Probabilistic Bigraphs

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Abstract. Bigraphs are a universal computational modelling formalism for the spatial and temporal evolution of a system in which entities can be added and removed. We extend bigraphs to probabilistic bigraphs, and then again to action bigraphs, which include non-determinism and rewards. The extensions are implemented in the BigraphER toolkit and illustrated through examples of virus spread in computer networks and data harvesting in wireless sensor systems. BigraphER also supports the existing stochastic bigraphs extension of Krivine \textit{et al.}, and using BigraphER we give, for the first time, a direct implementation of the membrane budding model used to motivate stochastic bigraphs [KMT08].

Keywords: Bigraphs, Probabilistic bigraphical reactive systems, Discrete Time Markov Chains, Markov Decision Processes

1. Introduction

Bigraphical reactive systems (BRSs) [Mil09] are a universal computational modelling formalism for systems that evolve in time and space. They consist of bigraphs, a graph based formalism that models entity relationships, both spatially and through (global) links, and a rewriting framework that allows models to evolve over time via a set of reaction (rewrite) rules. Applying a reaction rule, $L \to R$, replaces an occurrence of bigraph $L$ (in a bigraph) with bigraph $R$. BRSs can represent a diverse range of phenomena including mixed-reality games [BCRS16], network management [CKSS14], wireless communication protocols [CS14], biological processes [KMT08], cyber-physical security [TPGN18], and indoor environments [WW12].

In practice, the systems we wish to model may be probabilistic, stochastic, or explicitly make non-deterministic choices. Standard BRSs have no notion of the first two concepts, and are implicitly non-deterministic in that if there is a match to $L$ then any rule can be applied.

Previously, Krivine \textit{et al.} [KMT08] extended bigraphs to stochastic bigraphs, by associating rates (rather than weights) with reaction rules. We build on that work, utilising similar ideas to create probabilistic bigraphs – a discrete variant. We then take the theory further to allow explicit non-determinism with action bigraphs that encode Markov decision processes [Bel57], by adding actions and rewards.

For each of the three types of system – probabilistic, stochastic, and action based – we provide an implementation of the theory in the BigraphER toolkit [SC16]. This allows, for the first time, an implementation and analysis of the Krivine \textit{et al.} stochastic bigraph example [KMT08] without requiring a separate PRISM [KNPV09] model.

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We make the following contributions:

- we extend standard BRSs with probabilistic reaction rules, to create probabilistic BRSs,
- we extend probabilistic BRSs with non-deterministic actions and reward structures, to create action BRSs,
- we provide an implementation in BigraphER [SC16] of probabilistic, stochastic, and action BRSs,
- we illustrate the new modelling capability through examples of virus spread through computer networks, the membrane budding example of [KMT08], and data harvesting in wireless sensor networks with mobile sinks.

Outline The paper is structured as follows. Bigraphs and BRSs are introduced in Sections 2.1 and 2.2 with emphasis on the important notion of matching/occurrence; probabilistic systems are introduced in Section 2.3. In Section 3 we introduce probabilistic BRSs by adding relative weights to reaction rules. Section 4 extends probabilistic bigraphs further by adding explicit actions that represent non-deterministic choice. We evaluate the approaches through a set of further examples, implemented in an extended BigraphER, in Section 5. We conclude in Section 6 with a discussion of the limitations of the approaches, how they relate to other probabilistic modelling frameworks, and future work.

2. Background

2.1. Bigraphs

We introduce bigraphs by example, formal definitions can be found elsewhere [Mil09]. Although we restrict ourselves to Milner’s original formulation of bigraphs (standard bigraphs), the probabilistic, stochastic, and non-deterministic variants are also applicable to, and implemented for, bigraphs with sharing [SC15] – an extension supporting overlapping spatial regions.

Bigraphs are a universal computational model for representing both the spatial configuration of entities, and their non-spatial interactions. A bigraph consists of two orthogonal structures: the *place graph*, that represents topological space in terms of containment, and the *link graph*, a hypergraph that expresses non-spatial relationships among entities. Each entity has a *type* that determines its (fixed) *arity*, i.e. number of links, and whether it is *atomic*, i.e. if it cannot contain other nodes.

Bigraphs have an equivalent diagrammatic and algebraic notation. Throughout this paper we use the intuitive diagrammatic notation where possible. An example bigraph is shown in Figure 1a. Entities are drawn as (coloured) shapes, with the label, e.g. A, B, ... determining the type. Where it is clear from the
context we will often omit the labels. Entities may be nested, e.g. A is inside B, and non-atomic entities can have any (finite) number of children. The green hyperlinks represent non-spatial links between entities, such as between the two A’s in different B’s. Entities have fixed arity, so the rightmost A in Figure 1a must have a single link, but in this case it is closed.

Bigraphs are compositional in nature, that is, we may combine smaller bigraphs to create larger models. To achieve this compositionality, alongside entities, bigraphs may contain regions, shown by clear dashed rectangles, which represent adjacent parts of a system: sites, shown by filled dashed rectangles, represent abstraction, i.e. an unspecified bigraph (possibly the empty bigraph) exists there; a set of inner names, e.g. \{z\}, allows names to be connected from below; and a set of outer names, e.g. \{x, y\}, allows these links to connect with a wider context. Capabilities to interact with an external environment are recorded formally in the interface of a bigraph. For example, in Figure 1a we write \( B : (1, \{z\}) \rightarrow (2, \{x, y\})\) to indicate that \( B \) has one site and inner name \( z \) (written \( (1, \{z\}) \)) and, two regions and outer names \( x, y \) (written \( (2, \{x, y\}) \)).

We use \( X, Y \) and \( K, I, J \) to denote sets of names and interfaces, respectively.

Composition of two bigraphs \( F : K \rightarrow I \) and \( G : I \rightarrow J \) is written

\[
G \circ F : K \rightarrow J
\]

and operates by placing the regions on \( F \) inside the sites of \( G \) and linking like outer names from \( F \) with inner names from \( G \). When the name sets are disjoint, bigraphs may also be combined horizontally by placing regions, which may contain any other bigraph, side-by-side. This is denoted by

\[
F_0 \otimes F_1 : \langle m_0 + m_1, X_0 \cup X_1 \rangle \rightarrow \langle n_0 + n_1, Y_0 \cup Y_1 \rangle
\]

with \( F_i : \langle m_i, X_i \rangle \rightarrow \langle n_i, Y_i \rangle \) and \( i = 0, 1 \).

