

COARSE-GRAINING OPEN MARKOV PROCESSES

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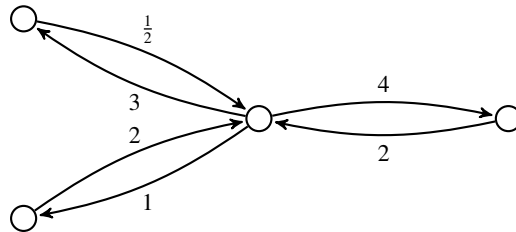
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ABSTRACT. Coarse-graining is a standard method of extracting a simpler Markov process from a more complicated one by identifying states. Here we extend coarse-graining to ‘open’ Markov processes: that is, those where probability can flow in or out of certain states called ‘inputs’ and ‘outputs’. One can build up an ordinary Markov process from smaller open pieces in two basic ways: composition, where we identify the outputs of one open Markov process with the inputs of another, and tensoring, where we set two open Markov processes side by side. In previous work, Fong, Pollard and the first author showed that these constructions make open Markov processes into the morphisms of a symmetric monoidal category. Here we go further by constructing a symmetric monoidal *double* category where the 2-morphisms include ways of coarse-graining open Markov processes. We also extend the already known ‘black-boxing’ functor from the category of open Markov processes to our double category. Black-boxing sends any open Markov process to the linear relation between input and output data that holds in steady states, including nonequilibrium steady states where there is a nonzero flow of probability through the process. To extend black-boxing to a functor between double categories, we need to prove that black-boxing is compatible with coarse-graining.

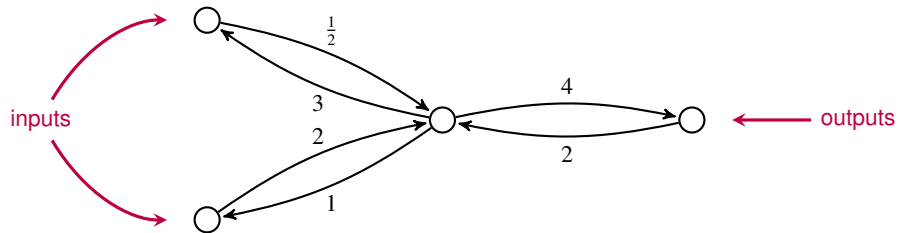
1. INTRODUCTION

A ‘Markov process’ is a stochastic model describing a sequence of transitions between states in which the probability of a transition depends only on the current state. The only Markov processes we consider here are continuous-time Markov processes with a finite set of states. These can be drawn as labeled graphs:



where the number labeling each edge describes the probability per time of making a transition from one state to another.

An ‘open’ Markov process is a generalization in which probability can also flow in or out of certain states designated as ‘inputs’ and ‘outputs’:



Open Markov processes can be seen as morphisms in a category, since we can compose two open Markov processes by identifying the outputs of the first with the inputs of the second. Composition lets us build a Markov process from smaller open parts—or conversely, analyze the behavior of a Markov process in terms of its parts [4, 5, 15, 22].

‘Coarse-graining’ is a widely used method of simplifying a Markov process by mapping its set of states X onto some smaller set X' in a manner that respects, or at least approximately respects, the dynamics [1, 8]. Here we introduce coarse-graining for open Markov processes. We show how to extend this notion to the case of maps $p: X \rightarrow X'$ that are not surjective, obtaining a general concept of morphism between open Markov processes.

Since open Markov processes are already morphisms in a category, it is natural to treat morphisms between them as morphisms between morphisms, or ‘2-morphisms’. We can do this using double categories. These were first introduced by Ehresmann [13, 14], and they have long been used in topology and other branches of pure mathematics [9, 10]. More recently they have been used to study open dynamical systems [21] and open discrete-time Markov chains [11]. So, it should not be surprising that they are also useful for open Markov processes.

