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**Generic Forward and Backward Simulations II:
Probabilistic Simulation**

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Generic Forward and Backward Simulations II: Probabilistic Simulation^{*}

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Abstract. Jonsson and Larsen’s notion of probabilistic simulation is studied from a coalgebraic perspective. The notion is compared with two generic coalgebraic definitions of simulation: Hughes and Jacobs’ one, and the one introduced previously by the author. We show that the first almost coincides with the second, and that the second is a special case of the last. We investigate implications of this characterization; notably the Jonsson-Larsen simulation is shown to be *sound*, i.e. its existence implies trace inclusion.

1 Introduction

Use of probabilistic algorithms in distributed and concurrent applications is common practice. Consequently, modeling and verification techniques for probabilistic systems have been extensively developed. One fundamental branch therein is about probabilistic (*bi*)simulation: it gives an answer when a probabilistic system is “equivalent” to another, or when one “refines” another.

In this paper we focus on simulation notions for purely probabilistic systems.³ For such systems it is standard to define a notion of simulation using *weight functions*. The idea is first devised by Jonsson and Larsen [12]; it has inspired a large body of work including [1]. Our aim in this paper is to shed fresh, mathematical light on the idea, from the viewpoint of *coalgebra*.

Coalgebra is a mathematical/categorical presentation of state-based systems. Its initial success was brought about by a generic, coalgebraic characterization of bisimulation that applies to a variety of systems, including probabilistic ones (see e.g. [11, 17, 19]). The theory has since been extended to include various aspects of concurrency theory—such as SOS and modal logic (see e.g. [13]). Simulation, as “one-sided bisimulation,” is one of such aspects.

Two approaches have been presented towards a coalgebraic theory of simulation: Hughes and Jacobs’ [10] and the current author’s [5]. Both approaches are generic, applicable to non-deterministic systems like LTS as well as probabilistic ones. In this paper we restrict them to a purely probabilistic setting and conduct a comparative study. The comparison is among the *Jonsson-Larsen simulation*, the *Hughes-Jacobs simulation*, and the one in the author’s previous work [5] which we call the *Kleisli simulation*.

^{*} This is an extended version of the paper [7] that is to appear in Proc. CONCUR 2010. The current version is supplied with additional proofs and examples.

³ Unlike e.g. Segala’s probabilistic automata [18], they do not feature non-determinism.

Among the three, the notion of Kleisli simulation is the most distinguishable: it is given not as a relation but as a function $X \rightarrow \mathcal{D}Y$, where X and Y are the state spaces of the involved systems. Therefore it is not suitable as a candidate of a *refinement relation*, the original motivation for the Jonsson-Larsen one. The Kleisli simulation rather follows the spirit of Lynch and Vaandrager [16]: it is a powerful tool for showing *trace inclusion*. While a direct proof of trace inclusion involves transitions within arbitrary many steps, finding a simulation is a stepwise matter. Indeed the notion of Kleisli simulation is precisely a coalgebraic generalization of the one in [16]; the former comes with the *forward* and *backward* variations just like the latter. The theory in [5] has been successfully applied to verification of probabilistic anonymity in [9].

Our findings are as follows. The standard Jonsson-Larsen simulation, defined in §3 concretely for a specific kind of probabilistic systems (we describe them in §2), is identified with a slightly restricted variant of the Hughes-Jacobs simulation (§4). This allows us to remove the unnecessary restriction that was hidden in the original concrete definition (§4.4), as well as provides a guideline in transferring the definition to other kinds of probabilistic systems (§4.5). On another link in the triangle, we identify the Hughes-Jacobs simulation as a special case of the Kleisli simulation (§5). From the generic *soundness theorem* [5]—existence of a Kleisli simulation implies (finite) trace inclusion—we thus conclude soundness of the Hughes-Jacobs notion, hence of the Jonsson-Larsen one. In §6 we present some example systems for further comparison of different simulations. They suggest the potential use of Kleisli simulation, whose definition we shall state also in concrete terms.

Our expedition will be in a leisurely pace. In particular, no categorical or coalgebraic prerequisites are assumed; they are introduced on our way, on a call-by-need basis.

Notations A square in a diagram which is not filled means that it *commutes*, that is, the equality symbol $=$ is implicit in it.

A probability (sub)distribution γ over a set X is often denoted like a table: $[x \mapsto \gamma(x)]_{x \in X}$. When an entry $x \in X$ is missing in the table, the probability 0 is assigned. Hence for example, when $x_0 \in X$ is a fixed element, $[x_0 \mapsto 1]$ means the distribution γ such that $\gamma(x_0) = 1$ and $\gamma(x) = 0$ for $x \neq x_0$.

2 Probabilistic System

We will be mainly interested in two kinds of purely probabilistic systems—GPAs and DTMCs—which we now define formally.

Definition 2.1 (Generative probabilistic automaton, GPA) Let \mathcal{A}_c be a fixed nonempty alphabet; we refer to its element as an *action*. A *generative probabilistic automaton (GPA)* over \mathcal{A}_c is a triple $\mathcal{X} = (X, x_0, c)$ where

- X is a nonempty set of *states*;
- $x_0 \in X$ is a chosen state which is called the *initial* one; and

- $c : X \rightarrow \mathcal{D}(\{\checkmark\} + \text{Ac} \times X)$ is a *transition function*. Here $\{\checkmark\}$ is a singleton; $+$ denotes the disjoint union; and \mathcal{D} is the *subdistribution* operation. For a set Y

$$\mathcal{D}Y = \{\gamma : Y \rightarrow [0, 1] \mid \sum_{y \in Y} \gamma(y) \leq 1\} . \quad (1)$$

Such $d \in \mathcal{D}Y$ is called a *sub-distribution* since its values add up to not more than 1, instead of precisely 1.

The subdistribution $c(x)$ tells the probabilistic behavior of a state x . The value $c(x)(a, x')$ with $a \in \text{Ac}$ and $x' \in X$ is the probability with which x makes the action a and moves to x' ; that is, $c(x)(a, x') = \Pr[x \xrightarrow{a} x']$. We interpret the symbol \checkmark as *successful termination*; thus with the probability $c(x)(\checkmark) = \Pr[x \rightarrow \checkmark]$ the state x is led to successful termination. The remaining probability $1 - c(x)(\checkmark) - \sum_{a, x'} c(x)(a, x')$ —which may be more than 0 since $c(x)$ is a subdistribution—is understood as the probability with which x gets into *deadlock*.

GPA's are said to be *generative*, in contrast to *reactive* systems whose transition function is given as, say, $c : \text{Ac} \times X \rightarrow \mathcal{D}(\{\checkmark\} + X)$. They differ in whether an action is chosen by the system or by the environment; see [4].

GPA's can be thought of as a probabilistic variant of labeled transition systems (LTSs). DTMCs, which we introduce shortly, are then probabilistic Kripke frames. The notion is standard, see e.g. [1, 14]. The definitions in the literature vary in details; the following one is adapted to fit the current context.

Definition 2.2 (Discrete-Time Markov Chain, DTMC) Let AP be a fixed set of *atomic propositions*. A *discrete-time Markov chain (DTMC)* over AP is a quadruple $\mathcal{X} = (X, x_0, l, p)$ where

- X is a nonempty set of *states*, among which $x_0 \in X$ is an *initial* state;
- $l : X \rightarrow \mathcal{P}(\text{AP})$ is a *labeling function* where \mathcal{P} denotes the powerset. This assigns to a state $x \in X$ the set $l(x)$ of atomic propositions that hold at x ;
- $p : X \rightarrow \mathcal{D}X$ is a *transition function*, where \mathcal{D} is the subdistribution operation in (1).

A DTMC has labels on its states, while a GPA has labels on its transitions.

3 Jonsson-Larsen Simulation

For DTMC and its variants, a standard definition of simulation [12] uses *weight functions*. Here we present the definition for DTMC taken from [1]. This family of simulation notions—based on weight functions—will be called *Jonsson-Larsen simulation*.

Definition 3.1 (JL-simulation for DTMC) Let $\mathcal{X} = (X, x_0, l, p)$ and $\mathcal{Y} = (Y, y_0, m, q)$ be DTMCs. A *Jonsson-Larsen simulation (JL-simulation)* from \mathcal{X} to \mathcal{Y} is a relation $R \subseteq X \times Y$ which satisfies the following.

1. The initial states are related, that is, $x_0 R y_0$.

2. Related states satisfy the same set of atomic propositions: xRy implies $l(x) = m(y)$.
3. For each $x \in X$ and $y \in Y$ such that xRy , there exists a *weight function*

$$\Delta_{x,y} : (\{\perp\} + X) \times (\{\perp\} + Y) \longrightarrow [0, 1]$$

such that

- (a) $\Delta_{x,y}(u, v) > 0$ implies either
 - $u = \perp$, or
 - $u = x' \in X, v = y' \in Y$ and $x'Ry'$;
- (b) $\Delta_{x,y}(\perp, \perp) + \sum_{y' \in Y} \Delta_{x,y}(\perp, y') = 1 - \sum_{x' \in X} p(x)(x')$;
- (c) for each $x' \in X$: $\Delta_{x,y}(x', \perp) + \sum_{y' \in Y} \Delta_{x,y}(x', y') = p(x)(x')$;
- (d) $\Delta_{x,y}(\perp, \perp) + \sum_{x' \in X} \Delta_{x,y}(x', \perp) = 1 - \sum_{y' \in Y} q(y)(y')$;
- (e) for each $y' \in Y$: $\Delta_{x,y}(\perp, y') + \sum_{x' \in X} \Delta_{x,y}(x', y') = q(y)(y')$.

