Coalgebraic Infinite Traces and Kleisli Simulations

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Abstract

Kleisli simulation is a categorical notion introduced by Hasuo to verify finite trace inclusion. They allow us to give definitions of *forward and backward simulation* for various types of systems. A generic categorical theory behind Kleisli simulation has been developed and it guarantees the soundness of those simulations wrt. *finite* trace semantics. Moreover, those simulations can be aided by *forward partial execution* (FPE) – a categorical transformation of systems previously introduced by the authors.

In this paper, we give Kleisli simulation a theoretical foundation that assures its soundness also wrt. *infinite* trace. There, following Jacobs' work, infinite trace semantics is characterized as the "largest homomorphism." It turns out that soundness of forward simulations is rather straightforward; that of backward simulation holds too, although it requires certain additional conditions and its proof is more involved. We also show that FPE can be successfully employed in the infinite trace setting to enhance the applicability of Kleisli simulations as witnesses of trace inclusion. Our framework is parameterized in the monad for branching as well as in the functor for linear-time behaviors; for the former we use the powerset monad (for nondeterminism) as well as the sub-Giry monad (for probability).

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1 Introduction

Language inclusion of transition systems is an important problem in both qualitative and quantitative verification. In a qualitative setting the problem is concretely as follows: for given two nondeterministic systems $\mathcal{X}$ and $\mathcal{Y}$, check if $L(\mathcal{X}) \subseteq L(\mathcal{Y})$ – that is, if the set of words generated by $\mathcal{X}$ is included in the set of words generated by $\mathcal{Y}$. In a typical usage scenario, $\mathcal{X}$ is a model of the *implementation* in question while $\mathcal{Y}$ is a model that represents the *specification* of $\mathcal{X}$. More concretely, $\mathcal{Y}$ is a system such that $L(\mathcal{Y})$ is easily seen not to contain anything "dangerous" – therefore the language inclusion $L(\mathcal{X}) \subseteq L(\mathcal{Y})$ immediately implies that $L(\mathcal{X})$ contains no dangerous output, either. Such a situation can also arise in a *quantitative setting* where a specification is about *probability*, *reward*, and so on.

▶ **Example 1.1.** In Fig. 1 are four examples of transition systems; $\mathcal{X}$ and $\mathcal{Y}$ are qualitative/nondeterministic; $\mathcal{Z}$ and $\mathcal{W}$ exhibit probabilistic branching. We shall denote the *finite* language of a system $\mathcal{A}$ by $L^*(\mathcal{A})$ and the *infinite* one by $L^\infty(\mathcal{A})$. We define that a generated finite word is one with a run that ends with the termination symbol ✓.

In the nondeterministic setting, languages are *sets* of words. We have $L^*(\mathcal{X}) = \{b\} \subseteq \{b, ab, aab, \ldots\} = L^*(\mathcal{Y})$, i.e. *finite* language inclusion from $\mathcal{X}$ to $\mathcal{Y}$. However $abb\ldots \in L^\infty(\mathcal{X})$ while $abb\ldots \notin L^\infty(\mathcal{Y})$, hence *infinite* language inclusion fails.

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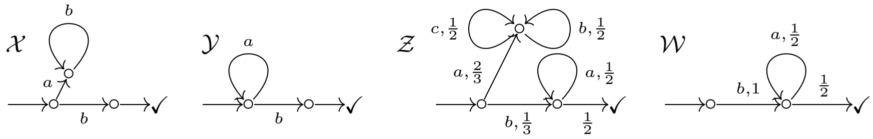

Figure 1 Examples of nondeterministic and probabilistic automata.

In the probabilistic setting, languages are naturally *probability distributions* over words; and language inclusion refers to the pointwise order between probabilities. For example $L^*(\mathcal{Z}) = [b \mapsto \frac{1}{6}, ba \mapsto \frac{1}{12}, baa \mapsto \frac{1}{24}, \ldots]$ and $L^*(\mathcal{W}) = [b \mapsto \frac{1}{2}, ba \mapsto \frac{1}{4}, baa \mapsto \frac{1}{8}, \ldots]$; since the former assigns no greater probabilities to all the words, we say that the finite language of $\mathcal{Z}$ is *included* in that of $\mathcal{W}$. This quantitative notion of trace inclusion is also useful in verification: it gives e.g. an upper bound for the probability for something bad.

Finally, the *infinite* languages for probabilistic systems call for measure-theoretic machinery since, in most of the cases, any infinite word gets assigned the probability 0 (which is also the case in $\mathcal{Z}$ and $\mathcal{W}$). Here it is standard to assign probabilities to *cylinder sets* rather than to individual words; see e.g. [2]. An example of a cylinder set is $\{aw \mid w \in \{b, c\}^\omega\}$. The language $L^\infty(\mathcal{Z})$ assigns $\frac{2}{3}$ to it, while $L^\infty(\mathcal{W})$ assigns 0; therefore we do not have *infinite* language inclusion from $\mathcal{Z}$ to $\mathcal{W}$.

There are many known algorithms for checking language inclusion. A well-known one for NFA is a complete one that reduces the problem to emptiness check; however it involves complementation, hence determinization, that incurs an exponential blowup.

One of the alternative approaches to language inclusion is by *simulation*. In the simulation-based verification we look for a simulation, that is, a witness for *stepwise* language inclusion. The notion of simulation is commonly defined so that it implies (proper, global) language inclusion – a property called *soundness*. Although its converse (*completeness*) fails in many settings, such simulation-based approaches tend to have an advantage in computational cost. One prototype example of such simulation notions is *forward* and *backward simulation* [14], by Lynch and Vaandrager, for nondeterministic automata. They are shown in [14] to satisfy soundness wrt. finite trace: explicitly, existence of a forward (or backward) simulation from $\mathcal{X}$ to $\mathcal{Y}$ implies $L(\mathcal{X}) \subseteq L(\mathcal{Y})$, where the languages collects all the *finite* words generated.

Kleisli simulation [8, 9, 18] is a categorical generalization of these notions of forward and backward simulation by Lynch and Vaandrager. It builds upon the use of coalgebras in a *Kleisli category*, in [10], where they are used to characterize finite traces. Specifically:

- A branching system $\mathcal{X}$ is represented as an F*-coalgebra* $c : X \nrightarrow FX$ in the Kleisli category $\mathcal{K}\ell(T)$, for a suitable choice of a functor F and a monad T. Here F and T are parameters that determine the (linear-time) *transition type* and the *branching type*, respectively, of the system $\mathcal{X}$. Examples are:
  - $F = 1 + \Sigma \times (\_)$ (terminate, or (output and continue)) and the *powerset monad* $T = \mathcal{P}$ on **Sets** (nondeterminism), if $\mathcal{X}$ is a nondeterministic automaton (with explicit termination); and
  - the same functor $F = 1 + \Sigma \times (\_)$ and the *sub-Giry monad* $T = \mathcal{G}$ [7] on the category **Meas** of measurable spaces and measurable functions, for their probabilistic variant.
- In [10], under certain conditions on F and T, it is shown that a *final* F*-coalgebra* in $\mathcal{K}\ell(T)$ arises as a lifting of an initial F-algebra in **Sets**. Moreover, it is observed that the natural notion of "finite trace semantics" or "(finite) languages" is captured by a unique homomorphism via finality. This works uniformly for a wide variety of systems, by changing F and T.

It is shown in [8] that, with respect to this categorical characterization of finite trace [10], both forward and backward Kleisli simulation are indeed sound. This categorical background allows us to instantiate Kleisli simulation for various concrete systems – including both qualitative and quantitative ones – and obtain simulation notions whose soundness wrt. *finite* traces comes for free [8, 9]. Like many other notions of simulation, the resulting simulation sometimes fails to be complete. This drawback of incompleteness wrt. finite trace can be partly mended by *forward partial execution* (FPE), a transformation of coalgebraic systems introduced in [18] that potentially increases the likelihood of existence of simulations.

Contributions. In this paper we continue our series of work [8, 9, 18] and study the relationship between Kleisli simulations and *infinite* traces. This turns out to be more complicated than we had expected, a principal reason being that *infinite* traces are less well-behaved than finite traces (that are characterized simply by finality).