A 2-morphism in a double category looks like this:

$$\begin{array}{ccc}
 A & \xrightarrow{M} & B \\
 f \downarrow & \Downarrow \alpha & \downarrow g \\
 C & \xrightarrow{N} & D
 \end{array}$$

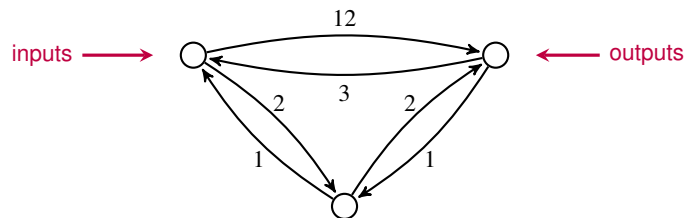
While a mere category has only objects and morphisms, here we have a few more types of entities. We call A, B, C and D ‘objects’, f and g ‘vertical 1-morphisms’, M and N ‘horizontal 1-cells’, and α a ‘2-morphism’. We can compose vertical 1-morphisms to get new vertical 1-morphisms and compose horizontal 1-cells to get new horizontal 1-cells. We can compose the 2-morphisms in two ways: horizontally by setting squares side by side, and vertically by setting one on top of the other. In a ‘strict’ double category all these forms of composition are associative. In a ‘pseudo’ double category, horizontal 1-cells compose in a weakly associative manner: that is, the associative law holds only up to an invertible 2-morphism, called the ‘associator’, which obeys a coherence law. This is just a quick sketch of the ideas; for full definitions see for example the works of Grandis and Paré [17, 18].

We construct a double category $\mathbb{M}\mathbf{ark}$ with:

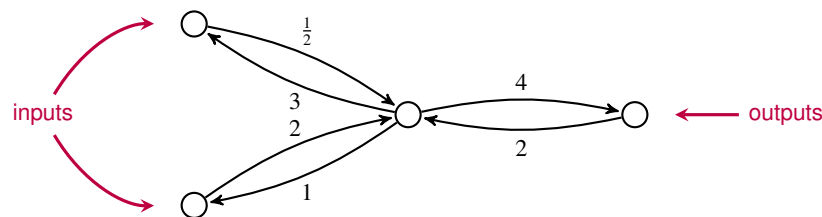
- (i) finite sets as objects,
- (ii) maps between finite sets as vertical 1-morphisms,
- (iii) open Markov processes as horizontal 1-cells,
- (iv) morphisms between open Markov processes as 2-morphisms.

Composition of open Markov processes is only weakly associative, so this is a pseudo double category.

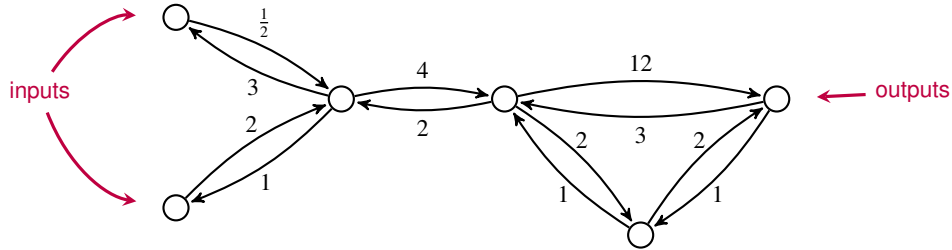
The plan of the paper is as follows. In Section 2 we define open Markov processes and steady state solutions of the open master equation. In Section 3 we introduce coarse-graining first for Markov processes and then open Markov processes. In Section 4 we construct the double category $\mathbb{M}\mathbf{ark}$ described above. We prove this is a symmetric monoidal double category in the sense of Shulman [23]. This captures the fact that we can not only compose open Markov processes but also ‘tensor’ them by setting them side by side. For example, if we compose this open Markov process:



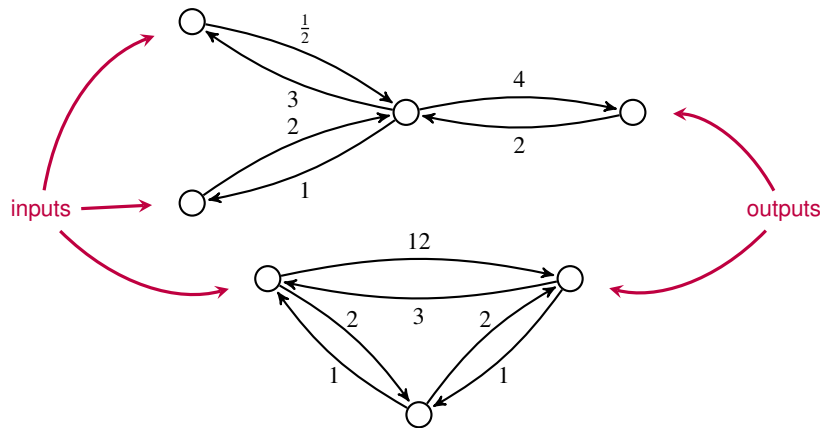
with the one shown before:



we obtain this open Markov process:



but if we tensor them, we obtain this:



As compared with an ordinary Markov process, the key new feature of an *open* Markov process is that probability can flow in or out. To describe this we need a generalization of the usual master equation for Markov processes, called the ‘open master equation’ [5]. In this equation the probabilities at input and output states are arbitrary specified functions of time, while the probabilities at other states obey the usual master equation. As a result, the probabilities are not necessarily normalized. We interpret this by saying probability can flow either in or out at both the input and the output states.

If we fix constant probabilities at the inputs and outputs, there typically exist solutions of the open master equation with these boundary conditions that are constant as a function of time. These are called ‘steady states’. Often these are *nonequilibrium* steady states, meaning that there is a nonzero net flow of probabilities at the inputs and outputs. For example, probability can flow through an open Markov process at a constant rate in a nonequilibrium steady state.

In previous work, Fong, Pollard and the first author studied the relation between probabilities and flows at the inputs and outputs that holds in steady state [5, 6]. They called the process of extracting this relation from an open Markov process ‘black-boxing’, since it gives a way to forget the internal workings of an open system and remember only its externally observable behavior. They proved that black-boxing is compatible with composition and tensoring. This result can be summarized by saying that black-boxing is a symmetric monoidal functor.

In Section 5 we show that black-boxing is compatible with morphisms between open Markov processes. To make this idea precise, we prove that black-boxing gives a map from the double category **Mark** to another double category, called **LinRel**, which has:

- (i) finite-dimensional real vector spaces U, V, W, \dots as objects,
- (ii) linear maps $f: V \rightarrow W$ as vertical 1-morphisms from V to W ,
- (iii) linear relations $R \subseteq V \oplus W$ as horizontal 1-cells from V to W ,
- (iv) squares

$$\begin{array}{ccc}
 V_1 & \xrightarrow{R \subseteq V_1 \oplus V_2} & V_2 \\
 f \downarrow & & \downarrow g \\
 W_1 & \xrightarrow{S \subseteq W_1 \oplus W_2} & W_2
 \end{array}$$

obeying $(f \oplus g)R \subseteq S$ as 2-morphisms.

Here a ‘linear relation’ from a vector space V to a vector space W is a linear subspace $R \subseteq V \oplus W$. Linear relations can be composed in the same way as relations [3]. The double category \mathbf{LinRel} becomes symmetric monoidal using direct sum as the tensor product, but unlike \mathbf{Mark} it is strict: that is, composition of linear relations is associative.

Maps between symmetric monoidal double categories are called ‘symmetric monoidal double functors’ [12]. Our main result, Thm. 5.5, says that black-boxing gives a symmetric monoidal double functor

$$\blacksquare: \mathbf{Mark} \rightarrow \mathbf{LinRel}.$$

The hardest part is to show that black-boxing preserves composition of horizontal 1-cells: that is, black-boxing a composite of open Markov processes gives the composite of their black-boxings. Luckily, for this we can adapt a previous argument [6]. Thus, the new content of this result concerns the vertical 1-morphisms and especially the 2-morphisms, which describe coarse-grainings.