Note that the condition (a) simplifies (c) and (d) into the following:

- (c') for each $x' \in X$: $\sum_{y' \in Y} \Delta_{x,y}(x', y') = p(x)(x')$;
- (d') $\Delta_{x,y}(\perp, \perp) = 1 - \sum_{y' \in Y} q(y)(y')$.

Although illustration of the previous definition is found e.g. in [1, Ex. 14], the definition hardly seems as “canonical” or “intuitive” as other notions such as (bi)simulation for ordinary LTS. For example, the only asymmetry between \mathcal{X} and \mathcal{Y} is found in Cond. 3.(a) where u , not v , is allowed to be \perp . One might wonder if it is possible to weaken this condition. Weakening = into \subseteq in Cond. 2 looks like another possibility. It is not clear either how to adapt this definition to GPA. Even less clear is whether the adapted notion satisfies soundness—existence of a simulation implies trace inclusion—which is a natural property to expect.

What we do in the rest of the paper is to put the above definition in a coalgebraic context. First it will be identified with a restriction of Hughes and Jacobs’ simulation (*HJ-simulation*) [10]. From this we immediately obtain natural generalizations of the original definition, which are hinted above. The generic theory in [10] can be used to conduct some “sanity checks” for the generalized definitions. Adaptation to GPA comes for free, too. After that we will identify HJ-simulation with a certain subclass of *Kleisli* simulation from [5]. Soundness of JL-simulation for GPA is its corollary.

4 Hughes-Jacobs Simulation

4.1 Coalgebraic Modeling

In the Hughes-Jacobs theory of coalgebraic simulation, a system is modeled as a *B-coalgebra*, which is a function c of the type on the right. The set X (which is arbitrary) is the system’s *state space*; the operation B specifies the kind of transitional behavior exhibited by the system; and the function c determines the system’s dynamic behavior. We now elaborate on the operation B , which takes a set X and returns another set BX .

$$\begin{array}{c} BX \\ c \uparrow \\ X \end{array}$$

Roughly speaking, it is the operation B which determines what kind of systems we are talking about. One choice of B makes a B -coalgebra an LTS; another choice of B is for a deterministic automaton (DA); and so on. Specifically,

B	$\mathcal{P}(\text{Ac} \times _)$	$2 \times (_)^{\text{Ac}}$	$(\text{Ac}_{\text{out}} \times _)^{\text{Ac}_{\text{in}}}$	$\mathcal{D}(\{\checkmark\} + \text{Ac} \times _)$	$\mathcal{P}(\text{AP}) \times \mathcal{D}(_)$
B -coalg.	LTS	DA	Mealy mach.	GPA	DTMC

When B is $\mathcal{D}(\{\checkmark\} + \text{Ac} \times _)$, a B -coalgebra is a function $c : X \rightarrow \mathcal{D}(\{\checkmark\} + \text{Ac} \times X)$; this is precisely a GPA (Def. 2.1) without an explicit initial state. For $B = \mathcal{P}(\text{AP}) \times \mathcal{D}(_)$, a B -coalgebra is a function $c : X \rightarrow \mathcal{P}(\text{AP}) \times \mathcal{D}X$, which is identified with a DTMC (without an initial state) via the following bijective projection-tupling correspondence.

$$\frac{X \longrightarrow \mathcal{P}(\text{AP}) \times \mathcal{D}X}{X \longrightarrow \mathcal{P}(\text{AP})} \quad X \longrightarrow \mathcal{D}X \quad \begin{array}{c} c \\ \Downarrow \cong \\ (\pi_1 \circ c, \pi_2 \circ c) \end{array} \quad \begin{array}{c} \langle l, p \rangle := \lambda x. (l(x), p(x)) \\ \uparrow \cong \\ (l, p) \end{array}$$

Here π_i denotes the i -th projection; $\langle l, p \rangle$ denotes the *tupling* of l and p .

To develop a “theory of systems” on top of this modeling, an operation B needs to be a *functor*. Leaving its detailed treatment to literature like [11], what it means is that the operation B not only applies to sets (i.e. $X \mapsto BX$) but also to functions. That is,

$$B : (X \xrightarrow{f} Y) \longmapsto (BX \xrightarrow{Bf} BY) .$$

Note the domain and the codomain of the resulting function Bf .

The previous examples of B have natural action on functions. For example, given a function $f : X \rightarrow Y$,

$$\begin{aligned} \mathcal{P}(\text{Ac} \times X) &\xrightarrow{\mathcal{P}(\text{Ac} \times f)} \mathcal{P}(\text{Ac} \times Y) , \quad u \longmapsto \{ (a, f(x)) \mid (a, x) \in u \} ; \\ \mathcal{D}(\{\checkmark\} + \text{Ac} \times X) &\xrightarrow{\mathcal{D}(\{\checkmark\} + \text{Ac} \times f)} \mathcal{D}(\{\checkmark\} + \text{Ac} \times Y) , \\ &\quad \gamma \longmapsto \left[\begin{array}{l} \checkmark \mapsto \gamma(\checkmark) \\ (a, y) \mapsto \sum_{x \in f^{-1}(\{y\})} \gamma(a, x) \end{array} \right] ; \\ \mathcal{P}(\text{AP}) \times \mathcal{D}X &\xrightarrow{\mathcal{P}(\text{AP}) \times \mathcal{D}f} \mathcal{P}(\text{AP}) \times \mathcal{D}Y , \quad (u, \gamma) \longmapsto (u, [y \mapsto \sum_{x \in f^{-1}(\{y\})} \gamma(x)]) . \end{aligned}$$

Lying under the latter two is \mathcal{D} 's action on functions:

$$\mathcal{D}X \xrightarrow{\mathcal{D}f} \mathcal{D}Y , \quad \gamma \longmapsto [y \mapsto \sum_{x \in f^{-1}(\{y\})} \gamma(x)] . \quad (2)$$

To be precise, such B is a functor of the type **Sets** \rightarrow **Sets**, from the category **Sets** of sets and functions to itself. We make a formal definition for the record.

Definition 4.1 (Functor, coalgebra) A *functor* $B : \mathbf{Sets} \rightarrow \mathbf{Sets}$ consists of its action on sets $X \mapsto BX$ and on functions $(X \xrightarrow{f} Y) \mapsto (BX \xrightarrow{Bf} BY)$, for each X and f . This is subject to the following conditions:

$$B(X \xrightarrow{\text{id}_X} X) = (BX \xrightarrow{\text{id}_{BX}} BX) ; \quad B(X \xrightarrow{f} Y \xrightarrow{g} U) = (BX \xrightarrow{Bf} BY \xrightarrow{Bg} BU) .$$

A B -coalgebra is a pair $(X, c : X \rightarrow BX)$ of a set and a function; we shall simply denote it by $X \xrightarrow{c} BX$.

The *functoriality* of B is crucial in the following definition of coalgebraic bisimulation (notice use of $B\pi_i$). The definition subsumes many known notions of bisimulation.

Definition 4.2 Let $B : \mathbf{Sets} \rightarrow \mathbf{Sets}$ be a functor and $c :$

$X \rightarrow BX$ and $d : Y \rightarrow BY$ be B -coalgebras. A *coalgebraic bisimulation* is a relation $R \subseteq X \times Y$ such that: there exists a function $r : R \rightarrow BR$ that makes the diagram on the right commute. Here π_1 and π_2 are obvious projections.

$$\begin{array}{ccccc} BX & \xleftarrow{B\pi_1} & BR & \xrightarrow{B\pi_2} & BY \\ c \uparrow & & r \uparrow & & \uparrow d \\ X & \xleftarrow{\pi_1} & R & \xrightarrow{\pi_2} & Y \end{array} \quad (3)$$

When B represents purely probabilistic systems such as DTMCs, the above coalgebraic bisimulation instantiates to the one that uses a weight function. It coincides with the more common formulation via equivalence classes [15]. The coincidence proof is implicit in [12, Thm. 4.6] and is much more systematically conducted in [19].

4.2 Hughes-Jacobs Simulation

Roughly speaking, simulation is “one-sided” bisimulation. When R is a simulation and xRy , we require y to exhibit “at least as much” behavior as x does, that is,

$$(x\text{'s behavior}) \sqsubseteq (y\text{'s behavior}) \quad (4)$$

in terms of a suitable preorder \sqsubseteq of “behavior inclusion.” Hughes and Jacobs [10] used this intuition and defined generic simulation as a variant of Def. 4.2. In order to do so, a functor $B : \mathbf{Sets} \rightarrow \mathbf{Sets}$ needs to come with a “behavior-inclusion” preorder \sqsubseteq .

Definition 4.3 (Functor with preorder) A *functor with preorder* consists of a functor $B : \mathbf{Sets} \rightarrow \mathbf{Sets}$ and a class of preorders $\{\sqsubseteq_{BX}\}_X$ for each set X , where \sqsubseteq_{BX} is on the set BX . Further, given a function $f : X \rightarrow Y$, its action $Bf : BX \rightarrow BY$ is required to be a monotone function. We often suppress the subscript in \sqsubseteq_{BX} .

Example 4.4 Let $B = \mathcal{P}(\text{Ac} \times _)$, for which B -coalgebras are LTSs. It is a functor with preorder, with a natural choice of \sqsubseteq_{BX} being the inclusion order.