For a suitable coalgebraic characterization of infinite traces we principally follow [11] – also relying on observations in [4, 12] – and characterize infinite traces in terms of *largest homomorphisms.* More specifically, we lift a final F-coalgebra in **Sets** to the Kleisli category $\mathcal{K}\ell(T)$ and exhibit that the latter admits a largest homomorphism. In this paper we (principally) work with: the powerset monad $\mathcal{P}$ (on **Sets**) and the sub-Giry monad $\mathcal{G}$ (on **Meas**), as a monad T for branching; and a polynomial functor F for linear-time behaviors.

Here are our concrete contributions. For each of the above combinations of T and F:

- We show that forward Kleisli simulations are sound with respect to inclusion of *infinite* languages. The proof of this general result is not hard, exploiting the above coalgebraic characterization of infinite languages as largest homomorphisms.
- We show that backward simulations are sound too, although here we have to impose suitable restrictions, like *totality* and *image-finiteness.* The soundness proofs are much more involved, too, and calls for careful inspection of the construction of infinite trace semantics. The proofs are separately for $T = \mathcal{P}$ and for $\mathcal{G}$.
- We show that *forward partial execution* (FPE) – a transformation from [18] that aids discovery of fwd./bwd. simulations – is applicable also to the current setting of *infinite* trace inclusion. More specifically we prove: *soundness* of FPE (discovery of a simulation after FPE indeed witnesses infinite language inclusion); and its *adequacy* (FPE does not destroy simulations that are already there).

Organization. §2 is devoted to categorical preliminaries; we fix notations there. In §3 we review the previous works that we rely on, namely coalgebraic infinite trace semantics [11], Kleisli simulation [8, 9, 18], and FPE [18]. Our technical contributions are in the subsequent sections: in §4 we study the nondeterministic setting (i.e. the powerset monad $\mathcal{P}$ on **Sets** and a polynomial functor F); §5 is for the probabilistic setting (where the monad T is the sub-Giry monad $\mathcal{G}$). In §6 we briefly discuss other monads like the *lift monad* $\mathcal{L}$ (for divergence) and the *subdistribution monad* $\mathcal{D}$ on **Sets** (for discrete probabilities).

Some definitions and results in §4–5 are marked with †. Those marked ones are essentially proofs of the results for specific settings (namely $T = \mathcal{P}$ and $T = \mathcal{G}$) but formulated in general terms with a general T. We do so in the hope that the axioms thus identified will help to discover new instances.

Most proofs are deferred to the appendices, that are found in the extended version [19] of this paper. Auxiliary definitions and examples are also found there.

2 Preliminaries

▶ **Definition 2.1.** A *polynomial functor* F on **Sets** is defined by the following BNF notation: $F ::= \mathrm{id} \mid A \mid F_1 \times F_2 \mid \coprod_{i\in I} F_i$. Here $A \in$ **Sets** and I is a countable set.

The notion of polynomial functor can be also defined for **Meas** – the category of measurable spaces and measurable functions between them.

▶ **Definition 2.2.** A *(standard Borel) polynomial functor* F on **Meas** is defined by the following BNF notation: $F ::= \mathrm{id} \mid (A, \mathfrak{F}_A) \mid F_1 \times F_2 \mid \coprod_{i\in I} F_i$. Here I is a countable set; and we require that $(A, \mathfrak{F}_A) \in$ **Meas** is a *standard Borel space* (see e.g. [6]). The σ-algebra $\mathfrak{F}_{FX}$ associated to FX is defined in the obvious manner. Namely: for $F = \mathrm{id}$, $\mathfrak{F}_{FX} = \mathfrak{F}_X$; for $F = (A, \mathfrak{F}_A)$, $\mathfrak{F}_{FX} = \mathfrak{F}_A$; for $F = F_1 \times F_2$, $\mathfrak{F}_{FX}$ is the smallest σ-algebra that contains $A_1 \times A_2$ for all $A_1 \in \mathfrak{F}_{F_1X}$ and $A_2 \in \mathfrak{F}_{F_2X}$; for for $F = \coprod_{i\in I} F_i$, $\mathfrak{F}_{FX} = \{\coprod_{i\in I} A_i \mid A_i \in \mathfrak{F}_{F_iX}\}$.

For arrows, F works in the same manner as a polynomial functor on **Sets**.

In what follows, a standard Borel polynomial functor is often called simply a *polynomial functor*.

The technical requirement of being standard Borel in the above will be used in the probabilistic setting of §5 (it is also exploited in [4, 17]). A standard Borel space is a measurable space induced by a Polish space; for further details see e.g. [6].

There is a natural correspondence between polynomial functors and *ranked alphabets*. In this paper a functor F for the (linear-time) transition type is restricted to a polynomial one; this means that we are dealing with (T-branching) systems that generate *trees* over some ranked alphabet. We collect some standard notions and notations for such trees in Appendix A.1; they will be used later in showing that our coalgebraic infinite traces indeed capture infinite tree languages of such systems.

We go on to introduce monads T for branching. We principally use two monads – the *powerset monad* $\mathcal{P}$ on **Sets** and the *sub-Giry* monad $\mathcal{G}$ on **Meas**. The latter is an adaptation of the *Giry monad* [7] and inherits most of its structure from the Giry monad; see Rem. 2.6.

▶ **Definition 2.3** (monads $\mathcal{P}$ and $\mathcal{G}$)**.** The *powerset monad* is the monad $(\mathcal{P}, \eta^{\mathcal{P}}, \mu^{\mathcal{P}})$ on **Sets** such that $\mathcal{P}X = \{A \subseteq X\}$ and $\mathcal{P}f(A) = \{f(x) \mid x \in A\}$. Its unit is given by the singleton set $\eta^{\mathcal{P}}_X(x) = \{x\}$ and its multiplication is given by $\mu^{\mathcal{P}}_X(M) = \bigcup_{A\in M} A$.

The *sub-Giry monad* is the monad $(\mathcal{G}, \eta^{\mathcal{G}}, \mu^{\mathcal{G}})$ on **Meas** such that

- $\mathcal{G}(X, \mathfrak{F}_X) = (\mathcal{G}X, \mathfrak{F}_{\mathcal{G}X})$, where the underling set $\mathcal{G}X$ is the set of all *subprobability measures* on $(X, \mathfrak{F}_X)$. The latter means those measures which assign to the whole space X a value in the unit interval $[0, 1]$.
- The σ-algebra $\mathfrak{F}_{\mathcal{G}X}$ on $\mathcal{G}X$ is the smallest σ-algebra such that, for all $S \in \mathfrak{F}_X$, the function $\mathrm{ev}_S : \mathcal{G}X \to [0, 1]$ defined by $\mathrm{ev}_S(P) = P(S)$ is measurable.
- $\mathcal{G}f(\nu)(S) = \nu(f^{-1}(S))$ where $f : (X, \mathfrak{F}_X) \to (Y, \mathfrak{F}_Y)$ is measurable, $\nu \in \mathcal{G}X$, and $S \in \mathfrak{F}_Y$.
- $\eta^{\mathcal{G}}_{(X,\mathfrak{F}_X)(x)}$ is given by the *Dirac measure*: $\eta^{\mathcal{G}}_{(X,\mathfrak{F}_X)}(x)(S)$ is 1 if $x \in S$ and 0 otherwise.
- $\mu^{\mathcal{G}}_{(X,\mathfrak{F}_X)}(\Psi)(S) = \int_{\mathcal{G}(X,\mathfrak{F}_X)} \mathrm{ev}_S\, d\Psi$ where $\Psi \in \mathcal{G}^2X$, $S \in \mathfrak{F}_X$ and ev_S is defined as above.

A monad gives rise to a category called its *Kleisli category* (see e.g. [15]).

▶ **Definition 2.4** (Kleisli category $\mathcal{K}\ell(T)$)**.** Given a monad (T, η, μ) on a category $\mathbb{C}$, the *Kleisli category* for T is the category $\mathcal{K}\ell(T)$ whose objects are the same as $\mathbb{C}$, and for each pair of objects X, Y, the homset $\mathcal{K}\ell(T)(X, Y)$ is given by $\mathbb{C}(X, TY)$. An arrow in $\mathcal{K}\ell(T)$ is referred to as a *Kleisli arrow*, and depicted by $X \nrightarrow Y$ for distinction. Note that it is nothing but an arrow $X \to TY$ in the base category $\mathbb{C}$.