An alternative approach to studying morphisms between open Markov processes uses bicategories rather than double categories [7, 24]. In Section 6 we use a result of Shulman [23] to construct symmetric monoidal bicategories \mathbf{Mark} and \mathbf{LinRel} from the symmetric monoidal double categories \mathbf{Mark} and \mathbf{LinRel} . We conjecture that the black-boxing double functor determines a functor between these symmetric monoidal bicategories. However, double categories seem to be a simpler framework for coarse-graining open Markov processes.

It is worth comparing some related work. Fong, Pollard and the first author constructed a symmetric monoidal category where the morphisms are open Markov processes [5, 6]. Like us, they only consider Markov processes where time is continuous and the set of states is finite. However, they formalized such Markov processes in a slightly different way than we do here: they defined a Markov process to be a directed multigraph where each edge is assigned a positive number called its ‘rate constant’. In other words, they defined it to be a diagram

$$(0, \infty) \xleftarrow{r} E \xrightleftharpoons[s]{t} X$$

where X is a finite set of vertices or ‘states’, E is a finite set of edges or ‘transitions’ between states, the functions $s, t: E \rightarrow X$ give the source and target of each edge, and $r: E \rightarrow (0, \infty)$ gives the rate constant of each edge. They explained how from this data one can extract a matrix of real numbers $(H_{ij})_{i, j \in X}$ called the ‘Hamiltonian’ of the Markov process, with two familiar properties:

- (i) $H_{ij} \geq 0$ if $i \neq j$,

(ii) $\sum_{i \in X} H_{ij} = 0$ for all $j \in X$.

A matrix with these properties is called ‘infinitesimal stochastic’, since these conditions are equivalent to $\exp(tH)$ being stochastic for all $t \geq 0$.

In the present work we skip the directed multigraphs and work directly with the Hamiltonians. Thus, we define a Markov process to be a finite set X together with an infinitesimal stochastic matrix $(H_{ij})_{i,j \in X}$. This allows us to work more directly with the Hamiltonian and the all-important ‘master equation’

$$\frac{dp(t)}{dt} = Hp(t)$$

which describes the evolution of a time-dependent probability distribution $p(t): X \rightarrow \mathbb{R}$.

Clerc, Humphrey and Panangaden have constructed a bicategory [11] with finite sets as objects, ‘open discrete labeled Markov processes’ as morphisms, and ‘simulations’ as 2-morphisms. In their framework, ‘open’ has a similar meaning as it does in works listed above. These open discrete labeled Markov processes are also equipped with a set of ‘actions’ which represent interactions between the Markov process and the environment, such as an outside entity acting on a stochastic system. A ‘simulation’ is then a function between the state spaces that map the inputs, outputs and set of actions of one open discrete labeled Markov process to the inputs, outputs and set of actions of another.

Another compositional framework for Markov processes is given by de Francesco Albasini, Sabadini and Walters [16] in which they construct an algebra of ‘Markov automata’. A Markov automaton is a family of matrices with non-negative real coefficients that is indexed by elements of a binary product of sets, where one set represents a set of ‘signals on the left interface’ of the Markov automata and the other set analogously for the right interface.

Notation and Terminology. Following Shulman, we use ‘double category’ to mean ‘pseudo double category’, and use ‘strict double category’ to mean a double category for which horizontal composition is strictly associative and unital. (In older literature, ‘double category’ often refers to a strict double category.)

It is common to use blackboard bold for the first letter of the name of a double category, and we do so here. Bicategories are written in boldface, while ordinary categories are written in roman font. Thus, three main players in this paper are a double category **Mark**, a bicategory **Mark**, and a category Mark, all closely related.

2. OPEN MARKOV PROCESSES

Before explaining open Markov processes we should recall a bit about Markov processes. As mentioned in the Introduction, we use ‘Markov process’ as a short term for ‘continuous-time Markov process with a finite set of states’, and we identify any such Markov process with the infinitesimal stochastic matrix appearing in its master equation. We make this precise with a bit of terminology that is useful throughout the paper.

