \times t_2$ ) list) and  $t_3 = T_3$  (( $t_1, (t_3, t_3)$  tree) tree)`

The definitions are legitimate, but the last group should be rejected if  $t_2$  is replaced by  $t_3$  in the constructor  $T_{11}$ .

What makes the problem interesting is our open-endedness assumption: The type constructors handled by the (co)datatype package are not syntactically predetermined. In particular, they are not restricted to polynomial functors—the user can register new type constructors in the package database after establishing a few semantic properties.

Our solution exploits the package’s abstract, functorial view of types. Each (co)datatype, and more generally each functor (type constructor) that participates in a definition, carries its own witnesses together with soundness proofs. Operations such as functorial composition, initial algebra, and final coalgebra derive their witnesses from those of the operands. Each computational step performed by the package is certified in HOL. The solution is complete: Given precise information about the functors participating in a definition, all nonempty datatypes are identified as such.

We start by recalling the package’s abstract layer, which is based on category theory (Section 2). Then we look at a concrete instance: a variation of context-free grammars acting on finite sets and their associated possibly infinite derivation trees (Section 3). The example supplies precious building blocks to the nonemptiness proofs (Section 4). It also displays some unique characteristics of the package, such as support for nested recursion through nonfree types. Other features and user conveniences are described elsewhere [8, 11]. The formalization covering the results presented here is publicly available [9]. It employs similar notations to this text but presents more details. The implementation is part of Isabelle [30] (Section 5).

*Conventions.* We work informally in a mathematical universe  $\mathcal{S}$  of sets but adopt many conventions from higher-order logic and functional programming. Function application is normally written in prefix form without parentheses (e.g.,  $f x y$ ). Sets are

ranged over by capital Roman letters ( $A, B, \dots$ ) and Greek letters ( $\alpha, \beta, \dots$ ). For  $n$ -ary functions, we often prefer the curried form  $f : \alpha_1 \rightarrow \dots \rightarrow \alpha_n \rightarrow \beta$  to the tuple form  $f : \alpha_1 \times \dots \times \alpha_n \rightarrow \beta$  but occasionally pass tuples to curried functions. Polymorphic operators are regarded as families of higher-order constants indexed by sets.

Operators on sets are normally written in postfix form:  $\alpha$  set is the powerset of  $\alpha$ , consisting of sets of elements of  $\alpha$ ;  $\alpha$  fset is the set of finite sets over  $\alpha$ . Given  $f : \alpha \rightarrow \beta$ ,  $A \subseteq \alpha$ , and  $B \subseteq \beta$ , image  $f A$ , or  $f \bullet A$ , is the image of  $A$  through  $f$ , and  $f^{-} B$  is the inverse image of  $B$  through  $f$ . The set unit contains a single element  $()$ , and  $[n] = \{1, \dots, n\}$ . Prefix and postfix operators bind more tightly than infixes, so that  $\alpha \times \beta$  set is read as  $\alpha \times (\beta \text{ set})$  and  $f \bullet g x$  as  $f \bullet (g x)$ .

The notation  $\bar{a}_n$ , or simply  $\bar{a}$ , denotes the tuple  $(a_1, \dots, a_n)$ . Given  $\bar{a}_m$  and  $\bar{b}_n$ ,  $(\bar{a}, \bar{b})$  denotes the flat tuple  $(a_1, \dots, a_m, b_1, \dots, b_n)$ . Given  $n$   $m$ -ary functions  $f_1, \dots, f_n$ , the notation  $\bar{f} \bar{a}$  stands for  $(f_1 \bar{a}, \dots, f_n \bar{a})$ , and similarly  $\bar{\alpha} \bar{F} = (\bar{\alpha} F_1, \dots, \bar{\alpha} F_n)$ . Depending on the context,  $\bar{\alpha}_n F$  either denotes the application of  $F$  to  $\bar{\alpha}$  or merely indicates that  $F$  is an  $n$ -ary set operator.

## 2 The Category Theory behind the Package

User-specified (co)datatypes and their characteristic theorems are derived from underlying constructions adapted from category theory. The central concept is that of bounded natural functors, a well-behaved class of functors with additional structure.

### 2.1 Functors and Functor Operations

We consider operators  $F$  on sets, which we call *set constructors*. We are interested in set constructors that are *functors* on the category of sets and functions, i.e., that are equipped with an action on morphisms commuting with identities and composition. This action is a polymorphic constant  $F\text{map} : (\alpha_1 \rightarrow \beta_1) \rightarrow \dots \rightarrow (\alpha_n \rightarrow \beta_n) \rightarrow \bar{\alpha} F \rightarrow \bar{\beta} F$  that satisfies  $F\text{map id} = \text{id}$  and  $F\text{map } (g_1 \circ f_1) \dots (g_n \circ f_n) = F\text{map } \bar{g} \circ F\text{map } \bar{f}$ . Formally, functors are pairs  $(F, F\text{map})$ . Basic instances are presented below.

*Identity functor* (ID, id). The identity maps any set and any function to itself.

*(n,  $\alpha$ )-Constant functor* ( $C_{n,\alpha}$ ,  $C\text{map}_{n,\alpha}$ ). The  $(n, \alpha)$ -constant functor  $(C_{n,\alpha}, C\text{map}_{n,\alpha})$  is the  $n$ -ary functor consisting of the set constructor  $\beta C_{n,\alpha} = \alpha$  and the action  $C\text{map}_{n,\alpha} f_1 \dots f_n = \text{id}$ . We write  $C_\alpha$  for  $C_{1,\alpha}$ .

*Sum functor* ( $+$ ,  $\oplus$ ). The sum  $\alpha_1 + \alpha_2$  consists of a copy  $\text{Inl } a_1$  of each element  $a_1 : \alpha_1$  and a copy  $\text{Inr } a_2$  of each element  $a_2 : \alpha_2$ . Given  $f_1 : \alpha_1 \rightarrow \beta_1$  and  $f_2 : \alpha_2 \rightarrow \beta_2$ , let  $f_1 \oplus f_2 : \alpha_1 + \alpha_2 \rightarrow \beta_1 + \beta_2$  be the function sending  $\text{Inl } a_1$  to  $\text{Inl } (f_1 a_1)$  and  $\text{Inr } a_2$  to  $\text{Inr } (f_2 a_2)$ .

*Product functor* ( $\times$ ,  $\otimes$ ). Let  $\text{fst} : \alpha_1 \times \alpha_2 \rightarrow \alpha_1$  and  $\text{snd} : \alpha_1 \times \alpha_2 \rightarrow \alpha_2$  denote the two projection functions from pairs. Given  $f_1 : \alpha \rightarrow \beta_1$  and  $f_2 : \alpha \rightarrow \beta_2$ , let  $\langle f_1, f_2 \rangle : \alpha \rightarrow \beta_1 \times \beta_2$  be the function  $\lambda a. (f_1 a, f_2 a)$ . Given  $f_1 : \alpha_1 \rightarrow \beta_1$  and  $f_2 : \alpha_2 \rightarrow \beta_2$ , let  $f_1 \otimes f_2 : \alpha_1 \times \alpha_2 \rightarrow \beta_1 \times \beta_2$  be  $\langle f_1 \circ \text{fst}, f_2 \circ \text{snd} \rangle$ .

$\alpha$ -Function space functor ( $\text{func}_\alpha, \text{comp}_\alpha$ ). Given a set  $\alpha$ , let  $\beta \text{ func}_\alpha = \alpha \rightarrow \beta$ . For all  $g : \beta \rightarrow \gamma$ , let  $\text{comp}_\alpha g : \beta \text{ func}_\alpha \rightarrow \gamma \text{ func}_\alpha$  be  $\text{comp}_\alpha g f = g \circ f$ .

Powerset functor ( $\text{set}, \text{image}$ ). For all  $f : \alpha \rightarrow \beta$ , the function  $\text{image } f : \alpha \text{ set} \rightarrow \beta \text{ set}$  sends each subset  $A$  of  $\alpha$  to the image of  $A$  through the function  $f : \alpha \rightarrow \beta$ .

Bounded  $k$ -powerset functor ( $\text{set}_k, \text{image}$ ). Given an infinite cardinal  $k$ , for all sets  $\alpha$ , the set  $\alpha \text{ set}_k$  carves out from  $\alpha \text{ set}$  only those sets of cardinality less than  $k$ . The finite powerset functor  $\text{fset}$  corresponds to  $\text{set}_{\aleph_0}$ .

Functors can be composed to form complex functors. Composition requires the functors  $F_j$  to take the same type arguments  $\bar{\alpha}$  in the same order. The operations of permutation and lifting, together with the identity and  $(n, \alpha)$ -constant functors, make it possible to compose functors freely. Let  $\text{Func}_n$  be the collection of  $n$ -ary functions.

*Composition.* Given  $\bar{\alpha} F_j$  for  $j \in [n]$  and  $\bar{\beta}_n G$ , the *functor composition*  $G \circ \bar{F}$  is defined as  $(\bar{\alpha} \bar{F}) G$  on objects and similarly on morphisms.

*Permutation.* Given  $F \in \text{Func}_n$  and  $i, j \in [n]$  with  $i < j$ , the  $(i, j)$ -permutation of  $F$ , written  $F^{(i, j)} \in \text{Func}_n$ , is defined on objects as  $\bar{\alpha} F^{(i, j)} = (\alpha_1, \dots, \alpha_{i-1}, \alpha_j, \alpha_{i+1}, \dots, \alpha_{j-1}, \alpha_i, \alpha_{j+1}, \dots, \alpha_n) F$  and similarly on morphisms.

*Lifting.* Given  $F \in \text{Func}_n$ , the *lifting* of  $F$ , written  $F^\dagger \in \text{Func}_{n+1}$ , is defined on objects as  $(\bar{\alpha}_n, \alpha_{n+1}) F^\dagger = \bar{\alpha}_n F$  and similarly on morphisms. In other words,  $F^\dagger$  is obtained from  $F$  by adding a superfluous argument  $\alpha_{n+1}$ .

Datatypes are defined by taking the initial algebra of a set of functors and codatatypes by taking the final coalgebra. Both operations are partial.

*Initial algebra.* Given  $n (m+n)$ -ary functors  $(\bar{\alpha}_m, \bar{\beta}_n) F_j$ , their *(mutual) initial algebra* consists of  $n$   $m$ -ary functors  $\bar{\alpha} \text{IF}_j$  that satisfy the isomorphism  $\bar{\alpha} \text{IF}_j \cong (\bar{\alpha}, \bar{\alpha} \text{IF}) F_j$  minimally (i.e., as the least fixpoint). The variables  $\bar{\alpha}$  are the passive parameters, and  $\bar{\beta}$  are the fixpoint variables. The functors  $\text{IF}_j$  are characterized by

- $n$  polymorphic *folding bijections* (constructors)  $\text{ctor}_j : (\bar{\alpha}, \bar{\alpha} \text{IF}) F_j \rightarrow \bar{\alpha} \text{IF}_j$  and
- $n$  polymorphic *iterators*  $\text{fold}_j : (\prod_{k \in [n]} (\bar{\alpha}, \bar{\beta}) F_k \rightarrow \beta_k) \rightarrow \bar{\alpha} \text{IF}_j \rightarrow \beta_j$

and subject to the following properties (for all  $j \in [n]$ ):

- Iteration equations:  $\text{fold}_j \bar{s} \circ \text{ctor}_j = s_j \circ \text{Fmap } \bar{\text{id}} (\bar{\text{fold}} \bar{s})$ .
- Unique characterization of iterators: Given  $\bar{\beta}$  and  $\bar{s}$ , the only functions  $f_j : \bar{\alpha} \text{IF}_j \rightarrow \beta_j$  satisfying  $f_j \circ \text{ctor}_j = s_j \circ \text{Fmap } \bar{\text{id}} f$  are  $\text{fold}_j \bar{s}$ .