Let $B = \mathcal{D}(\{\checkmark\} + \text{Ac} \times _)$; a B -coalgebra is a GPA. For $\gamma, \delta \in BX$ we define

$$\gamma \sqsubseteq_{BX} \delta \stackrel{\text{def.}}{\iff} \gamma(\checkmark) \leq \delta(\checkmark) \quad \text{and} \quad \gamma(a, x) \leq \delta(a, x) \quad \text{for each } a \text{ and } x.$$

Note that \sqsubseteq_{BX} need not be reduced to the equality, since γ and δ are *subdistributions*.

Let $B = \mathcal{P}(\text{AP}) \times \mathcal{D}(_)$; a B -coalgebra is then a DTMC. There are a few natural candidates for the preorder \sqsubseteq_{BX} . One is:

$$(u, \gamma) \sqsubseteq_{BX}^\equiv (v, \delta) \stackrel{\text{def.}}{\iff} u = v \quad \text{and} \quad \gamma(x) \leq \delta(x) \quad \text{for each } x.$$

We denote this order by \sqsubseteq^\equiv . Noting that u and v are subsets of AP, we could replace the condition $u = v$ by $u \subseteq v$, for example. The resulting order will be denoted by \sqsubseteq^\subseteq .

Definition 4.5 (HJ-simulation) Let (B, \sqsubseteq) be a functor

with preorder, and $X \xrightarrow{c} BX, Y \xrightarrow{d} BY$ be B -coalgebras. A *Hughes-Jacobs simulation* (HJ-simulation) from c to d is a relation $R \subseteq X \times Y$ such that: there exists a function $r : R \rightarrow BR$ which makes the inequalities on the right hold.

$$\begin{array}{ccccc} BX & \xleftarrow{B\pi_1} & BR & \xrightarrow{B\pi_2} & BY \\ c\uparrow & \sqsubseteq & r\uparrow & \sqsubseteq & \uparrow d \\ X & \xleftarrow{\pi_1} & R & \xrightarrow{\pi_2} & Y \end{array} \quad (5)$$

That is to be precise: for each $(x, y) \in R$

$$(c \circ \pi_1)(x, y) \sqsubseteq_{BX} (B\pi_1 \circ r)(x, y) \quad \text{and} \quad (B\pi_2 \circ r)(x, y) \sqsubseteq_{BY} (d \circ \pi_2)(x, y) .$$

Noting e.g. $\pi_1(x, y) = x$, this means: for each x and y such that xRy ,

$$c(x) \sqsubseteq_{BX} (B\pi_1 \circ r)(x, y) \quad \text{and} \quad (B\pi_2 \circ r)(x, y) \sqsubseteq_{BY} d(y) .$$

The formulation is different from the original one [10] where a lax relation lifting is used. The equivalence is proved in Appendix A.1.

4.3 Jonsson-Larsen Simulation as Hughes-Jacobs Simulation

Here is the first main observation in this paper: JL is HJ. The order $\sqsubseteq^=$ is from Ex. 4.4.

Theorem 4.6 Let $\mathcal{X} = (X, x_0, l, p)$ and $\mathcal{Y} = (Y, y_0, m, q)$ be DTMCs, and let R be a JL-simulation from \mathcal{X} to \mathcal{Y} . Then R is a HJ-simulation from the coalgebra $\langle l, p \rangle$ to $\langle m, q \rangle$: there exists r that makes the following (in)equalities hold.

$$\begin{array}{ccccccc} \mathcal{P}(\text{AP}) \times \mathcal{D}X & \xleftarrow{\mathcal{P}(\text{AP}) \times \mathcal{D}\pi_1} & \mathcal{P}(\text{AP}) \times \mathcal{D}R & \xrightarrow{\mathcal{P}(\text{AP}) \times \mathcal{D}\pi_2} & \mathcal{P}(\text{AP}) \times \mathcal{D}Y & & \\ \langle l, p \rangle \uparrow & = & \pi_1 & r \uparrow & \sqsubseteq^= & \uparrow \langle m, q \rangle & \\ X & \xleftarrow{\quad} & R & \xrightarrow{\quad} & Y & & \end{array} \quad (6)$$

Proof. We need to find $r = \langle r_1, r_2 \rangle$ with $r_1 : R \rightarrow \mathcal{P}(\text{AP})$ and $r_2 : R \rightarrow \mathcal{D}R$. We set $r_1(x, y) := l(x)$, which is equal to $m(y)$ by Cond. 2 of Def. 3.1. A weight function Δ is used to define r_2 ; specifically

$$r_2(x, y) := \lambda(x', y') \in R. \Delta_{x, y}(x', y') .$$

We verify the equality (left) and the inequality (right) in (6). They obviously hold with respect to the first component, i.e. equalities between functions $R \rightarrow \mathcal{P}(\text{AP})$. We focus on the second component, i.e. (in)equalities between functions $R \rightrightarrows \mathcal{D}X$ and $R \rightrightarrows \mathcal{D}Y$.

$$\begin{aligned} & (\mathcal{D}\pi_1 \circ r_2)(x, y)(x') \\ &= \sum_{\{(x'', y'') \in R \mid \pi_1(x'', y'') = x'\}} r_2(x, y)(x'', y'') \quad \text{by def. of } \mathcal{D}\pi_1 \text{ (2)} \\ &= \sum_{\{y'' \mid x'Ry''\}} \Delta_{x, y}(x', y'') \quad \text{by def. of } r_2 \\ &= \sum_{y'' \in Y} \Delta_{x, y}(x', y'') \quad \text{by Cond. 3.(a) of Def. 3.1} \\ &= p(x)(x') \quad \text{by Cond. 3.(c') of Def. 3.1.} \end{aligned}$$

This proves the equality on the left. Regarding the inequality on the right,

$$\begin{aligned}
& (\mathcal{D}\pi_2 \circ r_2)(x, y)(y') \\
&= \sum_{x'' \in X} \Delta_{x, y}(x'', y') \quad \text{much like the above} \\
&= q(y)(y') - \Delta_{x, y}(\perp, y') \quad \text{by Cond. 3.(e) of Def. 3.1} \\
&\leq q(y)(y') .
\end{aligned} \quad \square$$

We include initial states (Cond. 1, Def. 3.1) and obtain the following characterization.

Theorem 4.7 (JL is HJ) *Let \mathcal{X} and \mathcal{Y} be DTMCs in Thm. 4.6. A relation $R \subseteq X \times Y$ is a JL-simulation if and only if there exist functions r and r_0 that make the following (in)equalities hold. The set $\{*\}$ is a singleton.*

$$\begin{array}{ccccc}
\mathcal{P}(\text{AP}) \times \mathcal{D}X & \xleftarrow{\mathcal{P}(\text{AP}) \times \mathcal{D}\pi_1} & \mathcal{P}(\text{AP}) \times \mathcal{D}R & \xrightarrow{\mathcal{P}(\text{AP}) \times \mathcal{D}\pi_2} & \mathcal{P}(\text{AP}) \times \mathcal{D}Y \\
\uparrow \langle l, p \rangle & & \uparrow r & & \uparrow \langle m, q \rangle \\
X & \xleftarrow{\pi_1} & R & \xrightarrow{\pi_2} & Y \\
\uparrow x_0 & & \uparrow r_0 & & \uparrow y_0 \\
& \xleftarrow{\quad} & \{*\} & \xrightarrow{\quad} &
\end{array} \quad (7)$$

Note that a function $x_0 : \{*\} \rightarrow X$ can be identified with an element $x_0 \in X$.

Proof. The bottom equalities force r_0 to be (x_0, y_0) . Hence the ‘only if’ part is a direct consequence of Thm. 4.6.

For the ‘if’ part, Cond. 1 follows from the bottom equalities. Cond. 2 follows from the upper (in)equalities’ first components. Note that this relies on the choice of $\sqsubseteq^=$ instead of, say, \sqsubseteq^{\subseteq} . Regarding Cond. 3, for $(x, y) \in R$ we define a weight function $\Delta_{x, y}$ by

$$\begin{aligned}
(x', y') &\mapsto \begin{cases} r_2(x, y)(x', y') & \text{if } (x', y') \in R \\ 0 & \text{otherwise} \end{cases}, \quad (x', \perp) \mapsto 0, \\
(\perp, y') &\mapsto q(y)(y') - \sum_{\{x' | x' R y'\}} r_2(x, y)(x', y'), \quad (\perp, \perp) \mapsto 1 - \sum_{y' \in Y} q(y)(y'),
\end{aligned}$$

where $r_2 := \pi_2 \circ r$. Then Cond. 3.(a) of Def. 3.1 is obvious. On Cond. 3.(b),

$$\begin{aligned}
& \Delta_{x, y}(\perp, \perp) + \sum_{y' \in Y} \Delta_{x, y}(\perp, y') \\
&= 1 - \sum_{y' \in Y} q(y)(y') + \sum_{y' \in Y} \left(q(y)(y') - \sum_{\{x' | x' R y'\}} r_2(x, y)(x', y') \right) \\
&= 1 - \sum_{x' \in X} \sum_{\{y' | x' R y'\}} r_2(x, y)(x', y') \\
&= 1 - \sum_{x' \in X} (\mathcal{D}\pi_1 \circ r_2)(x, y)(x') \quad \text{by def. of } \mathcal{D}\pi_1 \\
&= 1 - \sum_{x' \in X} p(x)(x') \quad \text{by the top-left equality in (7).}
\end{aligned}$$

Cond. 3.(c') and 3.(e) are verified as follows. Cond. 3.(d') is obvious.

$$\begin{aligned}
& \sum_{y' \in Y} \Delta_{x,y}(x', y') \\
&= \sum_{\{y' | x' R y'\}} r_2(x, y)(x', y') \\
&= (\mathcal{D}\pi_1 \circ r_2)(x, y)(x') \quad \text{by def. of } \mathcal{D}\pi_1 \\
&= p(x)(x') \quad \text{by the top-left equality in (7),} \\
&\Delta_{x,y}(\perp, y') + \sum_{x' \in X} \Delta_{x,y}(x', y') \\
&= q(y)(y') - \sum_{\{x' | x' R y'\}} r_2(x, y)(x', y') + \sum_{\{x' | x' R y'\}} r_2(x, y)(x', y') \\
&= q(y)(y') \quad . \quad \square
\end{aligned}$$

4.4 Generalized Jonsson-Larsen Simulation

Thm. 4.7 shows that JL-simulation does not reach the full generality of HJ-simulation: the top-left square is an equality in (7), which is not necessary. Translating HJ-simulation into the Jonsson-Larsen style concrete terms, we are led to the following definition.