Moreover, for two sequential Kleisli arrows $f : X \nrightarrow Y$ and $g : Y \nrightarrow Z$, their composition is given by $\mu_Z \circ Tg \circ f$ and denoted by $g \odot f$. The *Kleisli inclusion functor* is the functor $J : \mathbb{C} \to \mathcal{K}\ell(T)$ such that $JX = X$ and $Jf = \eta_Y \circ f$ for $f : X \to Y$ in $\mathbb{C}$.

It is known that a functor $F : \mathbb{C} \to \mathbb{C}$ canonically lifts to a functor $\overline{F} : \mathcal{K}\ell(T) \to \mathcal{K}\ell(T)$, given that there exists a natural transformation $\lambda : FT \Rightarrow TF$ that is compatible with the unit and the multiplication of T. Such a natural transformation is called a *distributive law*. For more details, see [16].

Throughout this paper, we fix the orders on the homsets of $\mathcal{K}\ell(\mathcal{P})$ and $\mathcal{K}\ell(\mathcal{G})$ as follows.

▶ **Definition 2.5** (order enrichment of $\mathcal{K}\ell(\mathcal{P})$ and $\mathcal{K}\ell(\mathcal{G})$)**.** We define an order on $\mathcal{K}\ell(\mathcal{P})(X, Y)$ by $f \sqsubseteq g \overset{\text{def}}{\Leftrightarrow} \forall x \in X.\, f(x) \subseteq g(x)$. We define an order on $\mathcal{K}\ell(\mathcal{G})(X, Y)$ by $f \sqsubseteq g \overset{\text{def}}{\Leftrightarrow} \forall x \in X.\, \forall A \in \mathfrak{F}_Y.\, f(x)(A) \leq g(x)(A)$. Here the last $\leq$ is the usual order in the unit interval $[0, 1]$.

▶ **Remark 2.6.** *The sub-Giry monad $\mathcal{G}$ is an adaptation of the* Giry monad *from [7]; in the original Giry monad we only allow (proper)* probability measures*, i.e. measures that map the whole space to* 1*. We work with the sub-Giry monad because, without this relaxation from probability to subprobability, the order structure in Def. 2.5 is reduced to the equality.*

3 Infinite Traces, Kleisli Simulations and Coalgebras in $\mathcal{K}\ell(T)$

In this section we review the categorical constructs, the relationship among which lies at the heart of this paper. They are namely: coalgebraic infinite trace semantics [11], Kleisli simulation [8, 9, 18] and forward partial execution (FPE) [18].

The following situation is identified in [11], (see also §A.2 and §A.5.3): the largest homomorphism to a certain coalgebra that we describe below is observed to coincide with the standard, conventionally defined notion of infinite language, for a variety of systems. An instance of it is shown to arise, in [11], when $\mathbb{C} = \mathbf{Sets}$, $T = \mathcal{P}$ and F is a polynomial functor. In §4 we will give another proof for this fact; the new proof will serve our goal of showing soundness of backward simulations.

▶ **Definition 3.1** (infinite trace situation)**.** Let F be an endofunctor and T be a monad on a category $\mathbb{C}$. We assume that each homset of the Kleisli category $\mathcal{K}\ell(T)$ carries an order $\sqsubseteq$. A functor F and a monad T constitute an *infinite trace situation* with respect to $\sqsubseteq$ if they satisfy the following conditions.

- There exists a final F-coalgebra $\zeta : Z \to FZ$ in $\mathbb{C}$.
- There exists a distributive law $\lambda : FT \Rightarrow TF$, yielding a lifting $\overline{F}$ on $\mathcal{K}\ell(T)$ of F.
- For each coalgebra $c : X \nrightarrow \overline{F}X$ in $\mathcal{K}\ell(T)$, the lifting $J\zeta : Z \nrightarrow \overline{F}Z$ of ζ admits the largest homomorphism. That is, there exists a homomorphism $\mathsf{tr}^\infty(c) : X \nrightarrow Z$ from c to $J\zeta$ such that, for any homomorphism f from c to $J\zeta$, $f \sqsubseteq \mathsf{tr}^\infty(c)$ holds.

In [8, 9, 18] we augment a coalgebra with an explicit arrow for initial states. The resulting notion is called a (T, F)-system.

$$\begin{tikzcd}
\overline{F}X \arrow[r, squiggly, "\overline{F}(\mathsf{tr}^\infty(c))"] & \overline{F}Z \\
X \arrow[u, "c"] \arrow[r, squiggly, "\mathsf{tr}^\infty(c)"] \arrow[ur, phantom, "="] & Z \arrow[u, "J\zeta"'] \\
1 \arrow[u, "s"]
\end{tikzcd}$$

▶ **Definition 3.2** (infinite trace semantics for (T, F)-systems [10, 11])**.** Let $\mathbb{C}$ be a category with a final object $1 \in \mathbb{C}$. A (T, F)*-system* is a triple $\mathcal{X} = (X, s, c)$ consisting of a *state space* $X \in \mathbb{C}$, a Kleisli arrow $s : 1 \nrightarrow X$ for *initial states*, and $c : X \nrightarrow \overline{F}X$ for *transition*.
Let us assume that the endofunctor F and the monad T on $\mathbb{C}$ constitute an infinite trace situation. The *coalgebraic infinite trace semantics* of a (T, F)-system $\mathcal{X} = (X, s, c)$ is the Kleisli arrow $\mathsf{tr}^\infty(c) \odot s : 1 \nrightarrow Z$ (see the diagram, in $\mathcal{K}\ell(T)$, on the right).

Suppose that we are given two (T, F)-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$. Let us say we aim to prove the inclusion between infinite trace semantics, that is, to show $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$ with respect to the order in the homset of $\mathcal{K}\ell(T)$. Our goal in this paper is to offer *Kleisli simulations* as a sound means to do so.

The notions of *forward* and *backward Kleisli simulation* are introduced in [8] as a categorical generalization of fwd./bwd. simulations in [14]. They are defined as Kleisli arrows between (the state spaces of) two (T, F)-system that are subject to certain inequalities – in short they are *lax/oplax coalgebra homomorphisms*. In [8] they are shown to be sound with respect to *finite* trace semantics – the languages of finite words, concretely; and the unique arrow to a lifted initial algebra (that is a final coalgebra, see [10] and the introduction), abstractly. In this paper we are interested in their relation to *infinite* trace semantics.

▶ **Definition 3.3** (fwd./bwd. Kleisli simulation [8])**.** Let F be an endofunctor and T be a monad on $\mathbb{C}$ such that each homset of $\mathcal{K}\ell(T)$ carries an order $\sqsubseteq$. Let $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$ be (T, F)-systems. A *forward Kleisli simulation* from $\mathcal{X}$ to $\mathcal{Y}$ is a Kleisli arrow $f : Y \mathrel{+\!\!\!\rightarrow} X$ that satisfies the following conditions (see the diagram).

$$\begin{tikzcd}
\overline{F}X & & \overline{F}Y \arrow[ll, "\overline{F}f"', "|" marking] \\
X \arrow[u, "c", "|" marking] \arrow[urr, phantom, "\sqsubseteq" description] & & Y \arrow[u, "d"', "|" marking] \arrow[ll, "f"', "|" marking] \\
& 1 \arrow[ul, bend left, "s", "|" marking] \arrow[ur, bend right, "t"', "|" marking] \arrow[u, phantom, "\sqsubseteq" description] &
\end{tikzcd}$$

$$s \sqsubseteq f \odot t, \quad \text{and} \quad c \odot f \sqsubseteq \overline{F}f \odot d.$$

We write $\mathcal{X} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ if there exists a forward simulation from $\mathcal{X}$ to $\mathcal{Y}$.
A *backward Kleisli simulation* from $\mathcal{X}$ to $\mathcal{Y}$ is a Kleisli arrow $b : X \mathrel{+\!\!\!\rightarrow} Y$ that satisfies the following conditions (see the diagram).

$$\begin{tikzcd}
\overline{F}X \arrow[rr, "\overline{F}b", "|" marking] & & \overline{F}Y \\
X \arrow[u, "c", "|" marking] \arrow[rr, "b", "|" marking] \arrow[urr, phantom, "\sqsubseteq" description] & & Y \arrow[u, "d"', "|" marking] \\
& 1 \arrow[ul, bend left, "s", "|" marking] \arrow[ur, bend right, "t"', "|" marking] \arrow[u, phantom, "\sqsubseteq" description] &
\end{tikzcd}$$

$$b \odot s \sqsubseteq t, \quad \text{and} \quad \overline{F}b \odot c \sqsubseteq d \odot f.$$

We write $\mathcal{X} \sqsubseteq_{\mathbf{B}} \mathcal{Y}$ if there exists a backward simulation from $\mathcal{X}$ to $\mathcal{Y}$.