The functorial actions  $\text{IFmap}_j$  for  $\text{IF}_j$  are defined by iteration in the standard way.

*Final coalgebra.* The final coalgebra operation is categorically dual to initial algebra. Given  $n (m+n)$ -ary functors  $(\bar{\alpha}_m, \bar{\beta}_n) F_j$ , their *(mutual) final coalgebra* consists of  $n$   $m$ -ary functors  $\bar{\alpha} \text{JF}_j$  that satisfy the isomorphism  $\bar{\alpha} \text{JF}_j \cong (\bar{\alpha}, \bar{\alpha} \text{JF}) F_j$  maximally (i.e., as the greatest fixpoint). The functors  $\text{JF}_j$  are characterized by

- $n$  polymorphic *unfolding bijections* (destructors)  $\text{dctor}_j : \bar{\alpha} \text{JF}_j \rightarrow (\bar{\alpha}, \bar{\alpha} \text{JF}) F_j$  and
- $n$  polymorphic *coiterators*  $\text{unfold}_j : (\prod_{k \in [n]} \beta_k \rightarrow (\bar{\alpha}, \bar{\beta}) F_k) \rightarrow \beta_j \rightarrow \bar{\alpha} \text{JF}_j$

and subject to the following properties:

- Coiteration equations:  $\text{dctor}_j \circ \text{unfold}_j \bar{s} = \text{Fmap } \bar{\text{id}} (\overline{\text{unfold } \bar{s}}) \circ s_j$ .
- Unique characterization of coiterators: Given  $\bar{\beta}$  and  $\bar{s}$ , the only functions  $f_j : \beta_j \rightarrow \bar{\alpha} \text{JF}_j$  satisfying  $\text{dctor}_j \circ f_j = \text{Fmap } \bar{\text{id}} \bar{f} \circ s_j$  are  $\text{unfold}_j \bar{s}$ .

The functorial actions  $\text{JFmap}_j$  for  $\text{JF}_j$  are defined by coiteration in the standard way.

## 2.2 Bounded Natural Functors

The (co)datatype package is based on a class  $\mathcal{B}$  of functors, called *bounded natural functors (BNFs)*. The particular axioms defining  $\mathcal{B}$  are described in previous papers [8, 39]. The class  $\mathcal{B}$  contains all the basic functors except for unbounded powerset and is closed under the operations described in Section 2.1.

Unlike the (co)datatype specification mechanisms of other proof assistants, in our package the involved types are not syntactically predetermined by a fixed grammar.  $\mathcal{B}$  includes the class of polynomial functors but is additionally open-ended in the sense that users can register further functors as members of  $\mathcal{B}$ .

Besides closure under functor operations, another important question for theorem proving is how to state induction and coinduction abstractly, irrespective of the shape of the functor. We know how to state induction on lists, or trees, but how about initial algebras of arbitrary functors?

The answer we propose enriches the structure of functors  $\bar{\alpha}_n F$  with additional data: For each  $i \in [n]$ , BNFs must provide a natural transformation  $\text{Fset}^i : \bar{\alpha} F \rightarrow \alpha_i$  set that gives, for  $x \in \bar{\alpha} F$ , the set of  $\alpha_i$ -atoms that take part in  $x$ . For example, if  $(\alpha_1, \alpha_2) F = \alpha_1 \times \alpha_2$ , then  $\text{Fset}^1(a_1, a_2) = \{a_1\}$  and  $\text{Fset}^2(a_1, a_2) = \{a_2\}$ ; if  $\alpha F = \alpha \text{ list}$  (the list functor, obtained as minimal solution to  $\beta \cong \text{unit} + \alpha \times \beta$ ), then  $\text{Fset} (= \text{Fset}^1)$  applied to a list  $x$  gives all the elements appearing in  $x$ .<sup>1</sup> The abstract (co)induction principles can be massaged to account for multiple carried constructors (Appendices B and C).

Given  $j \in [n]$ , the elements of  $\text{Fset}_j^{m+k} x$  (for  $k \in [n]$ ) are the recursive components of  $\text{ctor}_j x$ . (Notice that subscripts select functors  $F_j$  in the tuple  $\bar{F}$ , whereas superscripts select  $\text{Fset}$  operators for different arguments of  $F_j$ .) The explicit modeling of the recursive components makes it possible to state induction and coinduction abstractly for arbitrary BNFs (Appendix A).

Briefly, the registration process is as follows. The user provides a type constructor  $F$  and its associated BNF structure (in the form of polymorphic HOL constants), including the  $\text{Fmap}$  functorial action on objects. Then the user establishes the BNF properties (e.g., that  $(F, \text{Fmap})$  is indeed a functor). After this, the new BNF is integrated and can appear nested in future (co)datatype definitions. Following this procedure, Isabelle users have already introduced the BNF  $\alpha$  bag of finite bags (multisets) over  $\alpha$  and the BNF  $\alpha$  pmf of probability mass functions with domain  $\alpha$ . Other nonstandard BNFs can be produced by using the quotient package [22, 23] and the nonfree datatype package [36].

<sup>1</sup> This  $\text{Fset}$  has similarities with Pierce’s notion of support from his account of (co)inductive types [33] and with Abel and Altenkirch’s urelement relation from their framework for strong normalization [1]. A distinguishing feature of our notion is the consideration of categorical structure [39].

As an example, the type constructor  $\alpha$  bag is registered as a BNF by the following command:

```
bnf  $\alpha$  bag
  map: bmap : ( $\alpha \rightarrow \beta$ )  $\rightarrow$   $\alpha$  bag  $\rightarrow$   $\beta$  bag
  sets: bset :  $\alpha$  bag  $\rightarrow$   $\alpha$  set
  bd:  $\aleph_0$  : ( $\text{nat} \times \text{nat}$ ) set
  wits:  $\{\#\}$  :  $\alpha$  bag
  rel: brel : ( $\alpha \rightarrow \beta \rightarrow \text{bool}$ )  $\rightarrow$   $\alpha$  bag  $\rightarrow$   $\beta$  bag  $\rightarrow$  bool
```

The command provides the necessary infrastructure that makes  $\alpha$  bag a BNF, consisting of various previously introduced constants (whose definitions are not shown here):

- the functorial action (bmap);
- the natural transformation (bset);
- a cardinal bound represented as minimal well-order relations [10] (here, that of natural numbers,  $\aleph_0$ );
- a witness term (the empty bag  $\{\#\}$ );
- a custom relator (brel).

The user is then requested to discharge the BNF assumptions [8, Section 2]:

$$\begin{array}{l} \text{bmap id} = \text{id} \quad \text{bmap } (f \circ g) = \text{bmap } f \circ \text{bmap } g \quad \frac{\forall x. x \in \text{bset } xs \Rightarrow f x = g x}{\text{bmap } f xs = \text{bmap } g xs} \\ |\text{bset } xs| \leq_o \aleph_0 \quad \text{bset} \circ \text{bmap } f = \text{image } f \circ \text{bset} \\ \text{brel } R x y \Leftrightarrow \exists z. \text{bset } z \subseteq \{(x, y) \mid R x y\} \wedge \text{bmap fst } z = x \wedge \text{bmap snd } z = y \\ \text{brel } R \circ \circ \text{brel } S \sqsubseteq \text{brel } (R \circ \circ S) \end{array}$$

(The operator  $\leq_o$  is a well-order on ordinals [10],  $\sqsubseteq$  denotes implication lifted to binary predicates, and  $\circ \circ$  denotes the relational composition of binary predicates.) In addition, the user is invited to discharge the nonemptiness witness property  $\text{bset } \{\#\} = \{\}$ .

### 3 Coinductive Derivation Trees

Before turning to the nonemptiness witnesses, we first study a concrete codatatype definable with our package. It consists of derivation trees for a context-free grammar, where we perform the following changes to the usual setting: Trees are possibly infinite and the generated words are not lists, but finite sets. The Isabelle formalization of this example [9] lays at the heart of the results presented in the next section. Indeed, this particular codatatype will provide the infrastructure for tracking nonemptiness of arbitrary (co)datatypes.

We take a few liberties with Isabelle notations to lighten the presentation; in particular, until Section 4, we always ignore the distinction between sets and types.

*Definition of Derivation Trees.* We fix a set  $T$  of *terminals* and a set  $N$  of *nonterminals*. The command

```
codatatype dtree = Node (root: N) (cont: (T + dtree) fset)
```

introduces a constructor  $\text{Node} : \mathbb{N} \rightarrow (\mathbb{T} + \text{dtree}) \text{fset} \rightarrow \text{dtree}$  and two selectors  $\text{root} : \text{dtree} \rightarrow \mathbb{N}$ ,  $\text{cont} : \text{dtree} \rightarrow (\mathbb{T} + \text{dtree}) \text{fset}$ . A tree has the form  $\text{Node } n \text{ as}$ , where  $n$  is a nonterminal (the tree's *root*) and  $\text{as}$  is a finite set of terminals and trees (its *continuation*). The `codatatype` keyword indicates that this tree formation rule may be applied an infinite number of times.

Given the above definition of `dtree`, the package first composes the input BNF to the final coalgebra operation  $\text{pre\_dtree} = (\times) \circ (\text{C}_{\mathbb{N}}, \text{fset} \circ ((+) \circ (\text{C}_{\mathbb{T}}, \text{ID})))$  from the constants  $\mathbb{N}$  and  $\mathbb{T}$ , identity, sum, product, and finite set. In the sequel, we prefer the more readable notation  $\alpha \text{pre\_dtree} = \mathbb{N} \times (\mathbb{T} + \alpha) \text{fset}$ . Then it constructs the final coalgebra `dtree` (= JF) from `pre_dtree` (= F).

The unfolding bijection  $\text{dtr} : \text{dtree} \rightarrow \text{dtree pre\_dtree}$  is decomposed in two selectors:  $\text{root} = \text{fst} \circ \text{dtr}$  and  $\text{cont} = \text{snd} \circ \text{dtr}$ . The constructor `Node` is defined as the inverse of the unfolding bijection. The basic properties of constructors and selectors (e.g., injectivity, distinctness) are derived from those of sums and products.

After some massaging that involves splitting according to the indicated destructors, the abstract coiterator from Section 2.2 leaves the stage to the `dtree` coiterator `unfold` :  $(\beta \rightarrow \mathbb{N}) \rightarrow (\beta \rightarrow (\mathbb{T} + \beta) \text{fset}) \rightarrow \beta \rightarrow \text{dtree}$  characterized as follows: For all sets  $\beta$ , functions  $r : \beta \rightarrow \mathbb{N}$ ,  $c : \beta \rightarrow (\mathbb{T} + \beta) \text{fset}$ , and elements  $b \in \beta$ ,

$$\text{root } (\text{unfold } r \ c \ b) = r \ b \quad \text{cont } (\text{unfold } r \ c \ b) = (\text{id} \oplus \text{unfold } r \ c) \cdot c \ b$$

Intuitively, the coiteration contract reads as follows: Given a set  $\beta$ , to define a function  $f : \beta \rightarrow \text{dtree}$  we must indicate how to build a tree for each  $b \in \beta$ . The root is given by  $r$ , and its continuation is given corecursively by  $c$ . Formally,  $f = \text{unfold } r \ c$ .

*A Variation of Context-Free Grammars.* We consider a variation of context-free grammars, acting on finite sets instead of sequences. We assume that the previously fixed sets  $\mathbb{T}$  and  $\mathbb{N}$ , of terminals and nonterminals, are finite and that we are given a set of *productions*  $\text{P} \subseteq \mathbb{N} \times (\mathbb{T} + \mathbb{N}) \text{fset}$ . The triple  $\text{Gr} = (\mathbb{T}, \mathbb{N}, \text{P})$  forms a (*set*) *grammar*, which is fixed for the rest of this section. Both finite and infinite derivation trees are of interest. The codatatype `dtree` constitutes a suitable universe for defining well-formed trees as a coinductive predicate.