We write \( \text{id}_X \) for the identity bigraph that maps like-names to like-names. We call bigraphs with no sites or inner names, e.g. those that cannot be composed with others, ground. In general, we define reactive systems over ground bigraphs, since these represent fully formed models. We use lowercase letters \( f, g, g_0, \ldots \) to denote ground bigraphs and uppercase for arbitrary bigraphs (including those that may be ground).

When constructing bigraph models we use abstract bigraphs, where entities are identified using their types, e.g. an entity \( A \). However, when rewriting models, to identity specific entities, we work instead with concrete bigraphs, \( F, G, \ldots, \tilde{g} \), where entities and closed links have distinct identifiers, e.g. \( v, u, e, \ldots \). For a bigraph \( G \), we assign an arbitrary concretion \( \tilde{G} \) by giving distinct labels to entities/closed links. We say two concrete bigraphs \( \tilde{F} \) and \( \tilde{G} \) are support equivalent, denoted \( \tilde{F} \simeq \tilde{G} \), if they are equal under a renaming of entities and links. A bigraph is trivially support equivalent to itself. An abstract bigraph \( B \) is a \( \simeq \)-equivalence class of concrete bigraphs, \( \tilde{B} = [\tilde{B}]_\simeq \) with \( \tilde{B} \) an arbitrary concretion of \( B \). An example of support equivalence is in Section 3.

### 2.2. Bigraphical Reactive Systems

A bigraph represents a system at a single point in time. To encode the dynamics of a system we create a Bigraphical Reactive System (BRS) using a set of reaction rules of the form \( L \Rightarrow R \), where \( L \) and \( R \) are bigraphs. Intuitively, a BRS operates by finding occurrences of \( L \) within a larger model and replacing these with \( R \).

To determine if a bigraph \( L \) is present in a bigraph \( B \) we need the following definition, which applies to both concrete and abstract bigraphs.

**Definition 1 (occurrence).** A bigraph \( L \) occurs in bigraph \( B \) if the equation \( B = C \circ (L \otimes \text{id}_X) \circ D \) holds for some set of names \( X \) and bigraphs \( C \) and \( D \). Two occurrences are equal if they differ only by a permutation or a bijective renaming on the composition interfaces; otherwise they are distinct.

The use of the identity bigraph \( \text{id}_X \) allows links to pass between \( C \) and \( D \). An important property is that it is possible to determine an abstract occurrence starting from a concrete one. In other words, a bigraph \( L \) occurs in \( B \) only if an arbitrary concretion \( \tilde{L} \) occurs in an arbitrary concretion \( \tilde{B} \). In a given bigraph, there

\[1^\text{In [M109], lean-support equivalence (\( \bowtie \)) is used instead. It corresponds to support equivalence (\( \simeq \)) after discarding idle links, i.e. links connecting zero entities or names.\]
may be multiple occurrences of another bigraph. For example, in Figure 1c bigraph $G$ occurs three times within bigraph $B$.

In general, the decomposition corresponding to the occurrence of a given bigraph might not be unique. To ensure distinct decompositions, following Krivine et al. [KMT08], we introduce the following class of bigraphs.

**Definition 2 (solid).** A bigraph is solid if:
- All regions contain at least one node, and all outer names are connected to at least one link.
- No two sites or inner names are siblings.
- No site has a region as a parent.
- No outer name is linked to an inner name.

This definition is important when determining a suitable probability to apply a rule.

**Definition 3 (reaction rule).** A reaction rule $R$ is a pair of bigraphs $R = (L, R)$, written $L \xrightarrow{R} R$, where $R$ and $L$ have the same interface and $L$ is solid.

We also say $R : L \xrightarrow{R} R$ is applicable to $g$ iff $L$ occurs in $g$. In general, we are interested in applying a reaction rule within a larger bigraph and as such provide the following reaction relation.

**Definition 4 (reaction relation).** Given a reaction rule $R : L \xrightarrow{R} R$, the reaction relation $\xrightarrow{R}$ over ground bigraphs is defined by

$$g \xrightarrow{R} g' \text{ iff } g = C \circ (L \otimes \text{id}_X) \circ d \text{ and } g' = C \circ (R \otimes \text{id}_X) \circ d$$

for some bigraph $C$, ground bigraph $d$, and set of names $X$.

**Definition 5 (bigraphical reactive system (BRS)).** A bigraphical reactive system is a pair $(B, R)$, where $B$ is a set of ground bigraphs and $R$ is a set of reaction rules defined over $B$. It has reaction relation $\xrightarrow{R} = \bigcup_{R \in R} \xrightarrow{R}$ which will be written $\xrightarrow{R}$ when $R$ is understood.

We indicate the set of reaction rules applicable to $g$ and yielding $g'$ with $R_g \xrightarrow{R} g'$. We also introduce the following notation to count the concrete occurrences of a reaction rule $R$ from $g$ to $g'$

$$\sigma_R[g, g'] = |\{\tilde{g}'' \mid \tilde{g} \xrightarrow{R} \tilde{g}'' \text{ and } \tilde{g}'' \equiv \tilde{g}' \}|$$

that is, we count how many concrete $\tilde{g}''$ that are support equivalent to a concretion of $g'$ can be obtained by applying $R$ to a concretion of $g$.

**Definition 6 (transition system).** A BRS with distinguished initial bigraph $g_0 \in B$ forms a transition system with bigraphs as states and state transitions defined by generating all possible rewrites (reactions) in $\xrightarrow{R}$ from $g_0$ until we hit a fixed point (the set of all states $B$).

This transition system view is useful for defining probabilistic, stochastic, and non-deterministic BRSs, where the transitions are assigned, for example, specific probabilities.

Finally, we allow states to be labelled by bigraph predicates which are also specified as bigraphs. A state $g$ satisfies a predicate bigraph $P$ if $P$ occurs in $g$. These can be used to, for example, identify invalid states for use in logical statements when performing verification.