Definition 4.8 (JL'-simulation for DTMC) A *JL'-simulation* is the same as a JL-simulation (Def. 3.1) except for the following.

- A weight function is of the type $\Delta_{x,y} : (\{\perp\} + X) \times (\{\perp\} + Y) \longrightarrow [-1, 1]$.
- Cond. 3.(a) is weakened: the value of $\Delta_{x,y}(u, v)$ must lie in the following range, according to u and v :

$u \backslash v$	\perp	$\dots y' \dots$
\perp	≤ 0	≥ 0
\vdots	\vdots	\vdots
x'	≤ 0	$\begin{cases} \geq 0 & (x' R y') \\ 0 & (\text{o.w.}) \end{cases}$
\vdots	\vdots	\vdots
- Cond. 3.(b) and 3.(d) are dropped.

Now a weight function can take negative values. Cond. 3.(b) and 3.(d) played no role in Thm. 4.6, hence are dropped. Similarly to JL-simulation, finding a weight function is filling in the matrix above on the right, in such a way that its rows and columns add up to the right values like $p(x)(x')$ or $q(y)(y')$. The task is easier with JL'-simulation because each entry can be picked from a broadened domain.

One can further generalize the previous definition by replacing $\sqsubseteq^=$ by \sqsubseteq^{\subseteq} (Ex. 4.4): in this case the system \mathcal{X} to be simulated satisfies no more atomic propositions than \mathcal{Y} does. This generalization is useful e.g. when we are interested in safety properties, and atomic propositions represent systems' actions.

Definition 4.9 (JL''-simulation for DTMC) A *JL''-simulation* is the same as a JL'-simulation (Def. 4.8), except that Cond. 2 is replaced by

2. $x R y$ implies $l(x) \subseteq m(y)$.

Proposition 4.10 Let \mathcal{X} and \mathcal{Y} be DTMCs as in Thm. 4.6, and $R \subseteq X \times Y$.

1. The relation R is a JL' -simulation if and only if there exist r and r_0 that validate the (in)equalities in (7), with the top-left equality replaced by $\sqsubseteq^=$.
2. The relation R is a JL'' -simulation if and only if there exist r and r_0 that validate the diagram (7), with the top two squares filled with $\sqsubseteq^=$. \square

Let us do some sanity checks. The following holds for JL'' instead of JL' too; also for the conventional notion of JL simulation (see [1]).

Proposition 4.11 *Let $\mathcal{X} = (X, x_0, l, p)$ and $\mathcal{Y} = (Y, y_0, m, q)$ be DTMCs.*

1. *If $R \subseteq X \times Y$ is a bisimulation, then R and R^{op} are both JL' -simulations.*
2. *The family of JL' -simulations from \mathcal{X} to \mathcal{Y} is closed under arbitrary unions. Therefore there is the largest JL' -simulation $\lesssim_{JL'}$, called JL' -similarity.*
3. *JL' -simulations are closed under composition. Hence $\lesssim_{JL'}$ is transitive.*

Proof. The claim follows from Lem. 4.2 and Prop. 5.4 of [10]. To apply the latter we need to show that the orders $\sqsubseteq^=$ and $\sqsubseteq^= \mathcal{P}(\text{AP}) \times \mathcal{D}(_)$ are *stable*, a technical condition from [10]. We prove that for $\sqsubseteq^=$; it is similar for $\sqsubseteq^=$. By the inequality (1) in [10] it suffices to show: for any function $f : Y \rightarrow X$ we have

$$\begin{aligned} & \{ (u, \gamma), (v, \delta) \mid (u, \gamma) \sqsubseteq^= (\mathcal{P}(\text{AP}) \times \mathcal{D}f)(v, \delta) \} \\ & \subseteq \{ ((\mathcal{P}(\text{AP}) \times \mathcal{D}f)(u', \delta'), (v', \delta'')) \mid (u', \delta') \sqsubseteq^= (v', \delta'') \} . \end{aligned}$$

Here $\gamma \in \mathcal{D}X$ and $\delta, \delta', \delta'' \in \mathcal{D}Y$. This is immediately reduced to:

Sublemma 1 *Assume $\gamma(x) \leq \sum_{y \in f^{-1}(\{x\})} \delta(y)$ for each $x \in X$. Then there exists $\delta' \in \mathcal{D}Y$ such that*

$$\delta'(y) \leq \delta(y) \quad \text{for each } y, \quad \text{and} \quad \gamma(x) = \sum_{y \in f^{-1}(\{x\})} \delta'(y) \quad \text{for each } x.$$

We construct such δ' by “discounting” δ . Concretely, we set

$$\delta'(y) := \frac{\gamma(f(y))}{\sum_{y' \in f^{-1}(\{f(y)\})} \delta(y')} \cdot \delta(y)$$

if the denominator is non-zero; otherwise $\delta'(y) := 0$. The first condition is obvious from the assumption. For the second one,

$$\begin{aligned} \sum_{y \in f^{-1}(\{x\})} \delta'(y) &= \sum_{y \in f^{-1}(\{x\})} \frac{\gamma(f(y))}{\sum_{y' \in f^{-1}(\{f(y)\})} \delta(y')} \cdot \delta(y) && \text{by def. of } \delta' \\ &= \sum_{y \in f^{-1}(\{x\})} \frac{\gamma(x)}{\sum_{y' \in f^{-1}(\{x\})} \delta(y')} \cdot \delta(y) && \text{by } f(y) = x \\ &= \frac{\sum_{y \in f^{-1}(\{x\})} \gamma(x) \cdot \delta(y)}{\sum_{y' \in f^{-1}(\{x\})} \delta(y')} = \gamma(x) , \end{aligned}$$

for each x such that $\sum_{y \in f^{-1}(\{x\})} \delta(y) > 0$. Otherwise we have $\gamma(x) = \sum_{y \in f^{-1}(\{x\})} \delta'(y) = 0$. This proves the sublemma, hence the proposition. \square

4.5 Jonsson-Larsen Simulation for GPA

Another implication of Thm. 4.7 is adaptation of JL-simulation for other kinds of probabilistic systems, via HJ-simulation which is general by definition.

Definition 4.12 (JL-simulation for GPA) Let $\mathcal{X} = (X, x_0, c)$ and $\mathcal{Y} = (Y, y_0, d)$ be GPAs. A *JL-simulation* from \mathcal{X} to \mathcal{Y} is a relation $R \subseteq X \times Y$ such that:

1. The initial states are related, that is, $x_0 R y_0$.
2. For each pair $(x, y) \in R$, there exists a weight function

$$\Delta_{x,y} : (\{\perp\} + \{\checkmark\} + \text{Ac} \times X) \times (\{\perp\} + \{\checkmark\} + \text{Ac} \times Y) \longrightarrow [-1, 1] \quad \text{such that}$$

- (a) $\Delta_{x,y}(u, v)$ lies in the range on the right. In particular, $\Delta_{x,y}((a, x'), (a', y')) > 0$ only if $a = a'$ and $x' R y'$;

$u \setminus v$	\perp	\checkmark	$\cdots (a_1, y'_1) \cdots$	$\cdots (a_2, y'_2) \cdots$
\perp	≤ 0	≥ 0	≥ 0	≥ 0
\checkmark	≤ 0	≥ 0	0	0
\vdots				
(a_1, x'_1)	≤ 0	0	$\begin{cases} \geq 0 & (x'_1 R y'_1) \\ 0 & (\text{o.w.}) \end{cases}$	0
\vdots				
(a_2, x'_2)	≤ 0	0	0	$\begin{cases} \geq 0 & (x'_2 R y'_2) \\ 0 & (\text{o.w.}) \end{cases}$
\vdots				

- (b) $c(x)(\checkmark) = \Delta_{x,y}(\checkmark, \perp) + \Delta_{x,y}(\checkmark, \checkmark)$;
(c) $c(x)(a, x') = \Delta_{x,y}((a, x'), \perp) + \sum_{y'} \Delta_{x,y}((a, x'), (a, y'))$ for each a and x' ;
(d) $d(y)(\checkmark) = \Delta_{x,y}(\perp, \checkmark) + \Delta_{x,y}(\checkmark, \checkmark)$;
(e) $d(y)(a, y') = \Delta_{x,y}(\perp, (a, y')) + \sum_{x'} \Delta_{x,y}((a, x'), (a, y'))$ for each a and y' .

The definition seems to appear for the first time. It coincides with HJ-simulation for $B = \mathcal{D}(\{\checkmark\} + \text{Ac} \times _)$, with B equipped with the order in Ex. 4.4 (the proof is easy). Properties like in Prop. 4.11 hold as well. Remaining is the issue of *soundness*; it is not obvious at all from the above complicated definition. One of our main contributions is the soundness proof later in §5.7, which uses the generic theory in [5].