Fixpoint (or Knaster–Tarski) (co)induction is provided in Isabelle/HOL by a separate package [32]. Fixpoint induction relies on the minimality of a predicate (the least fixpoint); dually, fixpoint coinduction relies on maximality (the greatest fixpoint). It is well known that datatypes interact well with definitions by fixpoint induction. For codatatypes, both fixpoint induction and fixpoint coinduction play an important role—the former to express safety properties, the latter to express liveness.

*Well-formed* derivation trees for  $\text{Gr}$  are defined coinductively as the greatest predicate  $\text{wf} : \text{dtree} \rightarrow \text{bool}$  such that, for all  $t \in \text{dtree}$ ,

$$\text{wf } t \Leftrightarrow (\text{root } t, (\text{id} \oplus \text{root}) \cdot \text{cont } t) \in \text{P} \wedge \text{root is injective on } \text{Inr}^- (\text{cont } t) \wedge \forall t' \in \text{Inr}^- (\text{cont } t). \text{wf } t'$$

Each nonterminal node of a well-formed derivation tree  $t$  represents a production. This is achieved by three conditions: (1) the root of  $t$  forms a production together with the terminals constituting its successor leaves and the roots of its immediate subtrees; (2) no two immediate subtrees of  $t$  have the same root; (3) properties 1 and 2 also hold for the



immediate subtrees of  $t$ . The definition's coinductive nature ensures that these properties hold for arbitrarily deep subtrees of  $t$ , even if  $t$  has infinite depth.

In contrast to well-formedness, the notions of subtree, interior (the set of nonterminals appearing in a tree), and frontier (the set of terminals appearing in a tree) require inductive definitions. The *subtree* relation  $\text{subtr} : \text{dtree} \rightarrow \text{dtree} \rightarrow \text{bool}$  is defined inductively as the least predicate satisfying the rules

$$\begin{aligned} & \text{subtr } t \ t \\ & \text{subtr } t \ t'' \wedge \text{Inr } t'' \in \text{cont } t' \Rightarrow \text{subtr } t \ t' \end{aligned}$$

We write  $\text{Subtr } t$  for the set of subtrees of  $t$ . The *interior*  $\text{ltr} : \text{dtree} \rightarrow \mathbb{N}$  set is defined inductively by the rules

$$\begin{aligned} & \text{root } t \in \text{ltr } t \\ & \text{Inr } t_1 \in \text{cont } t \wedge n \in \text{ltr } t_1 \Rightarrow n \in \text{ltr } t \end{aligned}$$

The *frontier*  $\text{Fr} : \text{dtree} \rightarrow \mathbb{N}$  set is defined inductively by

$$\begin{aligned} & \text{Inl } t \in \text{cont } t \Rightarrow t \in \text{Fr } t \\ & \text{Inr } t_1 \in \text{cont } t \wedge t \in \text{Fr } t_1 \Rightarrow t \in \text{Fr } t \end{aligned}$$

The language generated by the grammar  $\text{Gr}$  from a nonterminal  $n \in \mathbb{N}$  (via possibly infinite derivation trees) is defined as  $\mathcal{L}_{\text{Gr}}(n) = \{\text{Fr } t \mid \text{wf } t \wedge \text{root } t = n\}$ .

*Regular Derivation Trees.* A derivation tree is *regular* if each subtree is uniquely determined by its root. Formally, we define *regular*  $t$  as the existence of a function  $f : \mathbb{N} \rightarrow \text{Subtr } t$  such that  $\forall t' \in \text{Subtr } t. f(\text{root } t') = t'$ . The regular language of a nonterminal is defined as  $\mathcal{L}_{\text{Gr}}^r(n) = \{\text{Fr } t \mid \text{wf } t \wedge \text{root } t = n \wedge \text{regular } t\}$ .

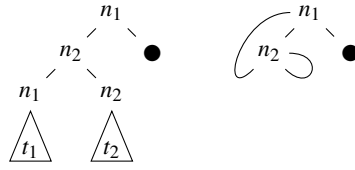
Given a possibly nonregular derivation tree  $t_0$ , a *regular cut* of  $t_0$  is a regular tree  $\text{rcut } t_0$  such that  $\text{Fr}(\text{rcut } t_0) \subseteq \text{Fr } t_0$ . Here is one way to perform the cut:

1. Choose a subtree of  $t_0$  for each interior node  $n \in \text{ltr } t_0$  via a function  $\text{pick} : \text{ltr } t_0 \rightarrow \text{Subtr } t_0$  with  $\forall n \in \text{ltr } t_0. \text{root}(\text{pick } n) = n$ .
2. Traverse  $t_0$  and substitute  $\text{pick } n$  for each subtree with root  $n$ . Perform this substitution hereditarily, i.e., also in the emerging subtree  $\text{pick } n$ .

This substitution task is elegantly achieved by the corecursive function  $\text{H} : \text{ltr } t_0 \rightarrow \text{dtree}$  defined as  $\text{unfold } r \ c$ , where  $r : \text{ltr } t_0 \rightarrow \mathbb{N}$  and  $c : \text{ltr } t_0 \rightarrow (\mathbb{T} + \text{ltr } t_0)$  fset are specified as follows:  $r \ n = n$  and  $c \ n = (\text{id} \oplus \text{root}) \cdot \text{cont}(\text{pick } n)$ . The function  $\text{H}$  is therefore characterized by the corecursive equations  $\text{root}(\text{H } n) = n$  and  $\text{cont}(\text{H } n) = (\text{id} \oplus (\text{H} \circ \text{root})) \cdot \text{cont}(\text{pick } n)$ . It is not hard to prove the following by fixpoint coinduction:

**Lemma 1.** For all  $n \in \text{ltr } t_0$ ,  $\text{H } n$  is regular and  $\text{Fr}(\text{H } n) \subseteq \text{Fr } t_0$ . Moreover,  $\text{H } n$  is well-formed provided  $t_0$  is well-formed.

*Proof.*  $\text{H } n$  is regular by construction: If a subtree of it has root  $n'$ , then it is equal to  $\text{H } n'$ . The frontier inclusion  $\text{Fr}(\text{H } n) \subseteq \text{Fr } t_0$  follows by routine fixpoint induction on the definition of  $\text{Fr}$  (since at each node  $n' \in \text{ltr}(\text{H } n)$  we only have the immediate leaves of  $\text{pick } n'$ , which is a subtree of  $\text{Fr } t_0$ ). Finally, assume that  $t_0$  is well-formed. Then the well-formedness of  $\text{H } n$  follows by routine fixpoint coinduction on the definition of  $\text{wf}$  (since, again, at each  $n' \in \text{ltr}(\text{H } n)$  we have the production of  $\text{pick } n'$ ).  $\square$



**Figure 1.** A derivation tree (left) and a minimal regular cut (right)

We define  $\text{rcut } t_0$  to be  $H(\text{root } t_0)$ . Figure 1 shows a derivation tree and a minimal regular cut. The bullets denote terminals, and  $t_1$  and  $t_2$  are arbitrary trees with roots  $n_1$  and  $n_2$ . The loop indicates an infinite tree that is its own subtree.

## 4 Computing Nonemptiness Witnesses

In the previous two sections, we referred to the codatatype  $\text{dtree}$  and other collections of elements as *sets*, ignoring an important aspect of HOL. While for most purposes sets and types can be identified in an abstract treatment of the logic, empty types are not allowed. The main primitive way to define custom types in HOL is to specify from an existing type  $\alpha$  a nonempty subset  $A : \alpha$  set that is isomorphic to the desired type. Hence, to register a collection of elements as a HOL type (and take advantage of the associated convenience, notably static type checking), it is necessary to prove it nonempty.

Datatype definitions are an instance of the above scenario, with the additional requirement that nonemptiness should be discharged automatically. When producing the relevant nonemptiness proofs, the package must take into consideration arbitrary combinations of basic and user-defined BNFs, datatypes, and codatatypes.

A first idea would be to follow the traditional approach of HOL datatype packages [6, 14]: Unfold all the definitions of the involved nested datatypes, inlining them as additional components of the mutual definition, until only sums of products remain, and then perform a reachability analysis. However, this approach is problematic in our framework. Due to open-endedness, there is no fixed set of basic types. Delving into nested types requires reproving nonemptiness facts, which scales poorly. Moreover, it is not clear how to unfold datatypes nested in codatatypes or vice versa.

By relying on all specifications being eventually reducible to the fixed situation of sums of products, the traditional approach needs to consider nonemptiness only at the point of a datatype definition. Here, we look for a prophylactic solution instead, trying to prepare the BNFs for future nonemptiness checks involving them. To this end, we ask: Given a mutual datatype definition involving several  $n$ -ary BNFs, what is the relevant information we need to know about their nonemptiness *without knowing what they look like* (hence, with no option to delve into them)? To answer this, we use a generalization of pointed types [20, 25], by maintaining witnesses that assert conditional nonemptiness for combinations of arguments. We introduce the solution by examples.

## 4.1 Introductory Examples

We start with the simple cases of products and sums. For  $\alpha \times \beta$ , the proof is as follows: Assuming  $\alpha \neq \emptyset$  and  $\beta \neq \emptyset$ , we construct the witness  $(a, b) \in \alpha \times \beta$  for some  $a \in \alpha$  and  $b \in \beta$ . For  $\alpha + \beta$ , two proofs are possible: Assuming  $\alpha \neq \emptyset$ , we can construct  $\text{Inl } a$  for some  $a \in \alpha$ ; alternatively, assuming  $\beta \neq \emptyset$ , we can construct  $\text{Inr } b$  for some  $b \in \beta$ .

With each BNF  $\bar{\alpha} F$ , we associate a set of witnesses, each of the form  $\text{Fwit} : \alpha_{i_1} \rightarrow \dots \rightarrow \alpha_{i_k} \rightarrow \bar{\alpha} F$  for a subset  $\{i_1, \dots, i_k\} \subseteq [n]$ . From a witness, we can construct a set-theoretic proof by following its signature, in the spirit of the Curry–Howard correspondence. Accordingly,  $\text{Inr} : \beta \rightarrow \alpha + \beta$  can be read as the following contract: Given a proof that  $\beta$  is nonempty,  $\text{Inr}$  yields a proof that  $\alpha + \beta$  is nonempty.

When BNFs are composed, so are their witnesses. The two possible witnesses for the list-defining functor  $(\alpha, \beta)$   $\text{pre\_list} = \text{unit} + \alpha \times \beta$  are  $\text{wit\_pre\_list}_1 = \text{Inl } ()$  and  $\text{wit\_pre\_list}_2 a b = \text{Inr } (a, b)$ . The first witness subsumes the second one, because it unconditionally shows the collection nonempty, regardless of the potential emptiness of  $\alpha$  and  $\beta$ . From this witness, we obtain the witness  $\text{list\_ctor wit\_pre\_list}_1$  (i.e.,  $\text{Nil}$ ).

Because they can store infinite objects, codatatype set constructors are never empty provided their arguments are nonempty. Compare the following:

```
datatype  $\alpha$  fstream = FSCons  $\alpha$  ( $\alpha$  fstream)
codatatype  $\alpha$  stream = SCons  $\alpha$  ( $\alpha$  stream)
```

The datatype definition fails because the optimal witness has a circular signature:  $\alpha \rightarrow \alpha \text{ fstream} \rightarrow \alpha \text{ fstream}$ . In contrast, the codatatype definition succeeds and produces the witness  $(\lambda a. \mu s. \text{SCons } a s) : \alpha \rightarrow \alpha \text{ stream}$ , namely the (unique) stream  $s$  such that  $s = \text{SCons } a s$  for a given  $a \in \alpha$ . This stream is easy to define by coiteration.