### 2.3. Probabilistic Models

In the following we assume basic familiarity with probability theory, see for example [Bil12].

Probabilistic systems can be described using Markov models/processes, where the probability/rate of moving to a new state is based (strictly) on the current state [KNP10]. A discrete time Markov chain (DTMC) labels each state transition with a probability $0 \leq p \leq 1$ such that the sum of all outgoing edges
from a state is equal to 1. That is, a DTMC draws the next state from a probability distribution of all possible states.

**Definition 7 (Probability Distribution).** A probability distribution over a countable set \( S \) is a function \( \mu : S \to [0, 1] \) satisfying \( \sum_{s \in S} \mu(s) = 1 \)

We use the notation \( \mu = [s_0 \mapsto p_0, s_1 \mapsto p_1, \ldots] \) to denote the distribution that chooses \( s_0 \) with probability \( p_0 \), and so on. We assume all other states are chosen with probability 0. To denote a set of probability distributions over \( S \) we use \( \mathcal{D}_S \), dropping the subscript \( S \) if it is clear from the context. For verification purposes, we usually work with finite probability distributions with \( S \) finite.

**Definition 8 (Discrete Time Markov Chain (DTMC)).** A DTMC is a tuple \( (S, s_0, P) \) where \( S \) is a set of states, \( s_0 \in S \) a distinguished initial state, and \( P : S \to \mathcal{D}_S \) is a function assigning to each state \( s \in S \) a probability distribution \( \mu_s \) such that \( \mu_s(s') : [0, 1] \) is the transition probability from \( s \) to \( s' \).

As distributions cannot be empty, each state \( s \in S \) has at least one transition. For terminal states \( s_t \), we have \( \mu_{s_t} = [s_t \mapsto 1] \) – the delta distribution.

To model continuous processes, we use continuous time Markov Chains (CTMCs) that assign stochastic rates, rather than probabilities, to state transitions.

**Definition 9 (Continuous Time Markov Chain (CTMC)).** A CTMC is a tuple \( (S, s_0, R) \) where \( S \) is a set of states, \( s_0 \in S \) a distinguished initial state, and \( R : S \times S \to \mathbb{R}_{\geq 0} \) the transition rate matrix matrix assigning a rate to each pair of states.

A transition between \( s \) and \( s' \) can only occur if \( R(s, s') > 0 \), and if so the probability of the transition occurring within time \( t \) is modelled as an exponential distribution, i.e. \( 1 - e^{-R(s,s')t} \). Unlike DTMCs, a CTMC allows terminal states where there is a 0 rate of transitioning.

Markov decision processes [Bel57, How60] model decision making in situations with both probabilistic outcomes and non-deterministic decision making. Intuitively, an MDP extends a DTMC by allowing a choice of possible actions at each state. Unlike a DTMC that provides a single probability distribution per state, the choice of action allows the multiple probability distributions per state.

**Definition 10 (Markov decision process (MDP)).** A MDP is a tuple \( (S, s_0, A, \text{Step}) \) where \( S \) is a set of states, \( s_0 \in S \) a distinguished initial state, \( A \) a set of actions, and \( \text{Step} : S \to 2^{A \times \mathcal{D}_S} \) a function assigning to each state a set of possible actions with associated probability distributions.

Unlike a DTMC, we allow states with no outgoing transitions, i.e. \( S \to \emptyset \). When the choice of action for each step is fixed an MDP is a DTMC.

To allow practical analysis of probabilistic models it is useful to define rewards associated with being in a particular state.

**Definition 11 (state reward function).** For a DTMC, CTMC, or MDP, a state reward function \( r_s : S \to \mathbb{R}_{\geq 0} \) assigns to each state a reward. For states where rewards are not required \( r_s \) maps the state to 0.

When working with bigraphs we associate rewards with bigraph predicates, allowing state rewards to be defined as simply the sum of the rewards of all matching predicates (0 if no predicates occur).

For MDPs we can also associate a reward for choosing a particular action.

**Definition 12 (action reward function).** An action reward structure for an MDP \( (S, s_0, A, \text{Step}) \) is a function \( r_a : S \times A \to \mathbb{R}_{\geq 0} \) that assigns to each state, action pair a reward for performing that particular action. For actions where rewards are not required \( r_a \) maps the action to 0.

Although we call these rewards, they are often used to model costs associated with states/actions.

### 3. Probabilistic Bigraphs

Given a state (bigraph), we want to control the probability of moving into a given next state (i.e. a bigraph). In other words, we require a DTMC where the states resulting from reactions are drawn from a probability distribution.
Our approach is similar to that of Bournez and Hoyrup [BH03] who consider abstract probabilistic rewrite systems. Here a weight is assigned to each rewrite rule which is then normalised based on which rules are applicable to a given state. Other approaches to modelling probabilistic systems are possible, for example, probabilistically determining which entities appear in the right-hand-side of a rule. We discuss these further in Section 6. Our approach allows re-use of existing probabilistic model checking tools such as PRISM [KNP11] or Storm [DJKV17a] for analysis/verification.

3.1. Probabilistic Bigraphical Reactive Systems

A probabilistic BRS adds weights to standard reaction rules to determine transitions probabilities when defining the reaction relation. This is, given a bigraph $g_0$ with $g_0 \rightarrow g_1$ and $g_0 \rightarrow g_2$ (for arbitrary rules) we wish to choose $g_1$ and $g_2$ from a probability distribution $\mu = [g_1 \mapsto p_1, g_2 \mapsto p_2]$, i.e. choose $g_1$ with probability $p_1$.

To account for multiple occurrences of a rule, we do not directly specify probabilities for rules but instead assign a weight which is then normalised to a probability.

Definition 13 (weighted reaction rule). A weighted reaction rule assigns to a reaction rule $L \rightarrow R$ a weight $w$, $w \in \mathbb{R}_{\geq 0}$. We write weighted reaction rules as $L^w \rightarrow R$.

The weight determines how likely a particular rule is to be applied relative to all other (applicable) rules. Rules with weight $w = 0$ are never applied. In the following, we write $\rightarrow R$ to indicate that a set of weighted reaction rules $R$ is treated as a set of standard reaction rules (see Definition 5) by dropping all the weights.