5 Kleisli Forward and Backward Simulation

We now describe the third kind of simulation from [5]. We shall refer to this family as *Kleisli simulation*, for the reason that is explained shortly. Kleisli simulation consists of four subclasses: *forward*, *backward*, and two *hybrid* ones, like in [16]. The most notable difference from JL- and HJ-notions is that a Kleisli simulation is a *function* $X \rightarrow \mathcal{D}Y$ or $Y \rightarrow \mathcal{D}X$ that satisfies certain conditions.

5.1 Kleisli Arrow

First we fix our domain of discourse—*Kleisli arrows*. They are arrows in a Kleisli category, a standard categorical construct. Our description is however in concrete terms.

Definition 5.1 (Kleisli arrow) Let X and Y be arbitrary sets. A *Kleisli arrow* from X to Y , denoted by $f : X \multimap Y$, is a function $f : X \rightarrow \mathcal{D}Y$. A few typical Kleisli arrows:

- The Kleisli arrow $\eta_X : X \multimap X$, for each X , is the function $\eta_X : X \rightarrow \mathcal{D}X$ that carries $x \in X$ to $[x \mapsto 1]$.
- Given consecutive Kleisli arrows $X \xrightarrow{f} Y$ and $Y \xrightarrow{g} U$, we have $g \odot f : X \multimap U$ by

$$g \odot f : X \longrightarrow \mathcal{D}U \quad , \quad x \longmapsto \lambda u. \sum_{y \in Y} g(y)(u) \cdot f(x)(y) \quad .$$

- For each (ordinary) function $f : X \rightarrow Y$, we have $Jf : X \multimap Y$ defined by $X \xrightarrow{f} Y \xrightarrow{\eta_Y} \mathcal{D}Y$. That is, $(Jf)(x) = [f(x) \mapsto 1]$. This generalizes η_X by: $\eta_X = J(\text{id}_X)$.

The following are straightforward; they say that Kleisli arrows form a category.

Proposition 5.2 1. *Composition of Kleisli arrows is associative: for three consecutive Kleisli arrows $X \xrightarrow{f} Y \xrightarrow{g} U \xrightarrow{h} V$, we have $h \odot (g \odot f) = (h \odot g) \odot f$.*
 2. *η is the unit of composition: for $X \xrightarrow{f} Y$ we have $\eta_Y \odot f = f = f \odot \eta_X$.* \square

One can think of a Kleisli arrow $f : X \multimap Y$ as a “function from X to Y , with implicit probabilistic branching”; or as a “probabilistic computation of input type X and output type Y .” The operator \odot realizes natural composition of such probabilistic computations. The embedding Jf of an ordinary function endows f with trivial branching. By moving from functions to Kleisli arrows, therefore, we have thrown probabilistic branching under the rug; this abstraction is useful in the subsequent development.

There is a natural order between parallel Kleisli arrows.

Definition 5.3 Between a parallel pair of Kleisli arrows $f, g : X \multimap Y$, we define an order $f \sqsubseteq g$ if: $f(x)(y) \leq g(x)(y)$ for each $x \in X$ and $y \in Y$.

5.2 Probabilistic Systems as Kleisli Coalgebras

A GPA $\mathcal{X} = (X, x_0, c)$ (Def. 2.1) can be presented by two Kleisli arrows:

$$\{*\} \xrightarrow{Jx_0} X \xrightarrow{c} \{\checkmark\} + \text{Ac} \times X \quad . \quad (8)$$

This is a prototype of the kind of systems on which we define Kleisli simulation. First we parametrize the ‘ $\{\checkmark\} + \text{Ac} \times (_)$ ’ part in the above.

Definition 5.4 (Polynomial functor) A *polynomial functor* is a functor $F : \mathbf{Sets} \rightarrow \mathbf{Sets}$ which is constructed

- from the identity functor $(_)$ and the constant functor C for each set C ,
- using finite products and arbitrary disjoint union (i.e. coproduct).

In the BNF notation: $F ::= (_) \mid C \mid F_1 \times F_2 \mid \coprod_{i \in I} F_i$.

The functor $\{\checkmark\} + \text{Ac} \times (_)$ is polynomial; so is e.g. $(\text{Ac} + _)^* = \coprod_{n < \omega} (\text{Ac} + _)^n$.

Lemma 5.5 *A polynomial functor F has canonical action on Kleisli arrows, carrying $X \xrightarrow{f} Y$ to $FX \xrightarrow{Ff} FY$.*

Proof. A general categorical proof is found in [8, §2.2]; one can also define such action concretely by induction on the construction of F . \square

In most cases F 's action on Kleisli arrows is obvious. For $F = \{\checkmark\} + \text{Ac} \times (_)$ and $f : X \rightarrow Y$, the Kleisli arrow $Ff : FX \rightarrow FY$ is given by the function $\{\checkmark\} + \text{Ac} \times X \rightarrow \mathcal{D}(\{\checkmark\} + \text{Ac} \times Y)$, defined by

$$\checkmark \mapsto [\checkmark \mapsto 1] \quad , \quad (a, x) \mapsto [(a, y) \mapsto f(x)(y)]_{y \in Y} \quad .$$

Definition 5.6 (Probabilistic F -system) Let F be a polynomial functor. A *probabilistic F -system* (or simply *F -system*) is a triple $\mathcal{X} = (X, s, c)$, where X is an arbitrary set and $\{*\} \xrightarrow{s} X \xrightarrow{c} FX$ are two Kleisli arrows. Recall that probabilistic branching is implicit in Kleisli arrows.

Example 5.7 A GPA induces an F -system, with $F = \{\checkmark\} + \text{Ac} \times (_)$; see (8). F -system is more general than GPA since the former allows a subdistribution on initial states (i.e. $s \in \mathcal{D}X$) rather than a single initial state. This additional generality is however not important.

A DTMC cannot be seen as an F -system as it is: its dynamics is given by a function $X \xrightarrow{\langle l, p \rangle} \mathcal{P}(\text{AP}) \times \mathcal{D}X$ which cannot be understood as a Kleisli arrow. We can fix it by moving “state labels” into “transition labels.” Let us define a function $c_{l,p}$ by

$$c_{l,p} : X \rightarrow \mathcal{D}(\mathcal{P}(\text{AP}) \times X) \quad , \quad x \mapsto [(l(x), x') \mapsto p(x)(x')]_{x' \in X} \quad ;$$

then the F -system $\{*\} \xrightarrow{Jx_0} X \xrightarrow{c_{l,p}} \mathcal{P}(\text{AP}) \times X$ represents a DTMC (X, x_0, l, p) .

The notion of (probabilistic) F -system is essentially a *Kleisli F -coalgebra* $X \xrightarrow{c} FX$ equipped with an explicit initial state $\{*\} \xrightarrow{s} X$. In coalgebraic studies it is usually unnecessary to speak about explicit initial states; we however need that in this paper for formulating the soundness result (Thm. 5.20). See [6, §3.2.4].

Let us compare the current *Kleisli coalgebraic modeling* of GPAs (Ex. 5.7) with the modeling in §4.1. They are the same in that the dynamics of a GPA is represented by a function $X \rightarrow \mathcal{D}(\{\checkmark\} + \text{Ac} \times X)$. In the Kleisli modeling, the functor $B = \mathcal{D}(\{\checkmark\} + \text{Ac} \times (_))$ is divided into \mathcal{D} (*branching part*) and $F = \{\checkmark\} + \text{Ac} \times (_)$ (*transition/action part*); the former is then “buried in the ground” using Kleisli arrows.

5.3 Kleisli Simulation

Definition 5.8 (Kleisli simulation) Let F be a polynomial functor and $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$ be F -systems. A *forward Kleisli simulation* from \mathcal{X} to \mathcal{Y} is a Kleisli arrow $f : Y \rightarrowtail X$ such that $c \odot f \sqsubseteq (Ff) \odot d$ and $s \sqsubseteq f \odot t$ (see below left). Note the direction of f . It is also called simply a *forward simulation*.

$$\begin{array}{ccc} \text{fwd.} & \begin{array}{c} FX \xleftarrow{Ff} FY \\ \begin{array}{ccc} c \uparrow & \sqsubseteq & f \\ X & \xleftarrow{f} & Y \\ \uparrow & \sqsubseteq & \uparrow \\ s & \{*\} & t \end{array} \end{array} & \text{bwd.} \quad \begin{array}{c} FX \xrightarrow{Fb} FY \\ \begin{array}{ccc} c \uparrow & \sqsubseteq & b \\ X & \xrightarrow{b} & Y \\ \uparrow & \sqsubseteq & \uparrow \\ s & \{*\} & t \end{array} \end{array} \end{array}$$

A *backward (Kleisli) simulation* is a Kleisli arrow $b : X \rightarrowtail Y$ such that $(Fb) \odot c \sqsubseteq d \odot b$ and $b \odot s \sqsubseteq t$ (see above right). Here the order \sqsubseteq refers to the one in Def. 5.3.

In fact, the last definition is an instance of *generic forward and backward simulation* in [5, 6]. The general definition has an extra parameter T that specifies a *branching type*. It is fixed to $T = \mathcal{D}$ in this paper, representing probabilistic branching. Another main example is $T = \mathcal{P}$, the powerset operation, for *non-deterministic* branching.