Let us now turn to a pair of examples involving nesting:

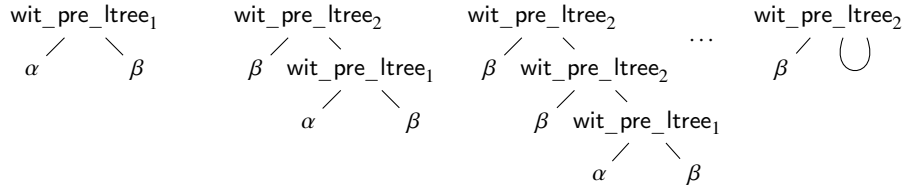
```
datatype  $(\alpha, \beta)$  tree = Leaf  $\beta$  | Branch (( $\alpha + (\alpha, \beta)$  tree) stream)
codatatype  $(\alpha, \beta)$  ltree = LNode  $\beta$  (( $\alpha + (\alpha, \beta)$  ltree) stream)
```

In the tree definition, the two constructors hide a sum BNF, giving us some flexibility. For the Leaf constructor, all we need is a witness  $b \in \beta$ , from which we construct Leaf  $b$ . For Branch, we can choose the left-hand side of the nested  $+$ , completely avoiding the recursive right-hand side: From a witness  $a \in \alpha$ , we construct Branch  $(\mu s. \text{SCons } (\text{Inl } a) s)$ .

For the ltree functor, the two arguments to LNode are hiding a product, so the ltree-defining functor is  $(\alpha, \beta, \gamma)$   $\text{pre\_ltree} = \beta \times (\alpha + \gamma)$  stream with  $\gamma$  representing the corecursive component. Composition yields two witnesses for pre\_ltree:

```
wit_pre_ltree1 a b = (b,  $\mu s. \text{SCons } (\text{Inl } a) s$ )
wit_pre_ltree2 b c = (b,  $\mu s. \text{SCons } (\text{Inr } c) s$ )
```

These can serve to build infinitely many witnesses for ltree. Figure 2 enumerates the possible combinations, starting with  $\text{wit\_pre\_ltree}_1$ . This witness requires only the noncorecursive components  $\alpha$  and  $\beta$  to be nonempty, and hence immediately yields a witness  $\text{wit\_ltree}_1 : \alpha \rightarrow \beta \rightarrow (\alpha, \beta) \text{ ltree}$  (by applying the constructor LNode). The second witness  $\text{wit\_pre\_ltree}_2$  requires both  $\beta$  and the corecursive component  $\gamma$  to be



**Figure 2.** Derivation trees for ltree witnesses

nonempty; it effectively “consumes” another ltree witness through  $\gamma$ . The consumed witness can again be either  $\text{wit\_pre\_ltree}_1$  or  $\text{wit\_pre\_ltree}_2$ , and so on. At the limit,  $\text{wit\_pre\_ltree}_2$  is used infinitely often. The corresponding witness  $\text{wit\_ltree}_2 : \beta \rightarrow (\alpha, \beta)$  ltree can be defined by coiteration as  $\lambda b. \mu t. \text{wit\_pre\_ltree}_2 \ b \ t$ . It subsumes  $\text{wit\_ltree}_1$  and all the other finite witnesses. But had ltree been defined as a datatype instead of a codatatype,  $\text{wit\_ltree}_1$  would have been its optimal witness.

## 4.2 A General Solution

The nonemptiness problem for an  $n$ -ary set constructor  $F$  and a set of indices  $I \subseteq [n]$  can be stated as follows: Is  $\bar{\alpha} F \neq \emptyset$  whenever  $\forall i \in I. \alpha_i \neq \emptyset$ , for all sets  $\bar{\alpha}_n$ ? We call  $F$   $I$ -witnessed if the answer is yes. Thus, set sum (+) is  $\{1\}$ -,  $\{2\}$ -, and  $\{1, 2\}$ -witnessed; set product ( $\times$ ) is  $\{1, 2\}$ -witnessed; and  $\alpha$  list is  $\emptyset$ - and  $\{1\}$ -witnessed. This leads to the following notion of soundness: Given an  $n$ -ary functor  $F$ , a set  $\mathcal{I} \subseteq [n]$  set is (*witness*-) *sound* for  $F$  if  $F$  is  $I$ -witnessed for all  $I \in \mathcal{I}$ .

The next question is: When is such a set  $\mathcal{I}$  also complete, in that it covers all witnesses? Clearly, if  $I_1 \subseteq I_2$ , then  $I_1$ -witnesshood implies  $I_2$ -witnesshood. Therefore, we are interested in retaining the witnesses completely only up to inclusion of sets of indices. A set  $\mathcal{I} \subseteq [n]$  set is (*witness*-) *complete* for  $F$  if for all  $J \subseteq [n]$  such that  $F$  is  $J$ -witnessed, there exists  $I \in \mathcal{I}$  such that  $I \subseteq J$ ; (*witness*-) *perfect* for  $F$  if it is both sound and complete.

Here are perfect sets  $\mathcal{I}_F$  for basic BNFs:

- Identity:  $\mathcal{I}_{\alpha \text{ ID}} = \{\{\alpha\}\}$
- Constant:  $\mathcal{I}_{C_{n,\alpha}} = \{\emptyset\}$  ( $\alpha \neq \emptyset$ )
- Sum:  $\mathcal{I}_{\alpha+\beta} = \{\{\alpha\}, \{\beta\}\}$
- Product:  $\mathcal{I}_{\alpha \times \beta} = \{\{\alpha, \beta\}\}$
- Function space:  $\mathcal{I}_{\beta \text{ func}_\alpha} = \{\{\beta\}\}$  ( $\alpha \neq \emptyset$ )
- Bounded  $k$ -powerset:  $\mathcal{I}_{\alpha \text{ set}_k} = \{\emptyset\}$

Parameters  $\alpha_j$  are identified with their indices  $j$  to improve readability.

Perfect sets must be maintained across BNF operations. Let us start with composition, permutation, and lifting.

**Theorem 1.** Let  $H = G \circ \bar{F}_n$ , where  $G \in \text{Func}_n$  has a perfect set  $\mathcal{I}$  and each  $F_j \in \text{Func}_m$  has a perfect set  $\mathcal{I}_j$ . Then  $\{\bigcup_{j \in J} I_j \mid J \in \mathcal{I} \wedge (I_j)_{j \in J} \in \prod_{j \in J} \mathcal{I}_j\}$  is a perfect set for  $H$ .

*Proof sketch.* Let  $\mathcal{K} = \{\bigcup_{j \in J} I_j \mid J \in \mathcal{J} \wedge (I_j)_j \in \prod_{j \in J} \mathcal{S}_j\}$ . We first prove that  $\mathcal{K}$  is sound for H. Let  $K \in \mathcal{K}$  and  $\bar{\alpha}_m$  be such that  $\forall i \in K. \alpha_i \neq \emptyset$ . By the definition of  $\mathcal{K}$ , we obtain  $J \in \mathcal{J}$  and  $(I_j)_{j \in J}$  such that (1)  $K = \bigcup_{j \in J} I_j$  and (2)  $\forall j \in J. I_j \in \mathcal{S}_j$ . Using (1), we have  $\forall j \in J. \forall i \in I_j. \alpha_i \neq \emptyset$ . Hence, since each  $\mathcal{S}_j$  is sound for  $F_j$ ,  $\forall j \in J. \bar{\alpha} F_j \neq \emptyset$ . Finally, since  $\mathcal{J}$  is sound for G, we obtain  $\bar{\alpha} \bar{F} G \neq \emptyset$ , i.e.,  $\bar{\alpha} H \neq \emptyset$ .

We now prove that  $\mathcal{K}$  is complete for H. Let  $K \subseteq [m]$  be such that H is  $K$ -witnessed. Let  $\bar{\beta}_n$  be defined as  $\beta_j = \text{unit}$  if  $j \in K$  and  $\emptyset$  otherwise, and let  $J = \{j \in [n] \mid \bar{\beta} F_j \neq \emptyset\}$ . Since H is  $K$ -witnessed, we obtain that  $\bar{\beta} H \neq \emptyset$ , i.e., (3)  $\bar{\beta} \bar{F} G \neq \emptyset$ .

We show that (4) G is  $J$ -witnessed. Let  $\bar{\gamma}_n$  such that  $\forall j \in J. \gamma_j \neq \emptyset$ . Thanks to the definition of  $J$ , we have  $\forall j \in [n]. F_j \neq \emptyset \Rightarrow \gamma_j \neq \emptyset$ , and therefore we obtain the functions  $(f_j : \bar{\beta} F_j \rightarrow \gamma_j)_{j \in [n]}$ . With  $\text{Gmap } \bar{f} : \bar{\beta} \bar{F} G \rightarrow \bar{\gamma} G$ , by (3) we obtain  $\bar{\gamma} G \neq \emptyset$ .

From (4), since  $J$  is complete for G, we obtain  $J_1 \in \mathcal{J}$  such that  $J_1 \subseteq J$ . Let  $j \in J_1$ . By the definition of  $J$ , we have  $\bar{\beta} F_j \neq \emptyset$ , making  $\bar{\beta} F_j$   $K$ -witnessed (by definition of  $\bar{\beta}$ ); hence, since  $\mathcal{S}_j$  is  $F_j$ -complete, we obtain  $I_j \in \mathcal{S}_j$  such that  $I_j \subseteq K$ . Then  $K_1 = \bigcup_{j \in J_1} I_j$  belongs to  $\mathcal{K}$  and is included in  $K$ .  $\square$

**Theorem 2.** Let  $\mathcal{J} \subseteq [n]$  set be a perfect set for F. Then  $\mathcal{J}$  and  $\mathcal{J}^{(i,j)}$  are perfect sets for  $F \uparrow$  and  $F^{(i,j)}$ , respectively, where  $\mathcal{J}^{(i,j)}$  is  $\mathcal{J}$  with  $i$  and  $j$  exchanged in each of its elements.

Theorems 1 and 2 hold not only for functors but also for plain set constructors (with a further cardinality-monotonicity assumption needed for the completeness part of Theorem 1). The most interesting cases are the genuinely functorial ones of initial algebras and final coalgebras. Witnesses for initial algebras and final coalgebras are essentially obtained by repeated compositions of the witnesses of the involved BNFs and the folding bijections, inductively in one case and coinductively in the other. The derivation trees from Section 3 turn out to be perfectly suited for recording the combinatorics of these compositions, so that both soundness and completeness follow easily.

For the rest of this subsection, we fix  $n$  ( $m+n$ )-ary functors  $\bar{\beta} F_j$  and assume each  $F_j$  has a perfect set  $\mathcal{K}_j$ . We start by constructing a (set) grammar  $\text{Gr} = (\text{T}, \text{N}, \text{P})$  with  $\text{T} = [m]$ ,  $\text{N} = [n]$ , and  $\text{P} = \{(j, \text{cp}(K)) \mid K \in \mathcal{K}_j\}$ , where, for each  $K \subseteq [m+n]$ ,  $\text{cp}(K)$  is its copy to  $[m] + [n]$  defined as  $\text{Inl} \cdot ([m] \cap K) \cup \text{Inr} \cdot \{k \in [n] \mid m+k \in K\}$ .