Definition 14 (total weight). Given a set of weighted reaction rules $R$, the total weight from $g$ to $g'$ is

$$\omega[g, g'] = \sum_{R \in R} w_R \cdot \sigma_R[g, g']$$

where $w_R$ is the weight of reaction rule $R$. Given a set of ground bigraphs $B$, the total weight from $g$ is

$$\omega[g, \_] = \sum_{g' \in B} \omega[g, g']$$

Definition 15 (reaction probability distribution). Given a set of ground bigraphs $B$, a set of weighted reaction rules $R$ and $g \in B$, the reaction probability distribution from $g$ is

$$\mu_g = [g_0 \mapsto p_0, g_1 \mapsto p_1, \ldots]$$

with

$$p_i = \frac{\omega[g, g_i]}{\omega[g, \_]}$$

for every $g_i \in B$ such that $g \rightarrow R g_i$. If there are no such $g_i$s, then $\mu_g = [g \mapsto 1]$.

Reaction probability distributions are then used to define a probabilistic reaction relation over ground bigraphs.

Definition 16 (probabilistic bigraphical reactive system (PBRS)). A probabilistic BRS is a pair $(B, R)$, where $B$ is a set of ground bigraphs, and $R$ is a set of weighted reaction rules. It has probabilistic reaction relation defined by

$$g \xrightarrow{p} g'$$

iff $\mu_g(g') = p$ with $g, g' \in B$.

The correspondence between PBRS and DTMC is as follows:

Lemma 1. A PBRS $(B, R)$ is a DTMC $(S, s_0, P : S \rightarrow D_S)$.

Proof. Take $S = B$, $s_0 = g_0 \in B$, and $P(s) = \mu_g$ [Definition 15] for $s \in S$, $g \in B$, and $s = g$. □

From a practical standpoint, the use of weighted reaction rules allows modelling only the relative probability a particular rule is executed. Unfortunately, this makes it difficult to specify an exact probability between states. Doing so is often impractical, requiring significant effort to control the applicable rules and...
3.2. Example PBRS

Consider a Wireless Sensor Network (WSN) with three sensor nodes (S) and a base-station (BS), as shown in Figure 2. The base station is represented by the rectangle and the three sensors are represented by circles. There is a link between the base station and the sensors. Due to hostile deployment environments, sensors often fail. We model failure using the reaction rule $\text{fail}$ that marks a sensor as failed (red circle) and unlinks it from the base-station. The rule $\text{recover}$ allows a failed sensor (red circle) to re-connect with the base-station. $\text{fail}$ (b) has weight $w_f$ and $\text{recover}$ (c) has weight $w_r$. Note that while $\text{fail}$ and $\text{recover}$ are behaviourally inverse rules, their weights differ.

The resulting transition system for this WSN is in Figure 3. From the initial state $g_0$, we determine the distribution of next states $\mu_{g_0}$. In this case, reaction rule $\text{recover}$ is not applicable and we can only apply $\text{fail}$. It may be surprising that even though there are three sensors, the probability of transitioning to $g_1$ is $\mu_{g_0}(g_1) = 1$. This is because support equivalent (concrete) bigraphs are combined when computing the states resulting from the application of a reaction rule. To see this more clearly, we show explicitly the three concrete occurrences of $\text{fail}$ from $g_0$ to $g_1$ in Figure 4. The key observation is that through renamings $v_2 \rightarrow v_1$ and $v_3 \rightarrow v_1$, these concrete bigraphs are support equivalent and therefore they correspond to the single abstract state $g_1$. Hence, we have $\sigma_{\text{fail}}[g_0, g_1] = 3$, $\omega[g_0, g_1] = 3w_f$, and $\omega[g_0, g_1] = 3w_f$, giving the overall reaction probability of 1.

In state $g_1$, with one failed sensor, we have $\sigma_{\text{fail}}[g_1, g_2] = 2$ and $\sigma_{\text{con}}[g_1, g_0] = 1$. Normalising this over the total weight $\omega[g_1, g_2] = 2w_f + w_r$, we obtain a $\frac{2w_f}{2w_f + w_r}$ probability that another sensor fails, and a probability $\frac{w_r}{2w_f + w_r}$ that the failed sensor recovers.

Importantly, due to support equivalence, transition probability corresponds to the probability that any sensor fails rather than the probability that a particular sensor fails (i.e. $\frac{w_r}{2w_f + w_r}$).

This process of normalising weights to probabilities continues until we obtain the full DTMC as shown.
4. Action Bigraphs

PBRSs allow a single distribution of possible next states defined over all rules \( \mathcal{R} \). However, for systems such as controllers, we want actions taken by the controller to affect the possible evolution of the system, e.g. by restricting the reaction rules. That is, we want multiple distributions that are determined by the action taken. To this end, we introduce action bigraphical reactive systems (ABRS), where the resulting transition system is a Markov decision processes (MDP – Definition 10).

ABRSs extend PBRSs by allowing a choice of probability distributions at each step. We call such choices actions.

**Definition 17 (Action).** An action is a non-empty set of weighted reaction rules (Definition 13) that determines the rewrites that can be performed if the action is chosen. We say an action is applicable to a bigraph \( g \) if at least one rule from the action is applicable to \( g \).

As actions are simply sets of rules, the same reaction rule may appear in multiple actions if required, e.g. if two different control actions allow updating of the same state. We use the notation \( |_A \) to restrict definitions to consider only rules in \( A \). For example \( \omega[g, g_i] |_A \) is the total weight between states \( g \) and \( g_i \) when considering only rules in \( A \) rather than in \( \mathcal{R} \).

To move from weighted to probabilistic rules, we apply, individually for each action, the normalisation procedure from PBRSs, i.e.

\[
p_i = \frac{\omega[g, g_i] |_A}{\omega[g, \cdot] |_A}
\]

After normalising, we obtain a set of probability distributions; one for each applicable action, allowing us to construct the MDP transition function \( \text{Step} : S \to 2^A \times 2^S \).

We then define an Action BRS as follows.