Forward partial execution (FPE) is a transformation of a (T, F)-system introduced in [18] for the purpose of aiding discovery of Kleisli simulations. Intuitively, it “executes” the given system by one step.

▶ **Definition 3.4** (FPE [18])**.** Let F be an endofunctor and T be a monad on $\mathbb{C}$. *Forward partial execution* (FPE) is a transformation that takes a (T, F)-system $\mathcal{X} = (X, s, c)$ as an input and returns a (T, F)-system $\mathcal{X}_{\mathsf{FPE}} = (\overline{F}X, c \odot s, \overline{F}c)$ as an output.

It is shown in [18] that FPE is a valid technique for establishing inclusion of *finite* trace semantics, in the technical senses of *soundness* and *adequacy*. Soundness asserts that discovery of a Kleisli simulation after applying FPE indeed witnesses trace inclusion between the original systems; adequacy asserts that if there is a Kleisli simulation between the original systems, then there is too between the transformed systems. In this paper, naturally, we wish to establish the same results for *infinite* trace semantics.

4 Systems with Nondeterministic Branching

In the rest of the paper we develop a coalgebraic theory of infinite traces and (Kleisli) simulations – the main contribution of the paper. We do so separately for the nondeterministic setting ($T = \mathcal{P}$) and for the probabilistic one ($T = \mathcal{G}$). This is because of the difference in the constructions of infinite traces, and consequently in the soundness proofs.

In this section we focus on the nondeterministic setting; we assume that F is a polynomial functor.

4.1 Construction of Infinite Traces

The following is already known from [11].

▶ **Theorem 4.1.** *The combination of polynomial F and $T = \mathcal{P}$ constitute an infinite trace situation (Def. 3.1).*

The proof in [11] combines fibrational intuitions with some constructions that are specific to **Sets**. Here we present a different proof. It exploits an order-theoretic structure of the Kleisli category $\mathcal{K}\ell(\mathcal{P})$; this will be useful later in showing soundness of (restricted) backward simulations. Our proof also paves the way to the probabilistic case in §5.

In fact, our proof of Thm. 4.1 is stated axiomatically, in the form of the following proposition. This is potentially useful in identifying new examples other than the combination of polynomial F and $T = \mathcal{P}$ (although we have not yet managed to do so). It is essentially the construction of a greatest fixed point by transfinite induction [5].

▶ **Proposition 4.2.**† *Let $\mathbb{C}$ be a category, F be an endofunctor on $\mathbb{C}$, and T be a monad on $\mathbb{C}$. Assume the following conditions.*

1. *There exists a final F-coalgebra $\zeta : Z \to FZ$ in $\mathbb{C}$.*
2. *There exists a distributive law $\lambda : FT \Rightarrow TF$, yielding a lifting $\overline{F}$ on $\mathcal{K}\ell(T)$ of F.*
3. *For each $X, Y \in \mathcal{K}\ell(T)$, the homset $\mathcal{K}\ell(T)(X, Y)$ carries a partial order $\sqsubseteq$. Moreover, $\overline{F}$'s action on arrows, as well as composition of arrows in $\mathcal{K}\ell(T)$, is monotone with respect to this order.*
4. *For each $X, Y \in \mathcal{K}\ell(T)$, every (possibly transfinite) decreasing sequence in $\mathcal{K}\ell(T)(X, Y)$ has the greatest lower bound. That is: let $\mathfrak{a}$ be a limit ordinal and $(g_\mathfrak{i} : X \nrightarrow Y)_{\mathfrak{i}<\mathfrak{a}}$ be a family of arrows such that $\mathfrak{i} \le \mathfrak{j}$ implies $g_\mathfrak{i} \sqsupseteq g_\mathfrak{j}$. Then $\bigsqcap_{\mathfrak{i}<\mathfrak{a}} g_\mathfrak{i}$ exists.*
5. *For each $X \in \mathbb{C}$, the homset $\mathcal{K}\ell(T)(X, Z)$ has the largest element $\top_{X,Z}$.*

Then T and F constitute an infinite trace situation with respect to $\sqsubseteq$.

Proof. Let $c : X \nrightarrow \overline{F}X$ be an $\overline{F}$-coalgebra in $\mathcal{K}\ell(T)$. We shall construct the largest homomorphism $\mathsf{tr}^\infty(c) : X \nrightarrow Z$ from c to $J\zeta$, by transfinite induction. We define an endofunction $\Phi_X : \mathcal{K}\ell(T)(X, Z) \to \mathcal{K}\ell(T)(X, Z)$ by $\Phi_X(f) = J\zeta^{-1} \odot \overline{F}f \odot c$. By the monotonicity of $\odot$ and $\overline{F}$ (Assumption 3), Φ_X is also monotone. For each ordinal $\mathfrak{a}$, we define $\Phi^\mathfrak{a}_X(\top_{X,Z}) \in \mathcal{K}\ell(T)(X, Z)$ by the following transfinite induction.

$$\begin{tikzcd} \overline{F}X \arrow[r, "\overline{F}\top_{X,Z}"] & \overline{F}Z \\ X \arrow[u, "c"] \arrow[r, "\top_{X,Z}"'] \arrow[ur, phantom, "\sqsubseteq"] & Z \arrow[u, "J\zeta"', "\cong"] \end{tikzcd}$$

- $\Phi^0_X(\top_{X,Z}) = \top_{X,Z}$.
- For a successor ordinal $\mathfrak{a}$, $\Phi^\mathfrak{a}_X(\top_{X,Z}) = \Phi_X(\Phi^{\mathfrak{a}-1}_X(\top_{X,Z}))$.
- For a limit ordinal $\mathfrak{a}$, $\Phi^\mathfrak{a}_X(\top_{X,Z}) = \bigsqcap_{\mathfrak{i}<\mathfrak{a}} \Phi^\mathfrak{i}_X(\top_{X,Z})$. (cf. Assumption 4)

We define $\mathfrak{l}$ to be the smallest ordinal such that the cardinality of $\mathfrak{l}$ is greater than that of $\mathcal{K}\ell(T)(X, Z)$. Then from [5], $\Phi^\mathfrak{l}_X(\top_{X,Z})$ is the greatest fixed point of Φ_X. This immediately implies that $\Phi^\mathfrak{l}_X(\top_{X,Z})$ is the largest homomorphism from c to $J\zeta$. ◀

Note that the local continuity of composition in $\mathcal{K}\ell(T)$ is not assumed. This is because $\mathcal{P}$ – our choice for T in this section – does not satisfy it. Indeed, consider $f : X \nrightarrow Y$ and a decreasing sequence $(g_i : Y \nrightarrow Z)_{i\in\omega}$, both in $\mathcal{K}\ell(\mathcal{P})$. Then we have $\left(\bigsqcap_{i\in\omega} g_i\right) \odot f(x) = \bigcup_{y\in f(x)} \bigcap_{i\in\omega} g_i(y)$ while $\bigsqcap_{i\in\omega}(g_i \odot f)(x) = \bigcap_{i\in\omega} \bigcup_{y\in f(x)} g_i(y)$, and these two are not equal in general (e.g. Example A.31). This failure of continuity prevents us from applying the (simpler) *Kleene fixed-point theorem*, in which induction terminates after ω steps.

There does exist a nondeterministic automaton for which the largest homomorphism is obtained after steps bigger than ω; see Example A.31.

It is easy to check that all the assumptions in Prop. 4.2 are satisfied by polynomial F and $T = \mathcal{P}$. This yields Thm. 4.1. We can also show that the resulting coalgebraic infinite trace semantics coincides with the usual definition of (infinite) tree languages for nondeterministic systems. See §A.2.1 for details.

4.2 Kleisli Simulations for Nondeterministic Systems

4.2.1 Forward Simulations

Soundness of forward simulation is not hard; we do not have to go into the construction in Prop. 4.2.

▶ **Theorem 4.3.** *Given two $(\mathcal{P}, F)$-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, $\mathcal{X} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ implies $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.*

The proof, again, is formulated as a general result, singling out some sufficient axioms.