The intuition is as follows. A mutual datatype definition introduces  $n$  isomorphisms  $\bar{\alpha} \text{IF}_j \cong (\bar{\alpha}, \bar{\alpha} \text{IF}_j, \dots, \bar{\alpha} \text{IF}_n) F_j$ . We are looking for conditions that guarantee nonemptiness of the functors  $\text{IF}_j$ . To this end, we traverse these isomorphisms from left to right, reducing nonemptiness of  $\bar{\alpha} \text{IF}_j$  to that of  $(\bar{\alpha}, \bar{\alpha} \text{IF}_1, \dots, \bar{\alpha} \text{IF}_n) F_j$ . Nonemptiness of the latter can be reduced to nonemptiness of some  $\alpha_{i_1}, \dots, \alpha_{i_p}$  and some  $\bar{\alpha} \text{IF}_{j_1}, \dots, \bar{\alpha} \text{IF}_{j_q}$ , via a witness for  $F_j$  of the form  $\{i_1, \dots, i_p, m+j_1, \dots, m+j_q\}$ . This yields a grammar production  $j \rightarrow \{\text{Inl } i_1, \dots, \text{Inl } i_p, \text{Inr } j_1, \dots, \text{Inr } j_q\}$ , where the  $i_k$ 's are terminals and the  $j_l$ 's are, like  $j$ , nonterminals. The ultimate goal is to reduce the nonemptiness of  $\bar{\alpha} \text{IF}_j$  to that of components of  $\bar{\alpha}$  alone, i.e., to terminals. This precisely corresponds to derivations in the grammar of terminal sets. It should be intuitively clear that by considering finite derivations, we obtain sound witnesses for  $\text{IF}_j$ . We actually prove more: For initial algebras, finite derivations are also witness-complete; for final coalgebras (substituting  $\bar{\text{JF}}$  for  $\bar{\text{IF}}$ ), accepting infinite derivations is sound and also required for completeness.

**Theorem 3.** Assume that the final coalgebra of  $\bar{F}$  exists and consists of  $n$   $m$ -ary functors  $\bar{\alpha}_m \text{JF}_j$  (cf. Section 2.1). Then  $\mathcal{L}_{\text{Gr}}^r(j)$  is a perfect set for  $\text{JF}_j$ , for  $j \in [n]$ .

To prove soundness, we define a nonemptiness witness to  $\bar{\alpha} \text{JF}_j$  corecursively (by abstract  $\text{JF}$ -corecursion). Showing completeness is more interesting: We define a function to  $\text{dtree}$  corecursively (by concrete tree corecursion), obtaining a derivation tree, from which we then cut a regular derivation tree by exploiting Lemma 1.

*Proof sketch.* Let  $j_0 \in [n]$ . We first show that  $\mathcal{L}_{\text{Gr}}^r(j_0)$  is sound. Let  $t_0$  be a well-formed regular derivation tree with root  $j_0$ . We must prove that  $\text{F}_{j_0}$  is  $\text{Fr } t_0$ -witnessed. For this, we fix  $\bar{\alpha}_m$  such that  $\forall i \in \text{Fr } t_0. \alpha_i \neq \emptyset$ , and aim to show that  $\bar{\alpha} \text{JF}_{j_0} \neq \emptyset$ .

For each  $j \in \text{ltr } t_0$ , let  $t_j$  be the corresponding subtree of  $t_0$ . (It is well-defined, since  $t_0$  is regular.) Note that  $t_0 = t_{j_0}$ . For each  $K$  such that  $(j, \text{cp}(K)) \in \text{P}$ , since  $K \in \mathcal{K}_j$  and  $\mathcal{K}_j$  is sound for  $\text{F}_j$ , we obtain a  $K$ -witness for  $\text{F}_j$ , i.e., a function  $w_{j,K} : (\gamma_k)_{k \in K} \rightarrow \bar{\gamma} \text{F}_j$  (polymorphic in  $\bar{\gamma}$ ).

Let  $\bar{\beta}_n$  be defined as  $\beta_j = \text{unit}$  if  $j \in \text{ltr } t_0$  and  $\emptyset$  otherwise. We build a coalgebra structure on  $\bar{\beta}$ ,  $(s_j : \beta_j \rightarrow (\bar{\alpha}, \bar{\beta}) \text{F}_j)_{j \in [n]}$ , as follows: If  $j \notin \text{ltr } t_0$ , then  $s_j$  is the unique function from  $\emptyset$ . Otherwise, let  $s_j () = w_{j,K} (a_i)_{i \in K \cap [m]} ()^{|\text{K} \cap [m+1, m+n]|}$ , where  $\text{cp}(K)$  is the right-hand side of the top production of  $t_j$ , i.e.,  $(\text{id} \oplus \text{root}) \cdot \text{cont } t_j$ . For each  $j \in \text{ltr } t_0$ ,  $\text{unfold}_j \bar{s} : \text{unit} \rightarrow \bar{\alpha} \text{JF}_j$  ensures the nonemptiness of  $\bar{\alpha} \text{JF}_j$ . In particular,  $\bar{\alpha} \text{JF}_{j_0} \neq \emptyset$ .

We now show that  $\mathcal{L}_{\text{Gr}}^r(j_0)$  is complete. Let  $I \subseteq [m]$  such that  $\text{JF}_{j_0}$  is  $I$ -witnessed. We must find  $I_1 \in \mathcal{L}_{\text{Gr}}^r(j_0)$  such that  $I_1 \subseteq I$ . Let  $\bar{\alpha}_m$  be defined as  $\alpha_i = \text{unit}$  if  $i \in I$  and  $\emptyset$  otherwise. Let  $J = \{j \mid \bar{\alpha} \text{F}_j \neq \emptyset\}$ . We define  $c : J \rightarrow ([m] + J)$  fset by  $c j = \text{cp}(K_j)$ , where  $K_j$  is such that  $(j, \text{cp}(K_j)) \in \text{P}$  and  $K_j \subseteq I \cup \{m+j \mid j \in J\}$ .

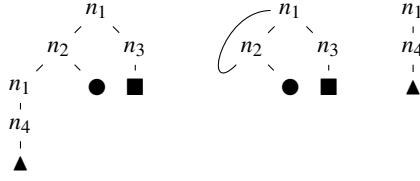
Now let  $g : J \rightarrow \text{dtree}$  be  $\text{unfold id } c$ . Thus, for all  $j \in J$ ,  $\text{root}(g j) = j$  and  $\text{cont}(g j) = (\text{id} \oplus g) \cdot c j = \text{Inl} \cdot (K_j \cap I) \cup \text{Inr} \cdot \{g j \mid m+j \in K_j\}$ . Taking  $t_0 = g j_0$  and using Lemma 1, we obtain the regular well-formed tree  $t_1$  such that  $\text{Fr } t_1 \subseteq \text{Fr } t_0 \subseteq I$ . Hence  $\text{Fr } t_1$  is the desired index set  $I_1$ .  $\square$

The above completeness proof provides an example of self-application of codatatypes: A specific codatatype, of infinite derivation trees, arises in the metatheory of general codatatypes. And this may well be unavoidable: While for soundness the regular trees are replaceable by some equivalent (finite) inductive items, it is not clear how completeness could be proved without first considering arbitrary infinite derivation trees and then cutting them down to regular trees.

An analogous result holds for initial algebras. For each  $i \in \mathbb{N}$ , let  $\mathcal{L}_{\text{Gr}}^{\text{rf}}(i)$  be the language generated by  $i$  by means of regular finite derivation trees for grammar  $\text{Gr}$ . Since  $\mathbb{N}$  is finite, these can be described more directly as trees for which every nonterminal path has no repetitions.

In the following proofs, we exploit an embedding of datatypes as finite codatatypes. Using this embedding, we can transfer the recursive definition and structural induction principles from  $\bar{\text{F}}$  to finite elements of  $\bar{\text{JF}}$ , and in particular from a datatype  $\text{fdtree}$  of finite trees (Appendix C) to finite trees in  $\text{dtree}$ .

The regular cut of a tree works well with respect to the metatheory of codatatypes, but for datatypes it has the disadvantage that it may produce infinite trees out of finite ones, as depicted in Figure 3 (left and middle). We need a slightly different concept for datatypes: the finite regular cut (right). Let  $t_0$  be a finite derivation tree. We define



**Figure 3.** A finite derivation tree (left), a regular cut (middle), and a finite regular cut (right)

the function  $\text{fpick} : \text{ltr } t_0 \rightarrow \text{Subtr } t_0$  similarly to pick from Section 3, but making sure that the choice of the subtrees  $\text{fpick } n$  is minimal, in that  $\text{fpick } n$  does not have  $n$  in the interior of a proper subtree (and hence does not have any proper subtree of root  $n$ ). Such a choice is possible owing to the finiteness of  $t_0$ . We define the finite regular cut of  $t_0$ ,  $\text{rfcut } t_0$ , analogously to  $\text{rcut } t_0$ , using  $\text{fpick}$  instead of pick.

**Lemma 2.** Assume  $t_0$  is a finite derivation tree. Then:

- (1) The statement of Lemma 1 holds if we replace  $\text{rcut}$  by  $\text{rfcut}$ .
- (2)  $\text{rfcut } t_0$  is finite.

*Proof.* (1) Similar to the proof of Lemma 1. (2) By routine induction on  $t_0$ .  $\square$

**Theorem 4.** Assume that the initial algebra of  $\bar{F}$  exists and consists of  $n$   $m$ -ary functors  $\bar{\alpha}_m \text{IF}_j$  (cf. Section 2.1). Then  $\mathcal{L}_{\text{Gr}}^{\text{rf}}(j)$  is a perfect set for  $\text{IF}_j$ , for  $j \in [n]$ .

*Proof.* Let  $j_0 \in [n]$ . We first show that  $\mathcal{L}_{\text{Gr}}^{\text{rf}}(j_0)$  is sound. Let  $t_0$  be a well-formed finite regular derivation tree with root  $j_0$ . We must prove that  $F_{j_0}$  is  $\text{Fr } t_0$ -witnessed. For this, we fix  $\bar{\alpha}_m$  such that  $\forall i \in \text{Fr } t_0. \alpha_i \neq \emptyset$ , and aim to show that  $\bar{\alpha} \text{IF}_{j_0} \neq \emptyset$ .

For each  $j \in \text{ltr } t_0$ , let  $t_j$  be the corresponding subtree of  $t_0$ . (It is well-defined, since  $t_0$  is regular.) Note that  $t_0 = t_{j_0}$ . For each  $K$  such that  $(j, \text{cp}(K)) \in \text{P}$ , since  $K \in \mathcal{K}_j$  and  $\mathcal{K}_j$  is sound for  $F_j$ , we obtain a  $K$ -witness for  $F_j$ , i.e., a function  $w_{j,K} : (\alpha_k)_{k \in K} \rightarrow \bar{\alpha} F_j$ .

We verify the following fact by induction on the finite derivation tree  $t$ : If  $\exists j \in \text{ltr } t_0. t = t_j$ , then  $\bar{\alpha} \text{IF}_j \neq \emptyset$ . The induction step goes as follows: Assume  $t = t_j$  has the form  $\text{Node } j \text{ as}$ , and let  $J$  be the set of all roots of the immediate subtrees of  $t$ , namely,  $\text{root} \bullet (\text{Inr}^- (\text{cont } t))$ . By the induction hypothesis,  $\bar{\alpha} \text{IF}_{j'} \neq \emptyset$  (say,  $b_{j'} \in \bar{\alpha} \text{IF}_{j'}$ ) for all  $j' \in J$ . Then  $w_{j,K} (a_i)_{i \in \text{Inl}^- t} (b_{j'})_{j' \in J} \in \bar{\alpha} \text{IF}_j$ , making  $\bar{\alpha} \text{IF}_j$  nonempty. In particular,  $\bar{\alpha} \text{IF}_{j_0} \neq \emptyset$ .