**Definition 18 (Action BRS (ABRS)).** An Action BRS is a triple \( (\mathcal{B}, \mathcal{R}, \mathcal{A}) \), where \( \mathcal{B} \) is a set of (ground) bigraphs, \( \mathcal{R} \) is a set of weighted reaction rules over \( \mathcal{B} \), and \( \mathcal{A} = \{A_0 \subseteq \mathcal{R}, \ldots, A_n \subseteq \mathcal{R} \} \) is a set of actions. It has a reaction relation defined by

\[
g \xrightarrow{(A_i, p)} g' \iff \mu_g(g') |_{A_i} = p
\]

for each applicable action \( A_i \in \mathcal{A} \) with \( g, g' \in \mathcal{B} \).

Just as a PBRS is a DTMC, an ABRS is an MDP:
Lemma 2. An ABRS \((B, R, A)\) is an MDP \((S, s_0, A, \text{Step}: S \rightarrow 2^{A \times D})\).

Proof. Take \(S = B\), \(s_0 = g_0 \in B\), \(A = A\), and for \(s = g\) with \(s \in S\) and \(g \in B\) define

\[
\text{Step}(s) = \begin{cases} 
\{(A_1, \mu_{g} | A_1), \ldots, (A_n, \mu_{g} | A_n)\} & \text{for all } A_i \in A \text{ applicable to } g \\
\emptyset & \text{if no action applies to } g
\end{cases}
\]

As with MDPs, we can assign rewards (Definition 12) for choosing a particular action to allow optimisation of decision processes.

Like MDPs, ABRS allow terminal states (the empty set of distributions) if there is no applicable action, however, for practical analysis, e.g. in PRISM, we usually require at least one action per state. In a similar manner to PBRS, in the case no action applies, we can add a trivial action containing the identity reaction for the current state.

4.1. Example ABRS

As an example, consider the model in Figure 5 representing another simple WSN. In this case, data can be sent between the sensor (S) and base-station (BS), and there is a non-deterministic choice whether the sensor should send data or wait.

There are three actions: \(A_{\text{send}} = \{\text{send suc}, \text{send fail}\}\), \(A_{\text{wait}} = \{\text{wait}\}\), and \(A_{\text{reset}} = \{\text{reset}\}\). The resulting Markov decision process is shown in Figure 6. From the initial state \(g_0\) the system has a choice of two actions: \(A_{\text{send}}\) or \(A_{\text{wait}}\). If the system chooses to send then the distribution of states is \(\mu_{g_0} | A_{\text{send}} = [g_1 \mapsto \frac{w_s + w_r}{w_s + w_r + w_f}, g_2 \mapsto \frac{w_f}{w_s + w_r + w_f}]\), while on a wait it is \(\mu_{g_0} | A_{\text{wait}} = [1 \mapsto g_2]\). In the case the send fails an additional action, \(A_{\text{reset}}\) reinitialises the state to allow another attempt.

5. Extended BigraphER and further examples

We have extended BigraphER\(^2\) \cite{SC16}, an open source toolkit for bigraphs, to support standard, probabilistic, stochastic, and action bigraphical reactive systems. BigraphER provides both a language for describing bigraphs and reaction rules algebraically, and support for simulating BRSs and generating transition systems. In the following we introduce the syntax of BigraphER by example, highlighting the new language constructs. A full reference is available \cite{SC16}.

BigraphER uses modern (probabilistic) model checkers by exporting transition systems to PRISM input format\(^3\). This enables quantitative model checking for probabilistic (DTMC), stochastic (CTMC) and action

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\(^2\) Available online: \url{https://uog-bigraph.bitbucket.io/}

\(^3\) These raw transition systems are often easily read by other model checkers.
(MDP) BRSs. We present examples of each type and show selected BigraphER implementation details and results.

Section 5.1 gives a probabilistic BRS model of virus spread through a computer network where firewalls are breached probabilistically.

When Stochastic Bigraphs were defined by Krivine et al. [KMT08] there was no tool support to analyse their membrane budding model, instead requiring a manual translation to a PRISM model. In Section 5.2 we revisit this model and for the first time, give a direct implementation in bigraphs.

Finally, in Section 5.3 we use an action BRS to model decisions in wireless sensor networks with mobile sinks: sensors decide whether to send immediately, or wait in the hope the sink moves closer.

Model files are available [ASC].

5.1. Probabilistic Bigraphs – Virus Spread in a Network

Viruses spread through computer networks in a probabilistic manner. The probability of infection may differ between nodes, depending on the effectiveness of firewalls. Although we focus on computer networks, similar models could be adapted to, for example, infection spread in populations. This example is based on an existing PRISM model [KNPV09].

In an arbitrary computer network, with the infection starting at a specified node, we wish to determine the likelihood of a virus infecting a particular node. We use the following infection process. Infected nodes attack, spreading the virus to uninfected neighbours. All (uninfected) neighbours are equally likely to be targets, i.e. the rule has fixed weight $w_{\text{attack}}$. A node that has been attacked is either protected by a firewall with weight $w_{\text{detect}}$, or become infected with weight $w_{\text{infect}}$. As we do not directly specify the probabilities, the important measure is the ratio of $w_{\text{detect}}$ to $w_{\text{infect}}$. This differs from the example PRISM model that adopts the more common approach of setting $p_{\text{detect}} = 1 - p_{\text{infect}}$.

The bigraph model is in Figure 7. An infected node attacks a neighbouring (through the green link) safe node (S, clear circle) with weight $w_{\text{attack}}$. An attacked node (A, indigo circle) enters the attacked state and from there has a $w_{\text{infect}}$ weight of becoming infected (I, red circle), or $w_{\text{detect}}$ of the firewall breaking the infection attempt.

Unlike Safe-Infected-Recovered (SIR) models [Het00], infected nodes remain infected for the entire run,
5.1.1. Syntax

Probabilistic rules are defined in BigraphER by using keyword `react` and by specifying a weight (any positive `float` expression) in the separator between the left-hand side and right-hand side of a rule. For example, rule `infect` is defined by the code snippet in line 8 of Listing 1 with weight $w_{\text{infect}}$. Entities are defined in lines 2-3 by using keyword `ctrl`. A PBRS is defined by construct `begin pbrs ... end` which also specifies the initial state, the state predicates, and the set of reaction rules (omitted).

Listing 1: Specifying probabilistic rules in BigraphER (snippet).