▶ **Lemma 4.4.**[†] *Let F be an endofunctor and T be a monad on $\mathbb{C}$; assume further that they constitute an infinite trace situation (with respect to $\sqsubseteq$). We assume the following conditions.*

1. *Each homset of $\mathcal{K}\ell(T)$ is ω-complete, that is, each increasing ω-sequence in it has the lub.*
2. *Composition $\odot$ of arrows in $\mathcal{K}\ell(T)$ and $\overline{F}$'s action on arrows are both ω-continuous (i.e. they preserve the lub. of an increasing ω-sequence). It follows that they are both monotone.*

For two (T, F)-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, if $f : Y \nrightarrow X$ is a forward simulation from $\mathcal{X}$ to $\mathcal{Y}$, then $\mathsf{tr}^\infty(c) \odot f \sqsubseteq \mathsf{tr}^\infty(d)$. As a consequence we have $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.

Proof. Let $\zeta : Z \to FZ$ be a final F-coalgebra in $\mathbb{C}$. We define a function $\Phi_Y : \mathcal{K}\ell(T)(Y, Z) \to \mathcal{K}\ell(T)(Y, Z)$ by $\Phi_Y(g) = J\zeta^{-1} \odot \overline{F}g \odot d$; note that ζ is a final coalgebra and hence an isomorphism. Then

$$
\begin{aligned}
\mathsf{tr}^\infty(c) \odot f &= J\zeta^{-1} \odot \overline{F}(\mathsf{tr}^\infty(c)) \odot c \odot f && (\mathsf{tr}^\infty(c) \text{ is a homomorphism}) \\
&\sqsubseteq \Phi_Y(\mathsf{tr}^\infty(c) \odot f) && (f \text{ is a fwd. sim., and the definition of } \Phi_Y).
\end{aligned}
$$

By the assumption that $\overline{F}$ and the composition are monotone, Φ_Y is also monotone. Therefore by repeatedly applying Φ_Y to the both sides of the above inequality, we obtain an increasing sequence $\mathsf{tr}^\infty(c) \odot f \sqsubseteq \Phi_Y(\mathsf{tr}^\infty(c) \odot f) \sqsubseteq \Phi_Y^2(\mathsf{tr}^\infty(c) \odot f) \sqsubseteq \cdots$ in $\mathcal{K}\ell(T)(Y, Z)$. As $\mathcal{K}\ell(T)(Y, Z)$ is ω-complete, the least upper bound $\bigsqcup_{i<\omega} \Phi^i(\mathsf{tr}^\infty(c) \odot f)$ exists. By the assumption that $\overline{F}$ and $\odot$ are both locally ω-continuous, Φ_Y is also ω-continuous. Therefore $\bigsqcup_{i<\omega} \Phi^i(\mathsf{tr}^\infty(c) \odot f)$ is a fixed point of Φ_Y, and hence a homomorphism from d to $J\zeta$. As $\mathsf{tr}^\infty(d)$ is the largest homomorphism from d to $J\zeta$, this implies $\mathsf{tr}^\infty(c) \odot f \sqsubseteq \bigsqcup_{i<\omega} \Phi^i(\mathsf{tr}^\infty(c) \odot f) \sqsubseteq \mathsf{tr}^\infty(d)$. Combining with the assumption that f is a forward simulation (its condition on initial states), we have $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(c) \odot f \odot t \sqsubseteq \mathsf{tr}^\infty(d) \odot t$. ◀

$$\begin{tikzcd}
\overline{F}Y \arrow[r, "\overline{F}f"'] \arrow[rr, bend left, "\overline{F}(\mathsf{tr}^\infty(d))"] \arrow[dr, phantom, "\sqsupseteq"] & \overline{F}X \arrow[r, "\overline{F}(\mathsf{tr}^\infty(c))"'] \arrow[dr, phantom, "="] & \overline{F}Z \\
Y \arrow[u, "d"'] \arrow[r, "f"] \arrow[rr, bend right, "\mathsf{tr}^\infty(d)"'] & X \arrow[u, "c"'] \arrow[r, "\mathsf{tr}^\infty(c)"] & Z \arrow[u, "J\zeta"'] \\
1 \arrow[u, "t"] \arrow[ur, "s"'] \arrow[ur, phantom, bend left, "\sqsupseteq"] & &
\end{tikzcd}$$

It is known from [10] that the combination of polynomial F and $T = \mathcal{P}$ satisfy the conditions of Lem. 4.4. Hence we obtain Thm. 4.3, i.e. soundness of fwd. simulation in the nondeterministic setting.

4.2.2 Backward Simulations

Next we wish to establish soundness of *backward* Kleisli simulations with respect to *infinite* traces (for finite traces it is shown in [8]). In fact, the desired soundness fails in general – a counterexample is in Example A.32. It turns out that we can impose certain restrictions on backward Kleisli simulations and ensure soundness.

▶ **Definition 4.5** (totality, image-finiteness, TIF-backward simulation)**.** Let $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$ be $(\mathcal{P}, F)$-systems. A backward simulation $b : X \nrightarrow Y$ from $\mathcal{X}$ to $\mathcal{Y}$ is *total* if $b(x) \neq \emptyset$ for all $x \in X$; it is *image-finite* if $b(x)$ is finite for all $x \in X$. If b satisfies both of the two conditions, it is called a *TIF-backward simulation.* We write $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}$ if there exists a TIF-backward simulation from $\mathcal{X}$ to $\mathcal{Y}$.

▶ **Theorem 4.6** (soundness of $\sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}}$)**.** *For two $(\mathcal{P}, F)$-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}$ implies $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.*

The proof of Thm. 4.6 is, yet again, via the following axiomatic development.

▶ **Definition 4.7** (TIF-backward simulation, generally)**.**† Let F be an endofunctor and T be a monad on $\mathbb{C}$ that satisfy the conditions in Prop. 4.2 wrt. $\sqsubseteq$. For two (T, F)-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, a *TIF-backward simulation* from $\mathcal{X}$ to $\mathcal{Y}$ is a backward simulation $b : X \nrightarrow Y$ that satisfies the following conditions.

1. The arrow $b : X \nrightarrow Y$ satisfies $\top_{Y,Z} \odot b = \top_{X,Z}$.
2. Precomposing $b : X \nrightarrow Y$ preserves the greatest lower bound of any decreasing transfinite sequence. That is, let $A \in \mathcal{K}\ell(T)$, $\mathfrak{a}$ be a limit ordinal, and $(g_{\mathfrak{i}} : Y \nrightarrow A)_{\mathfrak{i}<\mathfrak{a}}$ be a family of Kleisli arrows such that $\mathfrak{i} \leq \mathfrak{j}$ implies $g_{\mathfrak{i}} \sqsupseteq g_{\mathfrak{j}}$. Then we have $\bigsqcap_{\mathfrak{i}\in\mathfrak{a}}(g_{\mathfrak{i}} \odot b) = (\bigsqcap_{\mathfrak{i}\in\mathfrak{a}} g_{\mathfrak{i}}) \odot b$.

We write $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}$ if there exists a TIF-backward simulation from $\mathcal{X}$ to $\mathcal{Y}$.

Assumption 2 of Def. 4.7 resembles how “finiteness” is formulated in category theory, e.g. in the definition of *finitary* objects.

This general TIF-backward simulation satisfies soundness. For its proof we have to look into the inductive construction of the largest homomorphism in §4.1.