We now show that  $\mathcal{L}_{\text{Gr}}^{\text{rf}}(j_0)$  is complete. Let  $I \subseteq [m]$  such that  $\text{IF}_{j_0}$  is  $I$ -witnessed. We must find  $I_1 \in \mathcal{L}_{\text{Gr}}^{\text{rf}}(j_0)$  such that  $I_1 \subseteq I$ . Let  $\bar{\alpha}_m$  be defined as  $\alpha_i = \text{unit}$  if  $i \in I$  and  $\emptyset$  otherwise. We verify, by structural  $\bar{\text{IF}}$ -induction on  $b$ , that for all  $j \in [n]$  and  $b \in \bar{\alpha} \text{IF}_j$ , there exists a finite well-formed derivation tree  $t$  such that  $\text{root } t = j$  and  $\text{Fr } t \subseteq I$ . For the inductive step, assume  $\text{ctor}_j x \in \bar{\alpha} \text{IF}_j$ , where  $x \in (\bar{\alpha}, \bar{\alpha} \bar{\text{IF}}) F_j$ . By the induction hypotheses, we obtain the finite well-formed derivation trees  $\bar{t}_n$  such that  $\text{root } \bar{t}_j = j$  and  $\text{Fr } \bar{t}_j \subseteq I$  for all  $j \in [n]$ . Let  $J = \{j' \in [n] \mid \bar{\alpha} \text{IF}_{j'} \neq \emptyset\}$ . Then  $F_j$  is  $(I \cup J)$ -witnessed, hence by the  $F_j$ -completeness of  $\mathcal{K}_j$  we obtain  $K \in \mathcal{K}_j$  such that  $K \subseteq I \cup \{m + j' \mid j' \in J\}$ . We take  $t$  to have  $j$  as root,  $I \cap K$  as leaves and  $(t_{j'})_{j' \in J}$  as immediate subtrees; namely,  $t = \text{Node } j (\text{Inl} \bullet I \cup \text{Inr} \bullet \{t_{j'} \mid j' \in J\})$ .

Let  $t_0$  be a tree as above corresponding to  $j_0$  (since  $\bar{\alpha} \Vdash_{j_0} \neq \emptyset$ ). Then, by Lemma 2,  $t_1 = \text{rcut } t_0$  is a well-formed finite derivation tree such that  $\text{Fr } t_1 \subseteq \text{Fr } t_0 \subseteq I$ . Thus, taking  $I_1 = \text{Fr } t_1$ , we obtain  $I_1 \in \mathcal{L}_{\text{Gr}}^{\text{rf}}(j_0)$  and  $I_1 \subseteq I$ .  $\square$

Let us see how Theorems 1 to 4 can be combined in establishing or refuting non-emptiness for some of our motivating examples from Sections 1 and 4.1.

- $\mathcal{I}_{(\alpha, \beta) \text{ pre\_list}} = \{\emptyset\}$  by Theorem 1;  $\mathcal{I}_{\alpha \text{ list}} = \{\emptyset\}$  by Theorem 4
- $\mathcal{I}_{(\alpha, \beta) \text{ pre\_fstream}} = \{\{\alpha, \beta\}\}$ ;  $\mathcal{I}_{\alpha \text{ fstream}} = \emptyset$  by Theorem 4 (i.e.,  $\alpha \text{ fstream}$  is empty)
- $\mathcal{I}_{(\alpha, \beta) \text{ pre\_stream}} = \{\{\alpha, \beta\}\}$ ;  $\mathcal{I}_{\alpha \text{ stream}} = \{\{\alpha\}\}$  by Theorem 3
- $\mathcal{I}_{(\alpha, \beta, \gamma) \text{ pre\_ltree}} = \{\{\alpha, \beta\}, \{\beta, \gamma\}\}$  by Theorem 1;  
 $\mathcal{I}_{(\alpha, \beta) \text{ ltree}} = \{\{\beta\}\}$  by Theorem 3
- $\mathcal{I}_{(\alpha, \beta, \gamma) \text{ pre\_t}_1} = \{\{\beta\}, \{\alpha, \gamma\}\}$ ,  $\mathcal{I}_{(\alpha, \beta, \gamma) \text{ pre\_t}_2} = \{\emptyset\}$ , and  
 $\mathcal{I}_{(\alpha, \beta, \gamma) \text{ pre\_t}_3} = \{\{\alpha\}, \{\gamma\}\}$  by Theorem 1;  $\mathcal{I}_{t_i} = \{\emptyset\}$  by Theorem 4

Since we have maintained perfect sets throughout all the BNF operations, we obtain the following central result.

**Theorem 5.** Any BNF built from other BNFs endowed with perfect sets of witnesses (in particular all basic BNFs discussed in this paper) by repeated applications of the composition, initial algebra, and final coalgebra operations has a perfect set defined as indicated in Theorems 1 to 4.

**Corollary 1.** The nonemptiness problem is decidable for arbitrarily nested, mutual (co)datatypes.

Consequently, a procedure implementing Theorems 1 to 4 will preserve enough nonemptiness witnesses to ensure that all specifications describing nonempty datatypes are accepted. The next subsection presents such a procedure.

### 4.3 Computational Aspects

Theorem 3 reduces the computation of perfect sets for final coalgebras to that of  $\mathcal{L}_{\text{Gr}}^{\text{r}}(n)$ . The use of infinite regular trees in the definition of  $\mathcal{L}_{\text{Gr}}^{\text{r}}(n)$  allows a simple proof of soundness, and the only natural proof of completeness we could think of, relating the coinductive nature of arbitrary mutual codatatypes with that of infinite trees. However, from a computational point of view, the use of infinite trees is excessive.

In fact,  $\mathcal{L}_{\text{Gr}}(n)$  and  $\mathcal{L}_{\text{Gr}}^{\text{f}}(n)$ , the nonregular versions of the generated languages, are computable by fixpoint iteration on finite sets. It is not hard to show that  $\mathcal{L}_{\text{Gr}}$  and  $\mathcal{L}_{\text{Gr}}^{\text{f}}$  are the greatest and least solutions of the following fixpoint equation, involving the variable  $X : \mathbb{N} \rightarrow ((\text{T} + \mathbb{N}) \text{ set}) \text{ set}$ , where the order is componentwise inclusion:

$$X n = \{ \text{Inl}^- ss \cup \bigcup_{n' \in \text{Inr}^- ss} K_{n'} \mid (n, ss) \in \text{P} \wedge K \in \prod_{n' \in \text{Inr}^- ss} X n' \}$$

The equation simply states the expected closure under the grammar productions, familiar from formal language theory. But since the “words” are finite sets and not lists, a fixpoint is reached after at most  $\text{card } \mathbb{N}$  iterations.



However, it is easier to settle this computational aspect by working with the regular versions  $\mathcal{L}_{Gr}^r(n)$  and  $\mathcal{L}_{Gr}^{rf}(n)$ , whose structure nicely exhibits boundedness. Namely, we prove for these languages a bounded version of the above fixpoint equation, featuring a decumulator that witnesses the finite convergence of the computation.

First, we relativize the notion of frontier to that of “frontier through  $ns$ ,”  $Fr\ ns\ t$ , containing the leaves of  $t$  accessible by paths of nonterminals from  $ns \subseteq N$ . We also define the corresponding  $ns$ -restricted regularly generated language  $\mathcal{L}_{Gr}^r\ ns\ n$ . Thus, what used to be denoted by  $Fr\ t$  and  $\mathcal{L}_{Gr}^r\ n$  now becomes  $Fr\ N\ t$  and  $\mathcal{L}_{Gr}^r\ N\ n$ .

In what follows, by “word” we mean “finite set of terminals.” We can think of a generated word as being more precise than another provided the former is a subword (subset) of the latter. This leads us to defining, for languages (sets of words), the notions of word-inclusion subsumption,<sup>2</sup>  $\leq$ , by  $L \leq L'$  iff  $\forall w \in L. \exists w' \in L'. w' \subseteq w$ , and equivalence,  $\equiv$ , by  $L \equiv L'$  iff  $L \leq L'$  and  $L' \leq L$ . It is easy to see that any set  $\equiv$ -equivalent to a perfect set is again perfect. Note also that Lemma 1 implies  $\mathcal{L}_{Gr}^r(n) \equiv \mathcal{L}_{Gr}(n)$ , which qualifies regular trees as a generated-language optimization of arbitrary trees.

We compute  $\mathcal{L}_{Gr}^r\ ns\ n$  up to word-inclusion equivalence  $\equiv$  by recursively applying available productions whose source nonterminals are in  $ns$ , removing each time from  $ns$  the expanded nonterminal. Thus, if  $n$  is in  $ns$ ,  $\mathcal{L}_{Gr}^r\ ns\ n$  calls  $\mathcal{L}_{Gr}^r\ ns'\ n'$  recursively with  $ns' = ns \setminus \{n\}$  for each nonterminal  $n'$  in the chosen production from  $n$ , and so on, until the current node is no longer in the decumulator  $ns$ :

**Theorem 6.** For all  $ns \subseteq N$  and  $n \in N$ ,  $\mathcal{L}_{Gr}^r\ ns\ n \equiv$

$$\begin{cases} \{\emptyset\} & \text{if } n \notin ns \\ \{\text{Inl}^- ss \cup \bigcup_{n' \in \text{Inr}^- ss} K_{n'} \mid (n, ss) \in P \wedge K \in \prod_{n' \in \text{Inr}^- ss} \mathcal{L}_{Gr}^r(ns \setminus \{n\}) n'\} & \text{otherwise} \end{cases}$$

*Proof sketch.*  $\mathcal{L}_{Gr}^r\ ns\ n \subseteq \{\emptyset\}$ , since  $Fr\ ns\ t = \emptyset$  for all  $t$  such that  $\text{root } t = n$ . It remains to show that  $\emptyset \in \mathcal{L}_{Gr}^r\ ns\ t$ , i.e., to find a derivation tree with root  $n$ . Using the assumption that there are no unused nonterminals, we can build a “default derivation tree”  $\text{deftr } n$  for each  $n$  as follows. We pick, for each  $n$ , a set  $S n \in (T + N)$  fset such that  $(n, S n) \in P$ . Then we define  $\text{deftr} : N \rightarrow \text{dtree}$  corecursively as  $\text{deftr} = \text{unfold id } S$ , i.e., such that  $\text{root}(\text{deftr } n) = n$  and  $\text{cont}(\text{deftr } n) = (\text{id} \oplus \text{deftr}) \bullet S n$ . It is easy to prove by fixpoint coinduction that  $\text{deftr } n$  is a derivation tree for each  $n$ .

Now assume  $n \notin ns$ , and let  $ns' = ns \setminus \{n\}$ . For the left-to-right direction, we prove more than  $\leq$ , namely, actual inclusion between  $\mathcal{L}_{Gr}^r\ ns\ n$  and the righthand side. Assume  $t$  is a well-formed regular derivation tree of root  $n$ . We must find  $ss \in (T + N)$  fset and  $U : \text{Inr}^- ss \rightarrow \text{dtree}$  such that, for all  $n' \in \text{Inr}^- ss$ ,  $U\ n'$  is a well-formed regular derivation tree of root  $n'$  and  $Fr\ ns\ t = \text{Inl}^- ss \cup \bigcup_{n' \in \text{Inr}^- ss} Fr\ ns'\ (U\ n')$ . Clearly,  $ss$  should be the right-hand side of the top production of  $t$ . As for  $U$ , the immediate subtrees of  $t$  would appear to be suitable candidates; however, these do not work, since our goal is to have  $Fr\ ns\ t$  covered by  $(\text{Inl}^- ss$  in conjunction with)  $Fr\ ns'\ (U\ n')$ , while the immediate subtrees only guarantee this property with respect to  $Fr\ ns\ (U\ n')$ , i.e., allowing paths to go through  $n$  as well. A correct solution is again offered by a corecursive definition: We build the tree  $t_0$  from  $t$  by substituting hereditarily each subtree with root  $n$  by  $t$ . Formally, we take  $t_0 = \text{unfold } r\ c$ , where  $r\ t' = \text{root } t'$  and  $c\ t' = \text{cont } t'$  if  $\text{root } t' = n$

<sup>2</sup> This is in effect the Smyth preorder extension [38] of the subword relation.

and  $c t' = \text{cont } t'$  otherwise. It is easy to prove that  $t_0$ , like  $t$ , is a regular derivation tree. Thus, we can define  $U$  to give, for any  $n'$ , the corresponding immediate subtree of  $t_0$ .