5.1.2. Evaluation

Consistent with the original PRISM model, we use a topology of nine nodes connected in a square grid layout as in Figure 8b. Using BigraphER we export the full (probabilistic) transition system for further analysis in PRISM. Figure 8a shows the probability that all nine nodes of the system are infected within the first $n$ timesteps (reactions), i.e. the Probabilistic Computation Tree Logic (PCTL) \cite{HJ94} formula $P_{=\exists} [ F^{\leq n} \text{all\_infected} ]$ where `all\_infected` is a predicate matching nine infected nodes as defined on line 12 of Listing 1. In the BigraphER languages, predicates are defined as bigraphs with keyword `big`. Iterated operator `par` allows to concisely place $n$ bigraphs side-by-side inside the same region.

We vary the detection weight $w_{\text{detect}}$ of the firewalls (5, 10, and 15) and, as expected, increasing $w_{\text{detect}}$, i.e. adding better firewalls, reduces the probability all nodes become infected within a given time period.

---

This corresponds to the iterated merge product operator in the algebraic form of bigraphs.
Table 1. Probability of full infection in $n$ steps when using 3 improved firewalls. In all cases $w_{detectBasic} = 5$.

| Max Steps | $w_{detectBasic}$ | $w_{detectAdv}$ |
|-----------|-------------------|-----------------|
| 5         | $1.09 \cdot 10^{-2}$ | $1.90 \cdot 10^{-1}$ |
| 10        | $1.19 \cdot 10^{-2}$ | $1.47 \cdot 10^{-1}$ |
| 15        | $1.29 \cdot 10^{-2}$ | $1.79 \cdot 10^{-1}$ |
| 250       | $1.00 \cdot 10^0$ | $9.99 \cdot 10^{-1}$ |
| 500       | $1.00 \cdot 10^0$ | $9.99 \cdot 10^{-1}$ |

5.1.3. Model Extensibility – Behaviour

As shown, better firewalls reduce the time to whole system infection, however this can be prohibitively expensive in a deployed system. Alternatively, we may wish to improve the firewalls on specific nodes. To test this, we add new entities BasicFW (light green squares) and AdvFW (yellow squares) representing a basic and more advanced (and expensive) firewall. We then split the detect rule into two rules, as shown in Figure 9 to account for the type of firewall. Because the sites abstract away internal node structure, the other rules remain the same. The only other change is to place the firewalls in the starting topology – in this case we place advanced firewalls in the nodes of the middle row.

The results of re-running the analysis are in Table 1. As expected, when $w_{detectBasic} = w_{detectAdv}$ the results match the previous experiment. Results like these can be used in a cost-benefit analysis, e.g. when determining how many advanced firewalls to deploy.

5.2. Stochastic Bigraphs – Membrane Budding

Stochastic Bigraphs were first introduced by Krivine, Milner, and Troina [KMT08], and allow BRS to form a CTMC (Definition 9) as an underlying transition system. Instead of assigning weights to reaction rule (as in PBRS), they assign a rate to each reaction rule. Because these rates are defined over rules, not states, similar to PBRS, a normalisation procedure is required to calculate a final exit rate based on the number of occurrences of each (applicable) rule.

The stochastic bigraphs paper presents a stochastic model of membrane budding, which describes a biological mechanism for particles to move between cells. In essence, coat proteins form on the surface of a membrane and, given enough coat proteins, a bud can form, accept some particles, and finally break off to carry particles out of a cell. Stochasticity comes from rates of coating, particle movement (into/out of the bud), and fission (breaking away).

No implementation of stochastic bigraphs was available when the example was developed, and analysis was given using a hand-coded PRISM model. As BigraphER now supports stochastic bigraphs, we revisit this example to recreate their analysis directly in bigraphs. We show a snippet of the model here, and refer the reader to the original source for full details of the model [KMT08].

We focus on the rule coat (rule 2 [KMT08]) that allows free Coat proteins to form on a Bud. The rule is shown in Figure 10. Free Coat proteins are distinguished from those already forming on a bud by the use of a closed link. The site abstracts over the particles within the Bud.

The rate $rc$ determines how quickly Coats form on the bud. Although it looks constant, because of the normalisation procedure, it in fact depends on the number of free coats, i.e. the number of occurrences increases and, in turn, so does the rate the rule applies. This is similar to the example in Section 3.2 where the probability any sensor failed was much higher than the probability a specific single sensor failed.

Stochastic rules are specified in a similar way to probabilistic rules in BigraphER by placing a float expression between the left and right-hand side of a rule. For example, the rule coat is as follows.
Listing 2: Specifying stochastic rules in BigraphER (snippet).

```plaintext
1 ctrl Bud = 1; # Arity 1
2 ctrl Coat = 1;
3 ctrl Gate = 1;
4 ctrl Particle = 0; # No links
5 # Coating rate
6 float rc = 1.0;
7
8 react coat =
9   Bud{x}.(id | Gate{z}) | /y Coat{y} -[rc]->
10   Bud{x}.(id | Gate{z}) | Coat{x};
11
12 # Predicate used for plotting.
13 # Determines the number of particles that have been transferred from a membrane when the bud breaks free
14 # par(n, b) = b | ... | b (n times)
15 fun big particles(n) = Bud{x}.(par(n, Particle));
16
17 begin sbrs
18   ...
19 end
```

Similarly, the initial state and the reaction rules of an SBRS are defined by construct `begin sbrs ... end`. For large models e.g. those with 50 free Coat entities, it is time consuming to count occurrences. To overcome this, we use a population model (a counter abstraction) that groups free coats etc. into a single entity Coats representing the number bound, and Fcoats representing the number that are still free. This allows coat to be alternatively written as shown in Figure 11. Entities such as Coats(c) are parameterised entities that can be seen as defining a family of Coats entities, one for each possible value of c. To calculate the number of free coats (Fcoats), we use the constant $c_{\text{max}}$ – the total number of coat proteins (free or bound); in our case 50. Coats are defined in the BigraphER language by the `fun ctrl` keywords. Similarly we augment the other rules to, for example, count the number of Protein(s) in the Bud. In this case we cannot rely on the occurrence count to determine the correct rate, so instead we explicitly scale the rate based on the number of remaining free coats.