▶ **Lemma 4.8.**† *Let F and T be as in Prop. 4.2. For two (T, F)-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}$ (in the sense of Def. 4.7) implies $\mathsf{tr}^\infty(c) \sqsubseteq \mathsf{tr}^\infty(d) \odot b$. Furthermore it follows that $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.*

Proof.

$$\begin{tikzcd}
\overline{F}X \arrow[r, "\overline{F}b"'] \arrow[rr, bend left, "\overline{F}\top_{X,Z}"] & \overline{F}Y \arrow[r, "\overline{F}\top_{Y,Z}"'] & \overline{F}Z \\
X \arrow[u, "c"] \arrow[r, "b"] \arrow[rr, bend right, "\top_{X,Z}"'] \arrow[ur, phantom, "\sqsubseteq"] & Y \arrow[u, "d"] \arrow[r, "\top_{Y,Z}"] \arrow[ur, phantom, "\sqsubseteq"] & Z \arrow[u, "J\zeta"', "\cong"]
\end{tikzcd}$$

Let $\zeta : Z \to FZ$ be a final F-coalgebra in $\mathbb{C}$. We define $\Phi_X : \mathcal{K}\ell(T)(X, Z) \to \mathcal{K}\ell(T)(X, Z)$ and $\Phi_Y : \mathcal{K}\ell(T)(Y, Z) \to \mathcal{K}\ell(T)(Y, Z)$ as in the proof of Prop. 4.2. Moreover, in the same manner as in the proof of Prop. 4.2, for each ordinal $\mathfrak{a}$, we define $\Phi^{\mathfrak{a}}_X(\top_{X,Z}) : X \nrightarrow Z$ and $\Phi^{\mathfrak{a}}_Y(\top_{Y,Z}) : Y \nrightarrow Z$ by the transfinite induction on $\mathfrak{a}$. As we have seen in the proof of Prop. 4.2, there exist ordinals $\mathfrak{l}_X$ and $\mathfrak{l}_Y$ s.t. $\mathsf{tr}^\infty(c) = \Phi^{\mathfrak{l}_X}_X(\top_{X,Z})$ and $\mathsf{tr}^\infty(d) = \Phi^{\mathfrak{l}_Y}_Y(\top_{Y,Z})$. Let $\mathfrak{l} = \max(\mathfrak{l}_X, \mathfrak{l}_Y)$. We shall now prove by transfinite induction that, for each $\mathfrak{a}$, we have $\Phi^{\mathfrak{a}}_X(\top_{X,Z}) \sqsubseteq \Phi^{\mathfrak{a}}_Y(\top_{Y,Z}) \odot b$; this will yield our goal by taking $\mathfrak{a} = \mathfrak{l}$.

For $\mathfrak{a} = 0$, from Assumption 1 of Def. 4.7, we have $\Phi^{\mathfrak{a}}_X(\top_{X,Z}) = \top_{X,Z} = \top_{Y,Z} \odot b = \Phi^{\mathfrak{a}}_Y(\top_{Y,Z}) \odot b$.

Assume that $\mathfrak{a}$ is a successor ordinal and $\Phi^{\mathfrak{a}-1}_X(\top_{X,Z}) \sqsubseteq \Phi^{\mathfrak{a}-1}_Y(\top_{Y,Z}) \odot b$. Then

$$\begin{aligned}
\Phi^{\mathfrak{a}}_X(\top_{X,Z}) &\sqsubseteq J\zeta^{-1} \odot \overline{F}(\Phi^{\mathfrak{a}-1}_Y(\top_{Y,Z})) \odot \overline{F}b \odot c && \text{(by induction hypothesis)} \\
&\sqsubseteq \Phi^{\mathfrak{a}}_Y(\top_{Y,Z}) \odot b && \text{(b is a bwd. simulation)}\,.
\end{aligned}$$

Let $\mathfrak{a}$ be a limit ordinal and assume that $\Phi^{\mathfrak{i}}_X(\top_{X,Z}) \sqsubseteq \Psi^{\mathfrak{i}}_Y(\top_{Y,Z}) \odot b$ for all $\mathfrak{i} < \mathfrak{a}$. Then

$$\begin{aligned}\Phi^{\mathfrak{a}}_X(\top_{X,Z}) &\sqsubseteq \textstyle\bigsqcap_{\mathfrak{i}<\mathfrak{a}} \left(\Phi^{\mathfrak{i}}_Y(\top_{Y,Z}) \odot b\right) && \text{(by induction hypothesis)}\\ &= \Phi^{\mathfrak{a}}_Y(\top_{Y,Z}) \odot b && \text{(by Assumption 2 of Def. 4.7)}\,.\end{aligned}$$

Thus $\mathsf{tr}^\infty(c) \sqsubseteq \mathsf{tr}^\infty(d) \odot b$. The last claim follows from b's condition on initial states. ◀

Proof of Thm. 4.6. In Lem. A.17 we prove that a TIF-backward simulation in the specific sense of Def. 4.5 is also a TIF-backward simulation in the general sense of Def. 4.7. Therefore Lem. 4.8 yields trace inclusion. ◀

Even with the additional constraints of totality and image-finiteness, backward Kleisli simulations are a viable method for establishing infinite trace inclusion. An example is in Example A.33 where a fwd. simulation does not exist but a TIF-bwd. simulation does.

4.3 Forward Partial Execution for Nondeterministic Systems

We now apply *forward partial execution* (FPE) [18] – a transformation of coalgebraic systems that potentially increases the likelihood of existence of simulations – in the current setting of nondeterminism and infinite traces. We follow the setting in [18] for the *finite* traces, and formulate FPE's "correctness" in the following theorem.

▶ **Theorem 4.9.** *Let F be a polynomial functor on* **Sets***. For $(\mathcal{P}, F)$-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, the following hold.*

1. **a.** (soundness of FPE for fwd. sim.) $\mathcal{X}_{\mathsf{FPE}} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ *implies* $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.
   b. (adequacy of FPE for fwd. sim.) $\mathcal{X} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ *implies* $\mathcal{X}_{\mathsf{FPE}} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$.
2. **a.** (soundness of FPE for bwd. sim.) $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}_{\mathsf{FPE}}$ *implies* $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.
   b. (adequacy of FPE for bwd. sim.) $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}$ *implies* $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}_{\mathsf{FPE}}$*, assuming that the following hold.*
      i. $d(y) \neq \emptyset$ *for all* $y \in Y$.
      ii. $d(y)$ *is finite for all* $y \in Y$.

Informally: *soundness* means that discovery after applying FPE still witnesses the trace inclusion between the original systems; and *adequacy* means that the relationship $\sqsubseteq_{\mathbf{F}}$ (or $\sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}}$) is not destroyed by application of FPE. The theorem also implies that FPE must be applied to the "correct side" of the desired trace inclusion: $\mathcal{X}$ in the search for a fwd. simulation; and $\mathcal{Y}$ in the search for a bwd. one.

Note that the adequacy property is independent from the choice of trace semantics (finite or infinite). Therefore the statement 1b of Thm. 4.9 is the same as its counterpart in [18]. For the statement 2b, however, we have to check that the TIF restriction (that is absent in [18]) is indeed carried over.

In [18] it is shown that FPE can indeed create a simulation that does not exist between the original systems. Its practical use is witnessed by experimental results in [18], too. It would not be hard to observe the same in the current setting for *infinite* traces.

For the proof of Thm. 4.9, once again, we turn to an axiomatic development.

▶ **Theorem 4.10** (FPE and fwd. sim.).[†] *Let F be an endofunctor and T be a monad on $\mathbb{C}$, as in Lem. 4.4 (that is, they constitute an infinite trace situation and satisfy the two additional assumptions.) Let $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$ be (T, F)-systems. Then we have:*

1. (soundness for fwd. sim.) $\mathcal{X}_{\mathsf{FPE}} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ *implies* $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.
2. (adequacy for fwd. sim.) $\mathcal{X} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ *implies* $\mathcal{X}_{\mathsf{FPE}} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$.

▶ **Theorem 4.11** (FPE and bwd. sim.).† *Let F be an endofunctor and T be a monad on $\mathbb{C}$ that satisfy the conditions in Prop. 4.2 (hence those in Lem. 4.8). Let $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$ be (T, F)-systems.*

1. (soundness for bwd. sim.) $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}_{\mathsf{FPE}}$ *implies* $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.
2. (adequacy for bwd. sim.) $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}$ *implies* $\mathcal{X} \sqsubseteq^{\mathrm{TIF}}_{\mathbf{B}} \mathcal{Y}_{\mathsf{FPE}}$ *if the following conditions are satisfied.*
   - **a.** *The coalgebra $d : Y \rightarrow\!\!\!\!\!\!\mapsto \overline{F}Y$ satisfies $\top_{\overline{F}Y,Z} \odot d = \top_{Y,Z}$.*
   - **b.** *Precomposing d preserves the glb. of a decreasing transfinite sequence.*

Proof of Thm. 4.9. 1 is immediate from Thm. 4.10. In a similar manner to Lem.A.17, we can prove 2 using Thm. 4.11. ◀

5 Systems with Probabilistic Branching

We now turn to probabilistic systems. They are modeled as $(\mathcal{G}, F)$-systems in the category **Meas**. Here we establish largely the same statements as in §4, but many constructions and proofs are different. Throughout this section F is assumed to be a (standard Borel) polynomial functor on **Meas** (Def. 2.2).