This extra parameter T is used in the definition of Kleisli arrow. Namely, $f : X \rightarrowtail Y$ is defined to be a function $f : X \rightarrow TY$. When $T = \mathcal{P}$, a Kleisli arrow $f : X \rightarrowtail Y$ is hence identified with a *binary relation* $R_f \subseteq X \times Y$, such that xR_fy if and only if $y \in f(x)$. In this case, if moreover $F = \text{Ac} \times (_)$ for which F -systems are ordinary LTSs, Kleisli simulation (Def. 5.8) coincides with the standard notions of forward and backward simulation for LTS (see e.g. [16]). This coincidence is illustrated in [6, §3.2.3]. To summarize: probabilistic Kleisli simulation (Def. 5.8) is a natural generalization of non-deterministic simulation in [16].

The directions of Kleisli arrows and inequalities in Def. 5.8 need some care. Notice that a *simulated* system always occurs on the smaller side of \sqsubseteq . The directions of f and b are best illustrated in a non-deterministic setting; see [6, §3.2.3].

5.4 Kleisli Simulation for GPA

We further instantiate the definition to GPA, i.e. $F = \{\checkmark\} + \text{Ac} \times (_)$. It demonstrates Kleisli simulation's affinity to the conventional simulation notions for LTS.

Notation 5.9 A forward simulation is a function $f : Y \rightarrow \mathcal{D}X$; we write $\Pr[y \dashrightarrow x]$ for the value $f(y)(x)$. We let $\Pr[x \rightarrow \checkmark]$ and $\Pr[x \xrightarrow{a} x']$ have their obvious meanings. We also compose events; for example

$$\Pr[y \dashrightarrow x \xrightarrow{a} x'] := \Pr[y \dashrightarrow x] \cdot \Pr[x \xrightarrow{a} x'] = f(y)(x) \cdot c(x)(a, x') .$$

For a backward simulation, we write $\Pr[x \dashrightarrow y]$ for $b(x)(y)$.

Definition 5.10 (Forward simulation for GPA) Let $\mathcal{X} = (X, x_0, c)$ and $\mathcal{Y} = (Y, y_0, d)$ be GPAs. A *forward (Kleisli) simulation* from \mathcal{X} to \mathcal{Y} is a function $f : Y \rightarrow \mathcal{D}X$ which satisfies the following (in)equalities.

$$\begin{aligned}
& \Pr[y_0 \dashrightarrow x_0] = 1 && \text{(INIT)} \\
& \sum_{x \in X} \Pr[y \dashrightarrow x \rightarrow \checkmark] \leq \Pr[y \rightarrow \checkmark] \quad \text{for each } y \in Y && \text{(TERM)} \\
& \sum_{x \in X} \Pr[y \dashrightarrow x \xrightarrow{a} x'] \leq \sum_{y' \in Y} \Pr[y \xrightarrow{a} y' \dashrightarrow x'] \\
& \quad \text{for each } y \in Y, a \in \text{Ac and } x' \in X && \text{(ACT)}
\end{aligned}$$

The condition (ACT) is illuminating. It can be depicted as the below left, which bears a clear affinity to the standard non-deterministic condition shown on the right.

$$\Pr \left[\begin{array}{c} y \\ \vdots \\ \bullet \end{array} \xrightarrow{a} x' \right] \leq \Pr \left[\begin{array}{c} y \xrightarrow{a} \bullet \\ \vdots \\ \bullet \end{array} \right] \quad \left(\begin{array}{c} y \\ \vdots \\ \bullet \end{array} \xrightarrow{a} x' \right) \text{ implies } \left(\begin{array}{c} y \xrightarrow{a} \exists \bullet \\ \vdots \\ \bullet \end{array} \right)$$

Definition 5.11 (Backward simulation for GPA) Let $\mathcal{X} = (X, x_0, c)$ and $\mathcal{Y} = (Y, y_0, d)$ be GPAs. A *backward (Kleisli) simulation* from \mathcal{X} to \mathcal{Y} is a function $b : X \rightarrow \mathcal{D}Y$ which satisfies the following inequalities.

$$\begin{aligned}
& \Pr[x_0 \dashrightarrow y_0] \leq 1 && \text{(INIT)} \\
& \Pr[x \rightarrow \checkmark] \leq \sum_{y \in Y} \Pr[x \dashrightarrow y \rightarrow \checkmark] \quad \text{for each } x \in X && \text{(TERM)} \\
& \sum_{x' \in X} \Pr[x \xrightarrow{a} x' \dashrightarrow y'] \leq \sum_{y \in Y} \Pr[x \dashrightarrow y \xrightarrow{a} y'] \\
& \quad \text{for each } x \in X, a \in \text{Ac and } y' \in Y && \text{(ACT)}
\end{aligned}$$

5.5 Hughes-Jacobs Simulation as Hybrid Kleisli Simulation

We follow [16] and introduce *hybrid* simulations which combine fwd. and bwd. ones.

Definition 5.12 (Hybrid simulation) Let $\mathcal{X} = (X, s, c)$ and $\mathcal{Y} = (Y, t, d)$ be F -systems. A *forward-backward (Kleisli) simulation* is a triple (\mathcal{U}, f, b) where

- $\mathcal{U} = (U, u, e)$ is an F -system called the *intermediate system*;
- f is a forward simulation from \mathcal{X} to \mathcal{U} , and
- b is a backward simulation from \mathcal{U} to \mathcal{Y} . See below on the left.

$$\begin{array}{ccc}
\text{fwd.-bwd.} & \begin{array}{c} FX \xleftarrow{Ff} FU \xrightarrow{Fb} FY \\ c \dashv \vdash \sqsubseteq f \dashv \vdash e \dashv \vdash b \sqsubseteq \dashv \vdash d \\ X \xleftarrow{f} U \xrightarrow{b} Y \\ \uparrow \sqsubseteq \dashv \vdash u \sqsubseteq \dashv \vdash t \uparrow \\ \quad \quad \quad \{*\} \end{array} & \text{bwd.-fwd.} \quad \begin{array}{c} FX \xrightarrow{Fb} FU \xleftarrow{Ff} FY \\ c \dashv \vdash \sqsubseteq b \dashv \vdash e \dashv \vdash f \sqsubseteq \dashv \vdash d \\ X \xrightarrow{f} U \xleftarrow{b} Y \\ \uparrow \sqsubseteq \dashv \vdash u \sqsubseteq \dashv \vdash t \uparrow \\ \quad \quad \quad \{*\} \end{array}
\end{array}$$

Similarly, a *backward-forward (Kleisli) simulation* is a triple (\mathcal{U}, b, f) of an intermediate system \mathcal{U} , a backward simulation b from \mathcal{X} to \mathcal{U} , and a forward simulation f from \mathcal{U} to \mathcal{Y} . See above on the right.

Proposition 5.13 *Let \mathcal{X}, \mathcal{Y} be F -systems. If there is a non-hybrid simulation from \mathcal{X} to \mathcal{Y} , then there are both fwd.-bwd. and bwd.-fwd. ones from \mathcal{X} to \mathcal{Y} .*

Proof. A forward simulation f from \mathcal{X} to \mathcal{Y} induces a backward-forward simulation $(\mathcal{X}, J(\text{id}), f)$; it has \mathcal{X} itself as an intermediate system. The other cases are similar. \square

The significance of bwd.-fwd. simulation is in its completeness; see [5, Thm. 6.2]. Fwd.-bwd. simulation is also important: it subsumes HJ-simulation, hence also JL-simulation. This is our second main observation.

Lemma 5.14 *Let F be a polynomial functor. Then the functor $\mathcal{D}F$ has the following natural order. This makes $(\mathcal{D}F, \sqsubseteq_{\mathcal{D}F})$ a functor with preorder (Def. 4.3).*

$$\gamma \sqsubseteq_{\mathcal{D}FX} \delta \xLeftrightarrow{\text{def.}} \gamma(u) \leq \delta(u) \text{ for all } u \in FX. \quad \square$$

When $F = \{\checkmark\} + \text{Ac} \times (_)$ and $B = \mathcal{D}F$, both B -coalgebras and probabilistic F -systems represent GPAs. In this case, the order on B in the previous definition coincides with the one in Ex. 4.4.

Theorem 5.15 (HJ is Kleisli) *Let $X \xrightarrow{c} \mathcal{D}FX$ and $Y \xrightarrow{d} \mathcal{D}FY$ be $\mathcal{D}F$ -coalgebras, $x_0 \in X$ and $y_0 \in Y$ be chosen (initial) states, and $R \subseteq X \times Y$ be a relation. Assume that there exists a function r that validates the inequalities in the diagram on the left, that is, that R is a HJ-simulation from c to d such that $x_0 R y_0$.*

$$\begin{array}{ccc} \mathcal{D}FX & \xleftarrow{\mathcal{D}F\pi_1} \mathcal{D}FR & \xrightarrow{\mathcal{D}F\pi_2} \mathcal{D}FY \\ \uparrow c & \sqsubseteq_{\mathcal{D}F} \uparrow r & \sqsubseteq_{\mathcal{D}F} \uparrow d \\ X & \xleftarrow{\pi_1} R & \xrightarrow{\pi_2} Y \\ \uparrow \text{ } & \uparrow \langle x_0, y_0 \rangle & \uparrow \text{ } \\ x_0 & \xrightarrow{\{*\}} y_0 & \end{array} \implies \begin{array}{ccc} FX & \xleftarrow{F(J\pi_1)} FR & \xrightarrow{F(J\pi_2)} FY \\ \uparrow c & \sqsubseteq \uparrow r & \sqsubseteq \uparrow d \\ X & \xleftarrow{J\pi_1} R & \xrightarrow{J\pi_2} Y \\ \uparrow \text{ } & \uparrow J\langle x_0, y_0 \rangle & \uparrow \text{ } \\ Jx_0 & \xrightarrow{\{*\}} Jy_0 & \end{array} \quad (9)$$

Then we have a fwd.-bwd. simulation from the F -system (X, Jx_0, c) to (Y, Jy_0, d) , shown above on the right. Note the order \sqsubseteq therein refers to the one in Def. 5.3.