For analysis, we have defined a family of bigraph predicates `particles(n)`, with $0 \leq n \leq 40$, that match a Bud with exactly n particles inside, allowing the probability that we end with n particles in a bud (that has broken off) to be determined through the PCTL formula: $P=?[\mathbf{F} \text{particles(n)}]$. This is defined in line 17 of Listing 2 by using the `fun` keyword.

We exported the BigraphER model to PRISM, where we successfully reproduced the “Particles in the formed bud” results from the appendix of stochastic bigraphs [KMT08], as shown in Figure 12. This figure shows the number of particles that are in the bud after fission, where $rd$ is the rate of diffusion of particles...
between the membrane and the bud (rule 3 [KMT08]). As expected, increasing the diffusion rate increases the expected number of particles in the formed bud. The rate of fission depends on the number of coat proteins (more coat proteins implying higher fission rates), and hence for \( rc = 2 \) the overall effect is to have less expected particles in the bud.

### 5.3. Action Bigraphs – Mobile Sinks in Wireless Sensor Networks

We use action bigraphs to model a well known decision problem in wireless sensor networks [BT08]. Traditionally, WSNs use multi-hop communication to move data between sensors and fixed sink (base-station). An alternative approach is for a moving sink to collect data directly from the sensors. Such an approach can be used, for example, when robots obtain information as they move through a space.

Given limited battery and memory capabilities of a sensor, when the sink moves into range a decision must be made: should the sensor send immediately, with high transmit power, or should it wait in the hope the sink moves closer, risking losing data by exhausting memory if the sink moves out of range before transmission can occur? Such decisions can be modelled as actions.

Model entities are shown in Figure 13a. There are three types: a (unique) Sink; a sensor Node that includes a Buffer with the number of slots filled; and Distance boundaries abstractly representing how close a sensor is to the sink, e.g. close, mid-range, or far. Nodes outwith the last Distance entity are considered out-of-range and cannot send.

The model updates in two phases: movement, where Nodes (possibly) move between Distance entities, and act, where Nodes non-deterministically decide whether to send or wait and receive data. Phases are scheduled in a round-robin fashion with each Node taking an action before moving onto the next phase.

Sink movement is modelled by moving Nodes between Distance boundaries, as shown in the reaction rule
Fig. 14. Send now or later: Actions, associated reaction rules, and costs

of Figure 14a. This models movement relative to the Sink, i.e. a Node moving to a closer Distance boundary implies a physical Sink move towards the Node. An additional rule (unshown) moves Nodes in/out of the outermost Distance boundary.

Non-determinism in the operation phase comes from the decision to send existing data, through one of the \texttt{A.send.close}, \texttt{A.send.mid}, \texttt{A.send.far} actions, or to receive new data through one of the \texttt{A.receive}, \texttt{A.receive.full} actions. Using multiple actions to model send/receive allows multiple action reward structures to be used. \texttt{A.receive} is shown in Figure 14b and consists of two reaction rules representing receipt or failure of new data with weight \( w_{\text{receive}} \). When the buffer is full (\( b = b_{\text{max}} \)), \texttt{A.receive} is no longer applicable, and instead \texttt{A.receive.full} (Figure 14c) represents a dropped sample and unit cost is incurred.

Actions/Rules for sending data in Figures 14d, 14e and 14f. In each case the buffer is fully emptied and a cost is incurred proportional to the distance from the sensor. We assume the cost is constant regardless of how much data is sent i.e. data always fits in a single radio packet. A more complex model could account for this through additional actions. Sending data is always successful but out-of-range sensors are unable to send any data, i.e. we do not fall back to hop-to-hop communication, and must always do a receive.

5.3.1. Syntax

To specify ABRSs we extend the BigraphER language to include an explicit \texttt{actions} declaration within \texttt{begin abrs ... end} blocks, as shown in Listing 3 (line 20). Each action consists of an identifier, \textit{e.g.}
Listing 3: Specifying actions BigraphER (snippet).

```plaintext
ctrl Sensor = 0;
fun ctrl Buffer(x) = 0;
fun ctrl Iden(i) = 0;

float w_suc = 5.0;
float w_fail = 1.0;

fun react receive(x,i) =
  Sensor.(Buffer(x) | Iden(i))
  -[w_suc]->
  Sensor.(Buffer(x + 1) | Iden(i))

fun react receive_fail(x,i) =
  Sensor.(Buffer(x) | Iden(i))
  -[w_fail]->
  Sensor.(Buffer(x) | Iden(i))

begin abrs
...
actions = [
  # Action[cost] = { rules }
  receive = { receive(x,i), receive_fail(x,i) },
  receive_full[1] = { receive(bmax,i) },
];
end
```

The model is analysed using PRISM [KNP11] by exporting the MDP transition system from BigraphER. PRISM does not support importing action rewards from a transition system, so we encode action rewards through state rewards which are fully supported. To do this we add additional entities (unshown) to the model when actions are taken, e.g. a SendClose entity if a sensor sends when the sink is close. These entities can be matched using state predicates to increase the cost. Importantly, this is an implementation detail to overcome tool support, and does not invalidate the theory.

We assume a single sink, two sensors, and 4 distance boundaries: close-range, mid-range, far-range, and out-of-range. Both sensors start in far-range of the sink.

First, consider the effect of increasing the maximum buffer size on the total cost, with the expected result being that an increased buffer size should reduce the overall cost, since sensors can wait longer before deciding to send data. Figure 15a shows how increasing the maximum buffer size effects the minimum possible cost in the first 4000 transitions, using the PCTL formula $R_{\min} = \mathbb{E}_{C \leq 4000}$. As expected, the minimum cost reduces as the buffer size increases as sensors can now delay sending for longer without incurring a penalty. The relationship is non-linear and we can see that increasing the buffer from 2 to 3 reading is much more beneficial than from 3 to 4.

Second, consider cost reduction by altering the probability that a sensor receives data when not sending – essentially reducing the sampling rate. Figure 15b shows how changing $w_{\text{receive}}$ affects the minimum possible cost for a fixed buffer size. As expected, increasing the likelihood of receiving data increases overall costs, as the buffers are likely to fill quickly and readings may be missed.