5.1 Construction of Infinite Traces

▶ **Theorem 5.1.** *The combination of polynomial F and $T = \mathcal{G}$ constitute an infinite trace situation (Def. 3.1).*

Our basic idea of the construction is similar to that for $\mathcal{P}$ (§4.1). Our goal is to construct the largest homomorphism from an $\overline{F}$-coalgebra c in to the lifted final coalgebra $J\zeta : Z \rightarrow\!\!\!\!\!\!\mapsto \overline{F}Z$; we do so inductively, starting from the top element and going down along a decreasing sequence. Compared to the nondeterministic case ($T = \mathcal{P}$), major differences are as follows.

- Composition of Kleisli arrows is ω^{op}-continuous in $\mathcal{K}\ell(\mathcal{G})$. This is an advantage, because we can appeal to the Kleene fixed point theorem and we only need inductive construction up-to ω steps (while, for $\mathcal{P}$, we needed transfinite induction).
- A big disadvantage, however, is the absence of the top element $\top_{X,Z}$ in $\mathcal{K}\ell(T)(X, Z)$. One can imagine a top element $\top_{X,Z}$ to assign 1 to every event – this is however not a (probability) measure.

To cope with the latter challenge, we turn to the *final F-sequence* in **Meas** that yields a final F-coalgebra as its limit. Instead of using a sequence like $\top \sqsupseteq \Phi(\top) \sqsupseteq \cdots$ in $\mathcal{K}\ell(T)(X, Z)$ (where the largest element $\top$ does not exist anyway), we use a decreasing sequence that goes along the final sequence.

$$\begin{tikzcd}
\overline{F}X \arrow[d, "\overline{F}(\mathsf{tr}^\infty(c))"', "\shortmid" marking] \arrow[dd, phantom, shift left=8ex, "="] & X \arrow[l, "c"', "\shortmid" marking] \arrow[dd, dashed, "\mathsf{tr}^\infty(c)"', "\shortmid" marking] \arrow[dr, "\pi_0", "\shortmid" marking] \arrow[drr, bend left, "\pi_1", "\shortmid" marking] \arrow[drrr, bend left=30, "\pi_2", "\shortmid" marking] & & & & \cdots \\
{} \arrow[d] & & 1 & \overline{F}1 \arrow[l, "J!"', "\shortmid" marking] & \overline{F}^2 1 \arrow[l, "JF!"', "\shortmid" marking] & \cdots \arrow[l, "JF^2!"', "\shortmid" marking] \\
\overline{F}Z & Z \arrow[l, "J\zeta"', "\cong", "\shortmid" marking] \arrow[ur, "J\gamma_0"', "\shortmid" marking] \arrow[urr, bend right, "J\gamma_1"', "\shortmid" marking] \arrow[urrr, bend right=30, "J\gamma_2"', "\shortmid" marking] & & & & \cdots
\end{tikzcd}$$

The precise construction is found in the proof of the following proposition (the proof is in Appendix A.4.

▶ **Proposition 5.2.**† *Let $\mathbb{C}$ be a category, F be an endofunctor on $\mathbb{C}$, and T be a monad on $\mathbb{C}$ where each homset of $\mathcal{K}\ell(T)$ carries an order $\sqsubseteq$. We assume the following conditions.*

1. *The category $\mathbb{C}$ has a final object 1; the final sequence $1 \xleftarrow{!_{F1}} F1 \xleftarrow{F!_{F1}} F^2 1 \xleftarrow{F^2!_{F1}} \dots$ has a limit $(Z, (\gamma_i : Z \to F^i 1)_{i \in \omega})$; and moreover, F preserves this limit. (Hence the limit carries a final F-coalgebra [1].)*
2. *There exists a distributive law $\lambda : FT \Rightarrow TF$, yielding a lifting $\overline{F}$ on $\mathcal{K}\ell(T)$ of F.*

3. *For $X, Y \in \mathcal{K}\ell(T)$, every decreasing ω-sequence $f_0 \sqsupseteq f_1 \sqsupseteq \dots$ in $\mathcal{K}\ell(T)(X,Y)$ has the greatest lower bound $\bigsqcap_{i\in\omega} f_i$. Moreover, composition of arrows in $\mathcal{K}\ell(T)$ and $\overline{F}$'s action on arrows are both ω^{op}-continuous. That is, for each $g : Z \nrightarrow X$ and $h : Y \nrightarrow W$, we have $g \odot (\bigsqcap_{i\in\omega} f_i) = \bigsqcap_{i\in\omega}(g \odot f_i)$, $(\bigsqcap_{i\in\omega} f_i) \odot h = \bigsqcap_{i\in\omega}(f_i \odot h)$, and $\overline{F}(\bigsqcap_{i\in\omega} f_i) = \bigsqcap_{i\in\omega}(\overline{F} f_i)$.*
4. *The lifting $J(!_X)$ of the unique arrow to 1 is the largest element of $\mathcal{K}\ell(T)(X,1)$.*
5. *The functor J lifts the limit in Assumption 1 to a 2-limit. Namely, for any cone $(X, (\pi_i : X \nrightarrow F^i 1)_{i\in\omega})$ over the sequence $1 \overset{J!_{F1}}{\nleftarrow} \overline{F}1 \overset{J\overline{F}!_{F1}}{\nleftarrow} \overline{F}^2 1 \overset{J\overline{F}^2!_{F1}}{\nleftarrow} \cdots$, there uniquely exists $l : X \nrightarrow Z$ s.t. $\pi_i = J\gamma_i \odot l$ holds for each $i \in \omega$. Moreover, if $l' : X \nrightarrow Z$ satisfies $J\gamma_i \odot l' \sqsubseteq J\gamma_i \odot l$ for each $i \in \omega$, then $l' \sqsubseteq l$ holds.*

Then F and T constitute an infinite trace situation with respect to $\sqsubseteq$.

In more elementary terms, Assumption 5 asserts that: J lifts the limit Z; and the lifted limit satisfies a stronger condition of "carrying over" the order between cones to the order between mediating maps.

Proof of Thm. 5.1. We have to check that polynomial F and $T = \mathcal{G}$ satisfy the assumptions in Prop. 5.2. The most nontrivial is Assumption 5; there we rely on Kolmogorov's consistency theorem, for the fact that a limit is lifted to a limit. That the latter is indeed a 2-limit is not hard, exploiting suitable monotonicity. Details are found in Lem. A.18. ◀

We can also show that the resulting coalgebraic infinite trace semantics coincides with the usual definition of (infinite) tree languages for probabilistic systems. See §A.2.2 for details.

5.2 Kleisli Simulations for Probabilistic Systems

5.2.1 Forward Simulations

Soundness of forward simulation, in the current probabilistic setting, follows immediately from the the axiomatic development in Lem. 4.4.

▶ **Theorem 5.3.** *Given two $(\mathcal{G}, F)$-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, $\mathcal{X} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ implies $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.*

5.2.2 Backward Simulations

Next we turn to backward simulations. Similarly to nondeterministic setting (§4.2.2), we have to impose a certain restriction on backward Kleisli simulations to ensure soundness. By the feature of $\mathcal{G}$ that composition in $\mathcal{K}\ell(\mathcal{G})$ is ω-continuous, the image-finiteness condition is no longer needed.

▶ **Definition 5.4** (totality, T-backward simulation)**.** Let $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$ be $(\mathcal{G}, F)$-systems. A backward simulation $b : X \nrightarrow Y$ from $\mathcal{X}$ to $\mathcal{Y}$ is *total* if $b(x)(Y) = 1$ for all $x \in X$. If b is total, it is called a *T-backward simulation*. We write $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}$ if there exists a T-backward simulation from $\mathcal{X}$ to $\mathcal{Y}$.

▶ **Theorem 5.5** (soundness of $\sqsubseteq^{\mathrm{T}}_{\mathbf{B}}$)**.** *For two $(\mathcal{G}, F)$-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}$ implies $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.*

The proof of Thm. 5.5 is via the following axiomatic development.