To prove the right-to-left direction, let  $ss \in (\mathbb{T} + \mathbb{N}) \text{ fset}$  and  $K \in \prod_{n' \in \text{Inr}^- ss} \mathcal{L}_{\text{Gr}}^r ns' n'$  such that  $ts = \text{Inl}^- ss \cup \bigcup_{n' \in \text{Inr}^- ss} K_{n'}$ . Unfolding the definition of  $\mathcal{L}_{\text{Gr}}^r$ , we obtain  $U : \text{Inr}^- ss \rightarrow \text{dtree}$  such that, for all  $n' \in \text{Inr}^- ss$ ,  $U n'$  is a regular derivation tree of root  $n'$  such that  $K_{n'} \in \text{Fr } ns' (U n')$ . Then the tree of immediate leafs  $\text{Inl}^- ss$  and immediate subtrees  $\{U n' \mid n' \in \text{Inr}^- ss\}$ , namely,  $\text{Node } n ((\text{id} \oplus U) \bullet ss)$ , is the desired regular derivation tree whose frontier is included  $ts$ .  $\square$

Theorem 6 provides an alternative, recursive definition of  $\mathcal{L}_{\text{Gr}}^r ns n$ . The definition terminates because the argument  $ns$  is finite and decreases strictly in the recursive case. This shows that the height of the recursive call stack is bounded by the number of non-terminals, which corresponds to the number of simultaneously introduced codatatypes.

Here is how the above recursion operates on the ltree example. We have  $\mathbb{T} = \{\alpha, \beta\}$ ,  $\mathbb{N} = \{\gamma\}$ , and  $\mathbb{P} = \{p_1, p_2\}$ , where  $p_1 = (\gamma, \{\text{Inl } \alpha, \text{Inl } \beta\})$  and  $p_2 = (\gamma, \{\text{Inl } \beta, \text{Inr } \gamma\})$ . Note that

- $\text{Inl}^- ss = \{\alpha, \beta\}$  and  $\text{Inr}^- ss = \emptyset$  for  $(n, ss) = p_1$
- $\text{Inl}^- ss = \{\beta\}$  and  $\text{Inr}^- ss = \{\gamma\}$  for  $(n, ss) = p_2$

The computation has one single recursive call, yielding

$$\begin{aligned}
\mathcal{L}_{\text{Gr}}^r \gamma &= \mathcal{L}_{\text{Gr}}^r \{\gamma\} \gamma \\
&\equiv \{\{\alpha, \beta\} \cup \emptyset\} \cup \{\{\beta\} \cup \bigcup_{n' \in \{\gamma\}} K_{n'} \mid K \in \prod_{n' \in \{\gamma\}} \mathcal{L}_{\text{Gr}}^r \emptyset n'\} \\
&= \{\{\alpha, \beta\}\} \cup \{\{\beta\} \cup K_\gamma \mid K_\gamma \in \mathcal{L}_{\text{Gr}}^r \emptyset \gamma\} \\
&= \{\{\alpha, \beta\}\} \cup \{\{\beta\} \cup \emptyset\} \\
&= \{\{\alpha, \beta\}, \{\beta\}\} \\
&\equiv \{\{\beta\}\}
\end{aligned}$$

For datatypes, the computation of  $\mathcal{L}_{\text{Gr}}^{\text{rf}}$  is achieved analogously to Theorem 6, defining  $\mathcal{L}_{\text{Gr}}^{\text{rf}} ns n$  as a generalization of  $\mathcal{L}_{\text{Gr}}^r n$ .

In what follows,  $nl$  ranges over lists of nonterminals and the centered dot operator  $(\cdot)$  denotes list concatenation. If  $n$  is a nonterminal,  $n$  also denotes the  $n$ -singleton list. The predicate  $\text{path } nl t$ , stating that  $nl$  is a path in  $t$  (starting from the root), is defined inductively as follows:

$$\begin{aligned}
&\text{path } (\text{root } t) t \\
&\text{Inr } t' \in \text{cont } t \wedge \text{path } nl t' \Rightarrow \text{path } ((\text{root } t) \cdot nl) t'
\end{aligned}$$

**Lemma 3.** Let  $t$  be a finite regular derivation tree. Then  $t$  has no paths that contain repetitions.

*Proof.* Assume, by absurdity, that a path  $nl$  in  $t$  contains repetitions, i.e., has the form  $nl_1 \cdot n \cdot nl_2 \cdot n$ , and let  $t_1$  and  $t_2$  be the subtrees corresponding to the paths  $nl_1 \cdot n$  and  $nl_2$ , respectively. Then  $t_2$  is a proper subtree of  $t_1$ ; on the other hand, by the regularity of  $t$ , we have  $t_1 = t_2$ , which is impossible since  $t_1$  and  $t_2$  are finite.  $\square$

**Theorem 7.** The statement of Theorem 6 still holds if we substitute  $\mathcal{L}_{Gr}^{rf}$  for  $\mathcal{L}_{Gr}^r$  and  $\emptyset$  for  $\{\emptyset\}$ .

*Proof.* By Lemma 3 and the properties of regular cuts, we have (1)  $\mathcal{L}_{Gr}^{rf} ns' n \equiv \mathcal{L}_{Gr}^{pf} ns' n$ , where  $\mathcal{L}_{Gr}^{pf} ns' n$  is the language defined like  $\mathcal{L}_{Gr}^{rf} ns' n$  but replacing “regular” with “having no paths that contain repetitions.” Moreover, it is easy to see that (2) the desired facts hold if we replace  $\mathcal{L}_{Gr}^{rf} ns' n$  with  $\mathcal{L}_{Gr}^{pf} ns' n$  and  $\equiv$  with equality. The result follows from (1) and (2).  $\square$

## 5 Implementation in Isabelle

The package maintains nonemptiness information for producing nonemptiness proofs arising when defining datatypes. The equations from Theorems 6 and 7 involve only executable operations over finite sets of numbers, sums, and products. Since the descriptions of Theorems 1 and 2 are also executable, the implementation task emerges clearly: Store a perfect set with each basic BNF, and have each BNF operation compute witnesses from those of its operands.

However, as it stands,  $I$ -witnesshood cannot be expressed in HOL because types are always nonempty: How can we state that  $(\alpha, \beta)$  tree  $\neq \emptyset$  conditionally on  $\alpha \neq \emptyset$  or  $\beta \neq \emptyset$ , in the context of  $\alpha$  and  $\beta$  being assumed nonempty in the first place? The solution is to work not with operators  $\bar{\alpha}F$  on HOL types directly but rather with their *internalization* to sets, expressed as a polymorphic function  $\text{Fin} : \alpha_1 \text{ set} \rightarrow \dots \rightarrow \alpha_n \text{ set} \rightarrow (\bar{\alpha} F) \text{ set}$  defined as  $\text{Fin } \bar{A} = \{x \mid \forall i \in [n]. \text{Fset}^i x \subseteq A_i\}$ .  $I$ -witnesshood is then expressible as  $(\forall i \in I. A_i \neq \emptyset) \Rightarrow \text{Fin } \bar{A} \neq \emptyset$ .

For each  $n$ -ary BNF  $F$ , the package stores a set of sets  $\mathcal{S}$  of numbers in  $[n]$  (the perfect set) and, for each set  $I \in \mathcal{S}$ , a polymorphic constant  $w_I : (\alpha_i)_{i \in I} \rightarrow \bar{\alpha} F$  and an equivalent formulation of  $I$ -witnesshood:  $\forall i \in I. \text{Fset}^i (w_I (a_j)_{j \in I}) \neq \emptyset$ .

Due to the logic’s restricted expressiveness, we cannot prove the theorems presented in this paper in their most general form for arbitrary functors and have the package instantiate them for specific functors. Instead, the package proves the theorems dynamically for the specific functors involved in the datatype definitions. Only the soundness part of the theorems is needed. Completeness is desirable, because in its absence some legitimate definitions would be rejected. To paraphrase Krauss and Nipkow [24], completeness belongs to the realm of metatheory and is not required to obtain actual nonemptiness proofs—it merely lets you sleep better.

A HOL definitional package bears the burden of computing terms and certifying the computation, i.e., ensuring that certain terms are theorems. The combinatorial computation of witnessing sets of indices described in Theorems 6 and 7 would be expensive if performed through Isabelle, that is, by executing the equations stated in these theorems as term rewriting in the logic. Instead, we perform the computation outside the logic, employing a Standard ML datatype aimed at efficiently representing the finite and the regular derivation trees inhabiting the Isabelle type `dtree` from Section 3:

```
datatype wit_tree = Wit_Leaf of int
                  | Wit_Node of (int * int * int list) * wit_tree list
```

Here, `Wit_Node ((i, j, is), ts)` stores the root nonterminal  $i$ , a numeric identifier of the used production  $j$ , and the continuation consisting of the terminals  $is$  and the further nonterminal expanded trees  $ts$ . Moreover, `Wit_Leaf i` stores, in the case of regular infinite trees, the nonterminal where a regularity loop occurs, i.e., such that it has a previous occurrence on the path to the root.

From this tree datatype, we produce witnesses represented as Isabelle constants of appropriate types (the  $w_I$ 's described above), by essentially mimicking the (co)recursive definitions employed in the proofs of the soundness parts of Theorems 3 and 4. We certify the witnesses by producing the relevant Isabelle proof goals and discharging them by mirroring the corresponding (co)inductive arguments from the aforementioned proofs. In summary: The witnesses are computed outside the logic, but they are verified by Isabelle's kernel. After introducing a BNF, redundant witnesses are silently removed.

The development devoted to the production and certification of witnesses amounts to about 1000 lines of Standard ML [9].

## 6 Related Work

Coinductive (or coalgebraic) datatypes have become popular in recent years in the study of infinite behaviors and nonterminating computation. Whereas inductive datatypes are well studied and widely available in most programming languages and proof assistants, coinductive types are still not mainstream, and their integration into existing systems poses many challenges.

In the context of theorem proving, much research has been done in the past few years on how to add coinductive types or improve support of coinductive proofs, notably in Agda [2], CIRC [27], and Coq [7, 29]. The work described in this paper is in line with this research. The results are applicable to other proof assistants from the HOL family.

In HOL-based systems, other definitional packages must also prove nonemptiness of newly defined types, but typically the proofs are easy. For example, Homeier's quotient package for HOL4 [19] exploits the observation that quotients of nonempty sets are nonempty, and Huffman's (co)recursive domain package for Isabelle/HOLCF [21] can rely on a minimal element  $\perp$ . For the traditional datatype packages introduced by Melham [28], and implemented in Isabelle/HOL by Berghofer and Wenzel [6], proving nonemptiness is nontrivial, but by reducing nested definitions to mutual definitions, they could employ a standard reachability analysis [6, §4.1]. To our knowledge, the completeness of the analysis has not been proved (or even formulated) for these.

Obviously, our overall approach to (co)datatypes is heavily inspired by category-theory developments [5, 12, 17, 18, 35]—this is discussed in detail in a previous paper [39], which puts forward a program for integrating insight from category theory in proof assistants based on higher-order logic, to achieve better structure and functionality. A similar program is pursued on a larger scale in the context of homotopy type theory [40], targeting proof assistants based on type theory, notably Agda and Coq. Our nonemptiness witness maintenance is similar to the preservation of enriched types along various constructions—for example, initial algebras and final coalgebras of pointed functors are also pointed [20]. However, existing analysis techniques are only concerned with soundness (not completeness) results.

## 7 Conclusion

We presented a complete solution to the nonemptiness problem for open-ended, mutual, nested codatatypes. This problem arose in the context of Isabelle’s new (co)datatype package and has broad practical applicability in terms of the popularity of HOL-based provers. The problem and its solution also enjoy an elegant metatheory, which itself is best expressed in terms of codatatypes. Our solution, like the rest of the definitional package, is part of the latest edition of Isabelle.