**Extensibility** As with the virus model [Section 5.1], a key benefit of bigraphs is the potential to quickly try out extensions to the model. For example, we could replace the movement system to have the sink move through a dynamic topology (rather than the sensors moving relative to the sink), or we could experiment with data dependent costs by adding structure to the buffer entity to allow it to record the type of data it received.

The existing model does not make use of linking, showing how we can utilise only the parts of the bigraph theory we require, without sacrificing expressiveness.
6. Discussion

6.1. Probabilistic Structure

Our approach is to generate probabilistic transition systems from a set of probabilistic reaction rules. An alternative approach is to keep the rewrite semantics unchanged and instead allow the bigraphs themselves to be probabilistic.

For example, given a non-ground bigraph, we could initialise it (probabilistically) with different parameters to simulate probabilistic phenomena and/or lack of information. This is the approach of term rewriting systems such as PMaude [AMS06], where rewriting can affect which variables are added in the substitution (the equivalent would be the instantiation of bigraph sites). This scenario can be modelled in probabilistic bigraphs as a set of rules, one for each possible right-hand side — where the set of rules act like a probability distribution.

Another approach, due to Syropoulos [Syr20], is to define the structure of bigraphs (i.e., the place and link graphs) in terms of fuzzy sets [Zad65]. An advantage of this formalisation is to allow a succinct representation of families of bigraphs. However, it is still an open question how to define bigraphs dynamics, i.e., matching and rewriting, in this setting. This makes it difficult to compare it directly with our approach.

6.2. Comparing Probabilistic/Stochastic Bigraphs and PRISM models

Since we use PRISM for analysis of exported systems from BigraphER, we compare bigraphs with the PRISM modelling language. The latter is based on the language of reactive modules [AH99]: a PRISM model consists of several modules, each with their own internal state, which are either updated independently or through shared (action) names. We make three observations.

First, consider creating new entities and arbitrary and dynamic topologies. PRISM employs renaming for this. For example, in the original PRISM model for virus spread our model is based on (Section 5.1), each node is represented by a module, links are (shared) actions. An infected node attacks by offering the action representing a link to another node — allowing the state of the attacked node to change. New nodes are created through module renaming, which creates a copy of the module with new state/action names. But PRISM modules have a fixed structure, so, for example, a module with 2 links (representing a corner node in Fig. 8b) cannot be reused for a module with 3 links (an internal node in Fig. 8b). Similarly, varying the firewall types requires a new module for each type of firewall. For this reason, creating arbitrary and dynamic topologies in PRISM is difficult and error prone. On the other hand, bigraphs allow arbitrary topologies to

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5 We discuss PRISM here, but the arguments are equally applicable to model checkers such as Storm [DJKV17].
be created easily by simply nesting additional links, and the graphical notation supports intuitive checking. This flexibility also allows nodes to be added/removed dynamically as the system progresses over time.

Second, consider \textit{exact} probabilities. PRISM allows these to be specified explicitly for \textit{module} transitions, \textit{e.g.} the probability for a particular node to block an infection. However, in probabilistic bigraphs, probabilities are assigned to pairs of states of the entire system, which requires the additional normalisation procedure to account for all possible (global) transitions. PRISM also includes a normalisation procedure to allow multiple modules to be used in parallel, \textit{i.e.} it combines states into a tuple and normalises probabilities \cite{PRI}.

In probabilistic bigraphs, as weights are defined as any positive real number, a modeller can use weights of the form $w_1 = p, 0 \leq p \leq 1$ and $w_2 = 1 - p$ if they prefer. However, we do not enforce transition of this form apply only to a single “modular” entity, \textit{i.e.} it is possible to define a single probabilistic transition where multiple entities change state.

Finally, PRISM models are often more efficient to analyse than those constructed from explicit transition systems, due to specialised symbolic analysis. It remains an open problem if similar techniques can be applied to bigraph models, especially those that reduce the state space.

\section*{6.3. Future Work}

\textbf{Additional Probabilistic Process Types} We currently support DTMC, CTMC, and MDP models, however many other probabilistic models are used in practice. For example MDPs have been extended in multiple ways, \textit{e.g.} partially observable MDPs (POMDPs) \cite{Ast65}, and these are candidates for further BRS extensions.

In POMDPs, agents cannot directly observe the current state and are instead assigned a set of observations/beliefs allowing decision making in uncertain environments. One possibility for BRSs is to fix the \textit{actual} and \textit{observed} states into two (bigraph) regions, where cross-region links connect the observations to the states they observe. Unfortunately while PRISM allows POMDPs to be specified, there is currently no way to import partially observable models.

Another extension of MDPs is Markov automata (MA) \cite{EHZ10, DH13}, combining probabilistic branching, non-determinism, and exponentially distributed delays. In a bigraph model, the probabilistic states of a MA would be treated as the states of an ABRS, while the Markovian states would behave like the states of a SBRS. However, rewriting for \textit{hybrid states}, \textit{i.e.} states where both non-deterministic choice over probability distributions and a distribution over states are available, requires a new definition.

\textbf{Bisimulations} Exploring the RPO framework in the presence of probabilistic rules likewise remains an open problem. It is likely RPOs exist for probabilistic rules, however these will have to also account for the normalised probabilities of specific matches (to ensure the contexts are equal).

\section*{7. Conclusion}

Bigraphical reactive systems (BRSs) have proved invaluable for modelling a wide range of systems, both virtual and physical, but are limited in the types of system they can represent. Real-world systems are often probabilistic, stochastic, and feature non-deterministic decisions, and these do not fit within standard BRSs.

We have shown how, by assigning \textit{weights} to standard BRS reaction rules we can model probabilistic systems (probabilistic BRSs – PBRSs), and extend this to support systems that make explicit decision (action) choices (action BRSs – ABRSs).

We have implemented both PBRS and ABRS in BigraphER, an open-source toolkit for working with bigraphs. To support stochastic systems we also implement \textit{stochastic bigraphs} as defined by Krivine et al. \cite{KMT08}. We show the new extensions are practical through a set of case study models: virus spread in computer networks, membrane budding in biological systems, and data harvesting in wireless sensor networks.

In conclusion, we have successfully extended the capabilities of BRSs and the toolkit BigraphER to model a wider range of systems, whilst preserving the high level nature and flexibility of the bigraph formalism.
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