▶ **Definition 5.6** (T-backward simulation, generally)**.**[†] Let F be an endofunctor and T be a monad on $\mathbb{C}$ that satisfy the conditions in Prop. 5.2 wrt. $\sqsubseteq$. For two (T, F)-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, a *T-backward simulation* from $\mathcal{X}$ to $\mathcal{Y}$ is a backward simulation $b : X \nrightarrow Y$ that satisfies the following condition:

1. The arrow $b : X \nrightarrow Y$ satisfies $J!_Y \odot b = J!_X$. Here $!_Y : Y \to 1$ is the unique function.
We write $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}$ if there exists a T-backward simulation from $\mathcal{X}$ to $\mathcal{Y}$.

This general T-backward simulation satisfies soundness. For its proof we have to look into the inductive construction of the largest homomorphism in §5.1 (Prop. 5.2).

▶ **Lemma 5.7.**[†] *Let F and T be as in Prop. 5.2. For two (T, F)-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}$ (in the sense of Def. 5.6) implies $\mathsf{tr}^\infty(c) \sqsubseteq \mathsf{tr}^\infty(d) \odot b$. Furthermore it follows that $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.*

Proof of Thm. 5.5. In Lem. A.19 we prove that a T-backward simulation in the specific sense of Def. 5.4 is also a T-backward simulation in the general sense of Def. 5.4. Therefore Lem. 5.7 yields trace inclusion. ◀

5.3 Forward Partial Execution for Probabilistic Systems

We show that FPE can be used to aid discovery of forward and backward simulations, also in the current probabilistic setting.

▶ **Theorem 5.8.** *Let F be a polynomial functor on* **Meas**. *For $(\mathcal{G}, F)$-systems $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$, the following hold.*

1. **a.** (soundness of FPE for fwd. sim.) $\mathcal{X}_{\mathsf{FPE}} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ *implies* $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.
b. (adequacy of FPE for fwd. sim.) $\mathcal{X} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$ *implies* $\mathcal{X}_{\mathsf{FPE}} \sqsubseteq_{\mathbf{F}} \mathcal{Y}$.

2. **a.** (soundness of FPE for bwd. sim.) $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}_{\mathsf{FPE}}$ *implies* $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.
b. (adequacy of FPE for bwd. sim.) $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}$ *implies* $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}_{\mathsf{FPE}}$, *assuming that: $d(y)(FY) = 1$ for all $y \in Y$.*

The item 1 for forward simulations follows immediately from Thm. 4.10. For the relationship to backward simulations, we develop another general result.

▶ **Theorem 5.9** (FPE and bwd. sim.).[†] *Let F be an endofunctor and T be a monad on $\mathbb{C}$ that satisfy the conditions in Prop. 5.2 (hence those in Lem. 5.7). Let $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$ be (T, F)-systems.*

1. (soundness for bwd. sim.) $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}_{\mathsf{FPE}}$ *implies* $\mathsf{tr}^\infty(c) \odot s \sqsubseteq \mathsf{tr}^\infty(d) \odot t$.

2. (adequacy for bwd. sim.) $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}$ *implies* $\mathcal{X} \sqsubseteq^{\mathrm{T}}_{\mathbf{B}} \mathcal{Y}_{\mathsf{FPE}}$, *assuming that: the coalgebra $d : Y \nrightarrow \overline{F}Y$ satisfies $J!_{FY} \odot d = J!_Y$.*

Proof of Thm. 5.8. The item 1 is immediate from Thm. 4.10. In a similar manner to Lem. A.19, we can prove the item 2 using Thm. 5.9. ◀

6 Systems with Other Branching Types

In this section we briefly discuss two more pairs of F and T that constitute infinite trace situations.

The first pair is a polynomial functor F on **Sets** and the *lift monad* $\mathcal{L}$. For a given set $X \in$ **Sets**, $\mathcal{L}X$ is given by $\{\perp\} + X$. The added element $\perp$ represents the aborting or non-termination of the program, and hence an $(\mathcal{L}, F)$-system can be regarded as a *tree automaton with exception*. To show that F and $\mathcal{L}$ constitute an infinite trace situation, we rely on Prop. 5.2 (but not Prop. 4.2, since $\mathcal{L}X$ does not have the greatest element). Therefore, much like for $\mathcal{G}$, we can check trace inclusion by forward or T-backward simulations (see §5.2). More details are found in §A.5.

The second pair is that of polynomial F on **Sets** and the *subdistribution monad* $\mathcal{D}$. For a given set $X \in$ **Sets**, $\mathcal{D}X$ is the set $\{d \colon X \to [0,1] \mid \sum_{x \in X} d(x) \leq 1\}$ of (discrete) subdistributions over X. The subdistribution monad $\mathcal{D}$ is similar to the sub-Giry monad $\mathcal{G}$, and a $(\mathcal{D}, F)$-system can be also regarded as a probabilistic tree automaton. We can prove that F and $\mathcal{D}$ constitute an infinite trace situation. The resulting infinite trace semantics has limited use, however, due to the discrete nature of an arrow $X \nrightarrow \mathcal{D}Z$ (it assigns a probability to a single tree and the probability is most of the time 0; see Example 1.1). Another difficulty is that infinite traces for $T = \mathcal{D}$ does not follow from either of our general results (Prop. 4.2 or Prop. 5.2) – in §A.6 we construct infinite traces for $T = \mathcal{D}$ in concrete terms. This prevents us from applying the general theories for Kleisli simulations in §4–5. For more details, see §A.6.

7 Related Work

The construction of the largest homomorphism given in Prop. 5.2 is based on the one in [4]. The latter imposes some technical conditions on a monad T, including a "totality" condition that excludes $T = \mathcal{P}$ from its instances (the nonempty powerset monad is an instance). Our assumption of lifting to a 2-limit (Assumption 5 in Prop. 5.2) is inspired by a condition in [4], namely that the limit Z is lifted to a *weak* limit in $\mathcal{K}\ell(T)$. It is not the case that Prop. 5.2 subsumes the construction in [4]: the former does not apply to the nonempty powerset monad (but our Prop. 4.2 does apply to it).

In [12], an explicit description of a (proper, not weakly) final $\overline{F}$-coalgebra is given for $F \in \big\{\, \Sigma \times (\_),\, 1 + \Sigma \times (\_) \,\big\}$ and $T \in \{\mathcal{G}, \mathcal{G}_{=1}\}$. Here $\mathcal{G}_{=1}$ is the *Giry monad* and restricts $\mathcal{G}$ to proper, not sub-, distributions. We do not use their results (proper finality) for characterization of infinite traces, because: 1) if $T = \mathcal{G}$ then the final coalgebras do not coincide with the set of possibly infinite words; and 2) if $T = \mathcal{G}_{=1}$ then language inclusion is reduced to the equality. We doubt about the value of developing simulation-based methods for the latter degenerate case, one reason being that trace inclusion is often a more difficult problem than trace equivalence. For example, finite trace inclusion for probabilistic systems is undecidable [3] while trace equivalence is decidable [13].

In [17], it is shown that: a limit of a ω^{op}-sequence consisting of standard Borel spaces and surjective measurable functions is preserved by a polynomial functor F (where constants are restricted to standard Borel spaces), and also by $\mathcal{G}$. It is also shown there that such a polynomial functor F preserves standard Borel spaces, and so does $\mathcal{G}$. These facts imply the existence of a final $\mathcal{G}F$-coalgebra in **Meas** for every polynomial functor F. Note however that this final $\mathcal{G}F$-coalgebra captures (probabilistic) bisimilarity, not trace semantics.

8 Conclusions and Future Work

We have shown that the technique forward and backward Kleisli simulations [8] and that of FPE [18] – techniques originally developed for witnessing *finite* trace inclusion – are also applicable to *infinite* trace semantics. We followed [11] (and also [4, 12]) to characterize infinite trace semantics in coalgebraic terms, on which we established properties of Kleisli simulations such as soundness. We developed our theory for two classes of instances: nondeterministic systems and probabilistic ones.

There are some directions for a future work. In [18], in addition to FPE, a transformation called *backward partial execution* (BPE) is introduced. Similarly to FPE, BPE can also aid forward and backward Kleisli simulation for finite trace in the sense that it satisfy soundness and adequacy. However, BPE is only defined for word automata (with T-branching) and not generally for (T, F)-systems. Defining BPE categorically and proving its soundness and adequacy with respect to infinite trace, possibly restricting to word automata, is one of the future work.

Another direction is implementation and experiments. As forward and backward Kleisli simulations in this paper are defined in almost the same way as [18], we can use the implementation already developed there to check infinite trace inclusion.

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