In short: a HJ-simulation between $\mathcal{D}F$ -coalgebras induces a fwd.-bwd. simulation between the corresponding F -systems.

Proof. The orders $\sqsubseteq_{\mathcal{D}F}$ and \sqsubseteq coincide by definition. Therefore we are done if we show that all the corresponding pairs of composites of arrows in (9) denote the same functions. That is,

$$\begin{aligned} c \circ \pi_1 &= c \odot (J\pi_1) && \text{as functions } R \rightarrow \mathcal{D}FX, \\ (\mathcal{D}F\pi_1) \circ r &= F(J\pi_1) \odot r && \text{as functions } R \rightarrow \mathcal{D}FX, \end{aligned}$$

and similar equalities regarding π_2 and d . The first one is immediate from the definition of $J\pi_1$ and \odot (Def. 5.1). The second one relies on the definition of F 's action on a Kleisli arrow $J\pi_1$ (Lem. 5.5). One can give a concrete proof again by induction on

construction of F ; we shall instead resort to categorical arguments. The prerequisites can be found in [8].

$$\begin{aligned}
F(J\pi_1) \odot r &= \mu_{FX}^{\mathcal{D}} \circ (\mathcal{D}FJ\pi_1) \circ r && \text{by def. of } \odot, \text{ using monad structure} \\
&= \mu_{FX}^{\mathcal{D}} \circ (\mathcal{D}JF\pi_1) \circ r && FJ = JF, [8, \text{Diagram (2.3)}] \\
&= \mu_{FX}^{\mathcal{D}} \circ (\mathcal{D}(\eta_{FX}^{\mathcal{D}} \circ F\pi_1)) \circ r && \text{by def. of } J \\
&= \mu_{FX}^{\mathcal{D}} \circ (\mathcal{D}\eta_{FX}^{\mathcal{D}}) \circ (\mathcal{D}F\pi_1) \circ r && \text{by functoriality of } \mathcal{D} \\
&= (\mathcal{D}F\pi_1) \circ r && \text{by the unit law for the monad } \mathcal{D}.
\end{aligned} \quad \square$$

The notion of fwd.-bwd. simulation instantiates to GPA, like in §5.4. Thm. 4.7 yields:

Corollary 5.16 (JL is Kleisli) *Let \mathcal{X} and \mathcal{Y} be GPAs. A JL-simulation R from \mathcal{X} to \mathcal{Y} induces a fwd.-bwd. (Kleisli) simulation from \mathcal{X} to \mathcal{Y} .* \square

5.6 Generic Trace Semantics

Like in [16], the principal aim of Kleisli simulation is to show *trace inclusion*—a refinement relation with respect to (linear time) *trace semantics* which is the coarsest in the spectrum of [3]. Our use of the generic notion of Kleisli coalgebra calls for a generic definition of trace semantics too. We employ the theory in [8]; here is its quick recap.

A polynomial functor F always has an *initial algebra* $\alpha : FA \xrightarrow{\cong} A$. The intuition is: F represents a set of datatype constructors; and A is the induced inductive datatype. The algebraic structure α always becomes an invertible function.

Example 5.17 The functor $F = \{\checkmark\} + \text{Ac} \times (_)$ is thought of as: a nullary constructor \checkmark and a family of unary constructors $a(_)$, for each $a \in \text{Ac}$. The induced inductive datatype is the set $\text{Ac}^* = \{a_1 a_2 \cdots a_n \checkmark \mid n < \omega, a_i \in \text{Ac}\}$ of (finite) lists over Ac . This set indeed carries an initial algebra: there is a canonical algebraic structure $\alpha : \{\checkmark\} + \text{Ac} \times \text{Ac}^* \xrightarrow{\cong} \text{Ac}^*$, namely

$$\checkmark \mapsto \checkmark \text{ (the empty sequence),} \quad (a, a_1 \cdots a_n \checkmark) \mapsto aa_1 \cdots a_n \checkmark.$$

The following is the main result in [8], adapted to the current context.

Theorem 5.18 (Generic (finite) trace semantics) *Let*

$\alpha : FA \rightarrow A$ *be an initial algebra. Given any F -system*
 $\mathcal{X} = (X, s, c)$, *there is a unique Kleisli arrow* $\text{tr}(c)$ *that*
makes the diagram on the right commute. In particular,
the Kleisli coalgebra $J(\alpha^{-1})$ *is a final coalgebra.*

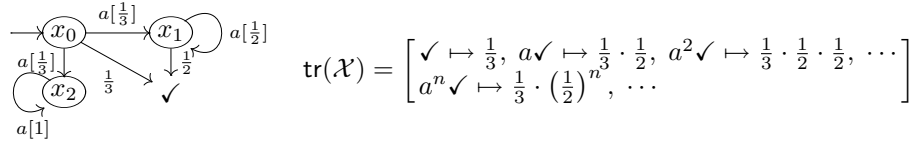
$$\begin{array}{ccc}
FX & \xrightarrow{F(\text{tr}(c))} & FA \\
\uparrow c \dashv \vdash & \text{tr}(c) & \uparrow J(\alpha^{-1}) \dashv \vdash \\
X & \xrightarrow{\text{tr}(c)} & A \\
\uparrow s & \text{tr}(c) \odot s & \uparrow \{*\}
\end{array} \quad (10)$$

We set $\text{tr}(\mathcal{X}) := \text{tr}(c) \odot s$. It is $\text{tr}(\mathcal{X}) : \{*\} \rightarrow \mathcal{D}A$ as a function, hence is a subdistribution over A . This $\text{tr}(\mathcal{X})$ is referred to as the (*finite*) *trace semantics* of \mathcal{X} . To summarize: the *action type* F determines the set A of *linear-time behavior*; \mathcal{X} 's trace semantics $\text{tr}(\mathcal{X})$ tells us which linear-time behavior is exhibited with how much likelihood.

Example 5.19 (Trace semantics for GPA) Let $F = \{\checkmark\} + \text{Ac} \times (_)$. The diagram (10) translates into the following conditions, where σ ranges over Ac^* .

$$\begin{aligned} \text{tr}(c)(x)(\checkmark) &= \Pr[x \rightarrow \checkmark] , \\ \text{tr}(c)(x)(a\sigma) &= \sum_{x' \in X} \Pr[x \xrightarrow{a} x'] \cdot \text{tr}(c)(x')(\sigma) ; \quad \text{and} \\ \text{tr}(\mathcal{X})(\sigma) &= \text{tr}(c)(x_0)(\sigma) \quad \text{when } s(*) = [x_0 \mapsto 1]. \end{aligned}$$

This is a reasonable definition of a “trace semantics” for GPA; resulting is a subdistribution $\text{tr}(\mathcal{X})$ over lists on Ac . For example, let \mathcal{X} be the GPA below on the left; then its trace semantics is as on the right.



Note that our trace semantics only captures *finite* behavior; infinite sequences like a^ω are not in its domain Ac^* . With infinite behavior included we no longer have a clean characterization like in Thm. 5.18.

Like the definition of Kleisli simulation, the generic trace semantics (Thm. 5.18) also applies to other kinds of branching such as non-determinism. See [8].

5.7 Soundness Theorems

We recall the soundness result [5] for Kleisli simulation, via which soundness of JL- and HJ-simulation immediately follows. Its short proof in [5] makes use of order-theoretic properties of the diagram (10).

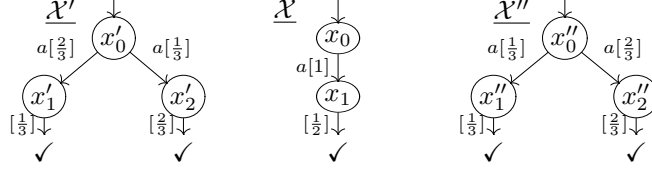
Theorem 5.20 (Soundness of Kleisli) *Let \mathcal{X}, \mathcal{Y} be F -systems. Existence of a Kleisli simulation from \mathcal{X} to \mathcal{Y} implies trace inclusion: $\text{tr}(\mathcal{X}) \sqsubseteq \text{tr}(\mathcal{Y})$. Here a Kleisli simulation can be any of forward, backward, or hybrid.* \square

Using Thm. 5.15 and Cor. 5.16, we immediately obtain soundness of JL-simulation (Def. 4.12). This is new to the best of the author’s knowledge. Therefore the notion of JL-simulation can also be used for proving trace inclusion between GPAs, a use that has not been investigated much in the literature. The same applies to JL- and JL’-simulation for DTMCs; we postpone detailed treatment to another venue.

6 Examples

For GPAs we have found several simulation notions: JL which is the same as HJ; forward; backward; backward-forward; and forward-backward. We have proved that the first is included in the last (Cor. 5.16); and that a non-hybrid Kleisli simulation induces a hybrid one (Prop. 5.13). In this section we present some examples that separate different simulation notions.

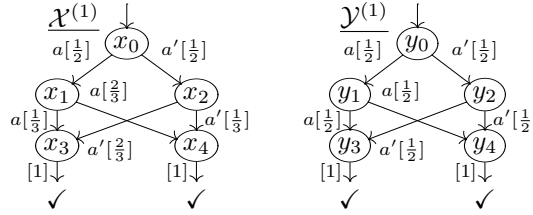
Example 6.1 Sometimes there is a forward (or a backward) simulation but not a JL-simulation. This does not contradict Prop. 5.13: to be a JL-simulation, a fwd.-bwd. simulation must be of a particular shape—the simulation arrows must be $J\pi_i$.