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## A Abstract (Co)induction

Using the atomic infrastructure described in Section 2.2, the induction principle can be expressed abstractly for the mutual initial algebra  $\bar{1}\bar{F}$  of functors  $\bar{F}$  as follows for sets  $\bar{\alpha}$  and predicates  $\varphi_j : \bar{\alpha} \mid \bar{F}_j \rightarrow \text{bool}$ :

$$\frac{\bigwedge_{j=1}^n \forall x \in (\bar{\alpha}, \bar{\alpha} \mid \bar{1}\bar{F}) \bar{F}_j. (\bigwedge_{k=1}^n \forall b \in \text{Fset}_j^{m+k} x. \varphi_k b) \Rightarrow \varphi_j (\text{ctor}_j x)}{\bigwedge_{j=1}^n \forall b \in \bar{\alpha} \mid \bar{F}_j. \varphi_j b}$$

For lists, this instantiates to

$$\frac{\forall x \in \text{unit} + \alpha \times \alpha \text{ list}. (\forall b \in \text{Fset}^2 x. \varphi b) \Rightarrow \varphi (\text{ctor } x)}{\forall b \in \alpha \text{ list}. \varphi b}$$

which, by taking  $\text{Nil} = \text{ctor} (\text{Inl } ())$  and  $\text{Cons } a b = \text{ctor} (\text{Inr } (a, b))$ , can be recast into the familiar rule

$$\frac{\varphi \text{ Nil} \quad \forall a \in \alpha. \forall b \in \alpha \text{ list. } \varphi b \Rightarrow \varphi (\text{Cons } a b)}{\forall b \in \alpha \text{ list. } \varphi b}$$

Moving to coinduction, we need a further well-known assumption: that our functors preserve weak pullbacks, or, equivalently, that they induce relators [34]. For a functor  $\bar{\alpha}_n F$ , we lift its action  $\text{Fmap} : (\alpha_1 \rightarrow \beta_1) \rightarrow \dots \rightarrow (\alpha_n \rightarrow \beta_n) \rightarrow \bar{\alpha} F \rightarrow \bar{\beta} F$  on functions to an action  $\text{Frel} : (\alpha_1 \rightarrow \beta_1 \rightarrow \text{bool}) \rightarrow \dots \rightarrow (\alpha_n \rightarrow \beta_n \rightarrow \text{bool}) \rightarrow (\bar{\alpha} F \rightarrow \bar{\beta} F \rightarrow \text{bool})$ , the *relator*, defined as follows:

$$\text{Frel } \bar{\varphi} x y \Leftrightarrow \exists z. \text{Fmap } \overline{\text{fst}} z = x \wedge \text{Fmap } \overline{\text{snd}} z = y \wedge \bigwedge_{i=1}^n \forall (a, b) \in \text{Fset}^i z. \varphi_i a b$$

Structural coinduction can also be expressed abstractly, for the mutual final coalgebra  $\bar{JF}$  of functors  $\bar{F}$ :

$$\frac{\bigwedge_{j=1}^n \forall a b \in (\bar{\alpha}, \bar{\alpha} \bar{JF}) F_j. \theta_j a b \Rightarrow \text{Frel}_j (=)^m \bar{\theta} (\text{dtor}_j a) (\text{dtor}_j b)}{\bigwedge_{j=1}^n \forall a b. \theta_j a b \Rightarrow a = b}$$

for sets  $\bar{\alpha}_n$  and binary predicates  $\theta_j \in \bar{\alpha} JF_j \rightarrow \bar{\alpha} JF_j \rightarrow \text{bool}$ . The rule is parameterized by predicates  $\theta_j : \bar{\alpha} JF_j \rightarrow \bar{\alpha} JF_j \rightarrow \text{bool}$  required by the antecedent to form an  $\bar{F}$ -bisimulation. The principle effectively states that equality is the largest  $\bar{F}$ -bisimulation [35].

## B Concrete Coiteration and Coinduction

*Coiteration.* The abstract coiteration principle described in Section 2.1 relies on a coiterator  $\text{unfold} : (\beta \rightarrow \beta \text{ pre\_dtree}) \rightarrow \beta \rightarrow \text{dtree}$  such that  $\text{dtor} \circ \text{unfold } s = \text{map\_pre\_dtree} (\text{unfold } s) \circ s$ . Writing  $s$  as  $\langle r, c \rangle$  for  $r : \beta \rightarrow \mathbb{N}$  and  $c : \beta \rightarrow (\mathbb{T} + \alpha) \text{ fset}$  and recasting the equation in pointful form yields  $\text{dtor} (\text{unfold } \langle r, c \rangle b) = \text{map\_pre\_dtree} (\text{unfold } s) (rb, cb)$ . This can be further improved by unfolding the definition of  $\text{map\_pre\_dtree}$ , expressing  $\text{dtor}$  as  $\langle \text{root}, \text{cont} \rangle$ , and splitting the result into a pair of equations:  $\text{root} (\text{unfold } \langle r, c \rangle b) = r b$  and  $\text{cont} (\text{unfold } \langle r, c \rangle b) = (\text{id} \oplus \text{unfold } \langle r, c \rangle) \cdot c b$ . The coiteration rule of Section 2.1 emerges by replacing  $\text{unfold}$  with the curried  $\text{unfold}' : (\beta \rightarrow \mathbb{N}) \rightarrow (\beta \rightarrow (\mathbb{T} + \beta) \text{ fset}) \rightarrow \beta \rightarrow \text{dtree}$  defined as  $\text{unfold}' r c = \text{unfold } \langle r, c \rangle$ .

*Coinduction.* The abstract coinduction principle of Appendix A is customized into the following concrete coinduction for  $\text{dtree}$ :

$$\frac{\forall t_1 t_2. \theta t_1 t_2 \Rightarrow \text{root } t_1 = \text{root } t_2 \wedge \text{fset\_rel} (\text{sum\_rel} (=) \theta) (\text{cont } t_1) (\text{cont } t_2)}{\theta t_1 t_2 \Rightarrow t_1 = t_2}$$

where the predicate  $\text{fset\_rel} (\text{sum\_rel} (=) \theta)$  is an instance of the abstract  $\text{Frel}$ : It gives the componentwise extension of  $\theta$  to  $(\mathbb{T} + \text{dtree}) \text{ fset}$ . Unfolding the characteristic theorems for  $\text{fset\_rel}$  and  $\text{sum\_rel}$  yields the antecedent

$$\begin{aligned} \forall t_1 t_2. \theta t_1 t_2 \Rightarrow & \text{root } t_1 = \text{root } t_2 \wedge \\ & \text{Inl}^- (\text{cont } t_1) = \text{Inl}^- (\text{cont } t_2) \wedge \\ & \forall t'_1 \in \text{Inr}^- (\text{cont } t_1). \exists t'_2 \in \text{Inr}^- (\text{cont } t_2). \theta t'_1 t'_2 \wedge \\ & \forall t'_2 \in \text{Inr}^- (\text{cont } t_2). \exists t'_1 \in \text{Inr}^- (\text{cont } t_1). \theta t'_1 t'_2 \end{aligned}$$



where  $\text{Inl}^-(\text{cont } t)$  is the set of  $t$ 's successor leaves and  $\text{Inr}^-(\text{cont } t)$  is the set of its immediate subtrees. Informally: If two trees are in relation  $\theta$ , then they have the same root and the same successor leaves and for each immediate subtree of one, there exists an immediate subtree of the other in relation  $\theta$  with it.

## C Concrete Iteration and Induction

Finite trees can be defined by

```
datatype fdtree = FNode (froot : N) (fcont : (T + dtree) fset)
```

This produces the operations `FNode`, `froot`, and `fcont`, with the same constructor-selector properties as `Node`, `root` and `cont` from the codatatype `dtree` introduced in Section 3. The differences concern (co)induction and (co)recursion.

*Iteration.* The general principle described in Section 2.1 employs in the unary case an iterator `fold` of (polymorphic) type  $(\beta \text{ pre\_fdtree} \rightarrow \beta) \rightarrow \text{fdtree} \rightarrow \beta$ , for which it yields  $\forall s : \beta \text{ pre\_fdtree} \rightarrow \beta. \text{fold } s \circ \text{ctor} = s \circ \text{map\_pre\_fdtree } (\text{fold } s)$ , that is,

$$\forall s : \beta \text{ pre\_fdtree} \rightarrow \beta. \forall k. \text{fold } s (\text{ctor } k) = s (\text{map\_pre\_fdtree } (\text{fold } s) k)$$

The `fdtree`-defining BNF coincides with the `dtree`-defining BNF:  $\beta \text{ pre\_fdtree} = \mathbb{N} \times (\mathbb{T} + \beta) \text{ fset}$  and  $\text{map\_pre\_fdtree } f = \text{id} \otimes (\text{image } (\text{id} \oplus f))$ .

The above characterization needs some customization. Using the `FNode` instead of `ctor` and unfolding the definition of `map\_pre\_fdtree`, we obtain  $\forall s : \mathbb{N} \times (\mathbb{T} + \beta) \text{ fset} \rightarrow \beta. \forall n \text{ as}. \text{fold } s (\text{FNode } n \text{ as}) = s (\text{map\_pre\_fdtree } (\text{fold } s) (n, \text{as}))$ . By unfolding the definition of `map\_pre\_fdtree`, we obtain

$$\forall s : \mathbb{N} \times (\mathbb{T} + \beta) \text{ fset} \rightarrow \beta. \forall n \text{ as}. \text{fold } s (\text{FNode } n \text{ as}) = s (n, (\text{id} \oplus \text{fold } s) \bullet \text{as})$$

Finally, replacing `fold` with its more convenient curried version  $\text{fold}' : (\mathbb{N} \rightarrow (\mathbb{T} + \beta) \text{ fset} \rightarrow \beta) \rightarrow \text{fdtree} \rightarrow \beta$  defined as  $\text{fold}' s = \text{fold } (\lambda(n, \text{as}). s \ n \ \text{as})$ , we obtain the following customized iteration principle, where we write `fold` instead of `fold'`: For all sets  $\beta$ , functions  $s : \mathbb{N} \rightarrow (\mathbb{T} + \beta) \text{ fset} \rightarrow \beta$  and elements  $n \in \mathbb{N}$  and  $\text{as} \in (\mathbb{T} + \text{fdtree}) \text{ fset}$ , it holds that  $\text{fold } s (\text{FNode } n \ \text{as}) = s \ n \ ((\text{id} \oplus \text{fold } s) \bullet \text{as})$ .

*Induction.* The induction principle from Section A yields for  $\varphi : \alpha \text{ fdtree} \rightarrow \text{bool}$

$$\frac{\forall k \in \alpha \text{ pre\_fdtree}. (\forall t \in \text{Fset } k. \varphi \ t) \Rightarrow \varphi (\text{ctor } k)}{\forall t \in \alpha \text{ fdtree}. \varphi \ t}$$

i.e., using the curried variation `FNode` of `ctor`,

$$\frac{\forall n \text{ as}. (\forall t \in \text{Fset } (n, \text{as}). \varphi \ t) \Rightarrow \varphi (\text{FNode } n \ \text{as})}{\forall t \in \alpha \text{ fdtree}. \varphi \ t}$$

Unfolding the definition of `Fset`, namely,  $\text{Fset } (n, \text{as}) = \text{Inr}^- \text{as}$ , we obtain the end-product customized induction for finite trees:

$$\frac{\forall n \text{ as}. (\forall t \in \text{Inr}^- \text{as}. \varphi \ t) \Rightarrow \varphi (\text{FNode } n \ \text{as})}{\forall t \in \alpha \text{ fdtree}. \varphi \ t}$$