We have a forward simulation f from \mathcal{X}' to \mathcal{X} : $f(x'_0) = [x'_0 \mapsto 1]$ and $f(x'_1) = [x'_1 \mapsto \frac{2}{3}, x'_2 \mapsto \frac{1}{3}]$. But not a JL-simulation; assume R is such. The only candidate for a weight function $\Delta_{x'_0, x_0}$ is: $((a, x'_1), (a, x_1)) \mapsto \frac{2}{3}$ and $((a, x'_2), (a, x_1)) \mapsto \frac{1}{3}$; this forces $x'_1 R x_1$ and $x'_2 R x_1$. However there is no weight function that witnesses the latter, hence a contradiction.

We have a backward simulation b from \mathcal{X} to \mathcal{X}'' : $b(x_0) = [x''_0 \mapsto 1]$ and $b(x_1) = [x''_1 \mapsto \frac{1}{3}, x''_2 \mapsto \frac{2}{3}]$. Assume R is a JL-simulation. In the same way as above, $x_1 R x''_1$ is forced, which is a contradiction.

Example 6.2 First let us consider the following pair.



In fact x_0 and y_0 are bisimilar; they are obviously so and finding suitable weight functions is straightforward. Assume f is a forward simulation from \mathcal{X} to \mathcal{Y} . By (INIT) in Def. 5.10 we have $f(y_0) = [x_0 \mapsto 1]$. Applying (ACT) for y_0 , a and x_1 , we are forced to have $f(y_1) = [x_1 \mapsto 1]$; similarly $f(y_2) = [x_2 \mapsto 1]$. Again applying (ACT) for the transitions on the second level, we have inequalities

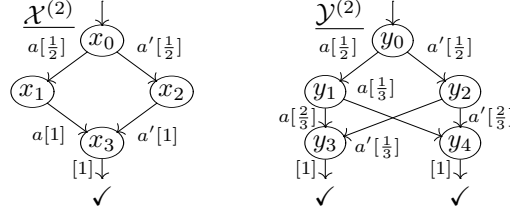
$$\begin{aligned} \frac{1}{3} &\leq \frac{1}{2}f(y_3)(x_3) + \frac{1}{2}f(y_4)(x_3) \quad , \quad \frac{2}{3} \leq \frac{1}{2}f(y_3)(x_4) + \frac{1}{2}f(y_4)(x_4) \quad ; \\ \frac{2}{3} &\leq \frac{1}{2}f(y_3)(x_3) + \frac{1}{2}f(y_4)(x_3) \quad , \quad \frac{1}{3} \leq \frac{1}{2}f(y_3)(x_4) + \frac{1}{2}f(y_4)(x_4) \quad . \end{aligned} \quad (11)$$

From the top-right one, we have

$$\frac{2}{3} \leq \frac{1}{2}f(y_3)(x_4) + \frac{1}{2}f(y_4)(x_4) \leq \frac{1}{2}(1 - f(y_3)(x_3)) + \frac{1}{2}(1 - f(y_4)(x_3)) \quad ;$$

the latter inequality is because $f(y_3)$ and $f(y_4)$ are subdistributions. From this we have $\frac{1}{2}f(y_3)(x_3) + \frac{1}{2}f(y_4)(x_3) \leq \frac{1}{3}$, which yields $\frac{1}{2}f(y_3)(x_3) + \frac{1}{2}f(y_4)(x_3) = \frac{1}{3}$ when combined with the top-left one in (11). In the same way we conclude $\frac{1}{2}f(y_3)(x_3) + \frac{1}{2}f(y_4)(x_3) = \frac{2}{3}$ from the bottom two in (11). There is no common solution of $f(y_3)(x_3)$ and $f(y_4)(x_3)$ for the last two equations; hence such f is impossible.

Let us now consider the following pair.



A JL-(bi)simulation is again obvious; assuming we have a backward simulation b , we derive a contradiction.

By (TERM), using some $p \in [0, 1]$ we can write $b(x_3) = [y_3 \mapsto p, y_4 \mapsto 1 - p]$. Applying (ACT) for the transitions on the second level, we have inequalities

$$\begin{aligned} p &\leq \frac{1}{3}b(x_1)(y_1) \quad , \quad 1 - p \leq \frac{2}{3}b(x_1)(y_1) \quad ; \\ p &\leq \frac{2}{3}b(x_2)(y_2) \quad , \quad 1 - p \leq \frac{1}{3}b(x_2)(y_2) \quad . \end{aligned} \quad (12)$$

From the top two we have $1 \leq b(x_1)(y_1)$, hence $b(x_1)(y_1) = 1$. Similarly from the bottom two we have $b(x_2)(y_2) = 1$. Using these in the original inequalities we have $p \leq \frac{1}{3}$, $1 - p \leq \frac{2}{3}$, $p \leq \frac{2}{3}$ and $1 - p \leq \frac{1}{3}$. The former two implies $p = \frac{1}{3}$, while the latter two says $p = \frac{2}{3}$. This is impossible.

A natural question is: does it happen that there is a JL-simulation, but neither forward nor backward simulation exists? At this point this is open.

7 Conclusions and Future Work

We have showed that JL-simulation is a special case of HJ-simulation, which is further a special case of Kleisli simulation. This allows to transfer general results for a latter notion to a former one, most notably soundness.

Finding a Kleisli simulation is reduced to solving a family of linear inequalities. Its algorithmic aspect is to be investigated. We also aim to exploit acquired genericity and apply our results to other kinds of systems. We are interested in *stochastic context-free grammars* which have their application in modeling the secondary structure of RNA [2].

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A Appendix

A.1 Formulation of Hughes-Jacobs simulation

The original formulation [10] of HJ-simulation (stated in fibrational terms) amounts to the following condition, which is shown to be equivalent to Def. 4.5.

Proposition A.1 *In Def. 4.5, the relation R is a HJ-simulation if and only if there exists a function $r' : R \rightarrow \text{Rel}_{\sqsubseteq}(B)(R)$ such that the following diagram commutes.*

$$\begin{array}{ccc} BX & \xleftarrow{\pi_1} \text{Rel}_{\sqsubseteq}(B)(R) & \xrightarrow{\pi_2} BY \\ c \uparrow & & \uparrow d \\ X & \xleftarrow{\pi_1} R & \xrightarrow{\pi_2} Y \end{array} \quad (13)$$

Here the relation $\text{Rel}_{\sqsubseteq}(B)(R) \subseteq BX \times BY$ is the lax relation lifting from [10].

The proof is similar to its bisimulation counterpart, which is standard in the theory of coalgebra (see e.g. [19, Lem. 3.6.4]).

Proof. First we recall the definition of (lax) relation lifting. Given a relation $R \subseteq X \times Y$, it is lifted to the *relation lifting* $\text{Rel}(B)(R) \subseteq BX \times BY$ via the following image-factorization (see e.g. [10]). We denote the surjective part by e .

$$\begin{array}{ccc} \text{Rel}(B)(R) & \xrightarrow{\quad} & BX \times BY \\ e \uparrow & \nearrow \langle B\pi_1, B\pi_2 \rangle & \\ BR & & \end{array} \quad (14)$$

Then the *lax relation lifting* $\text{Rel}_{\sqsubseteq}(B)(R)$ is defined to be $\sqsubseteq \circ \text{Rel}(B)(R) \circ \sqsubseteq$, that is, the relational composition of

$$\sqsubseteq_{BX} \subseteq BX \times BX, \quad \text{Rel}(B)(R) \subseteq BX \times BY, \quad \text{and} \quad \sqsubseteq_{BY} \subseteq BY \times BY. \quad (15)$$

For the ‘if’ part of the statement, take arbitrary $x \in X$ and $y \in Y$ such that xRy ; we shall define the value $r(x, y)$ for r in (5). The function r' in (13) is forced to be $r'(x, y) = (c(x), d(y))$ by commutativity. Since the value $r'(x, y)$ lies in the relation $\text{Rel}_{\sqsubseteq}(B)(R)$, there exist $\gamma \in BX$ and $\delta \in BY$ such that

$$c(x) \sqsubseteq \gamma, \quad (\gamma, \delta) \in \text{Rel}(B)(R), \quad \text{and} \quad \delta \sqsubseteq d(y) \quad (16)$$

by the definition of lax relation lifting. Then by (14) there exists $\beta \in BR$ such that $e(\beta) = (\gamma, \delta)$, using the axiom of choice. Now define r in (5) by $r(x, y) = \beta$. We have

$$(B\pi_1 \circ r)(x, y) = (\pi_1 \circ e)(\beta) = \pi_1(\gamma, \delta) = \gamma;$$

similarly $(B\pi_2 \circ r)(x, y) = \delta$. By (16) this function r makes the inequalities in (5) hold.

For the ‘only if’ part, define a function $r' : R \rightarrow \text{Rel}_{\sqsubseteq}(B)(R)$ by $r'(x, y) := (c(x), d(y))$. That makes the diagram commute; we have to show that $(c(x), d(y)) \in \text{Rel}_{\sqsubseteq}(B)(R)$. By the condition on r in Def. 4.5 we have $c(x) \sqsubseteq (B\pi_1)(r(x, y))$ and $(B\pi_2)(r(x, y)) \sqsubseteq d(y)$. Hence by the definition of a lax relation lifting, we are done if we show $((B\pi_1)(r(x, y)), (B\pi_2)(r(x, y))) \in \text{Rel}(B)(R)$, which is immediate from (14). \square