We call a function $v: X \rightarrow \mathbb{R}$ a ‘vector’ and call its values at points $x \in X$ its ‘components’ v_x . We define a ‘probability distribution’ on X to be a vector $p: X \rightarrow \mathbb{R}$ whose components are nonnegative and sum to 1. As usual, we use \mathbb{R}^X to denote the vector space of functions $v: X \rightarrow \mathbb{R}$. Given a linear operator $T: \mathbb{R}^X \rightarrow \mathbb{R}^Y$ we have $(Tv)_i = \sum_{j \in X} T_{ij}v_j$ for some ‘matrix’ $T: Y \times X \rightarrow \mathbb{R}$ with entries T_{ij} .

Definition 2.1. *Given a finite set X , a linear operator $H: \mathbb{R}^X \rightarrow \mathbb{R}^X$ is **infinitesimal stochastic** if*

(i) $H_{ij} \geq 0$ for $i \neq j$ and

(ii) $\sum_{i \in X} H_{ij} = 0$ for each $j \in X$.

The reason for being interested in such operators is that when exponentiated they give stochastic operators.

Definition 2.2. Given finite sets X and Y , a linear operator $T: \mathbb{R}^X \rightarrow \mathbb{R}^Y$ is **stochastic** if for any probability distribution p on X , Tp is a probability distribution on Y .

Equivalently, T is stochastic if and only if

- (i) $T_{ij} \geq 0$ for all $i \in Y, j \in X$ and
- (ii) $\sum_{i \in Y} T_{ij} = 1$ for each $j \in X$.

If we think of T_{ij} as the probability for $j \in X$ to be mapped to $i \in Y$, these conditions make intuitive sense. Since stochastic operators are those that preserve probability distributions, the composite of stochastic operators is stochastic.

In Lemma 3.7 we recall that a linear operator $H: \mathbb{R}^X \rightarrow \mathbb{R}^X$ is infinitesimal stochastic if and only if its exponential

$$\exp(tH) = \sum_{n=0}^{\infty} \frac{(tH)^n}{n!}$$

is stochastic for all $t \geq 0$. Thus, given an infinitesimal stochastic operator H , for any time $t \geq 0$ we can apply the operator $\exp(tH): \mathbb{R}^X \rightarrow \mathbb{R}^X$ to any probability distribution $p \in \mathbb{R}^X$ and get a probability distribution

$$p(t) = \exp(tH)p.$$

These probability distributions $p(t)$ obey the **master equation**

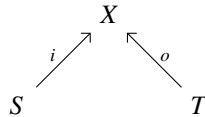
$$\frac{dp(t)}{dt} = Hp(t).$$

Moreover, any solution of the master equation arises this way.

All the material so far is standard. We now turn to open Markov processes.

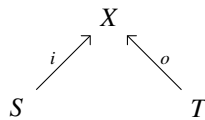
Definition 2.3. We define a **Markov process** to be a pair (X, H) where X is a finite set and $H: \mathbb{R}^X \rightarrow \mathbb{R}^X$ is an infinitesimal stochastic operator. We also call H a Markov process on X .

Definition 2.4. We define an **open Markov process** to consist of finite sets X, S and T and injections



together with a Markov process (X, H) . We call the S the set of **inputs** and T the set of **outputs**.

In general, a diagram of this shape in any category:



is called a **cospan**. The objects S and T are called the **feet**, the object X is called the **apex**, and the morphisms i and o are called the **legs**. We use FinSet to stand for the category

of finite sets and functions. Thus, an open Markov process is a cospan in FinSet with injections as legs and a Markov process on its apex. We often abbreviate an open Markov process as

$$\begin{array}{ccc} & (X, H) & \\ i \nearrow & & \nwarrow o \\ S & & T \end{array}$$

or simply $S \xrightarrow{i} (X, H) \xleftarrow{o} T$.

Given an open Markov process we can write down an ‘open’ version of the master equation, where probability can also flow in or out of the inputs and outputs. To work with the open master equation we need two well-known concepts:

Definition 2.5. Let $f: A \rightarrow B$ be a map between finite sets. The linear map $f^*: \mathbb{R}^B \rightarrow \mathbb{R}^A$ sends any vector $v \in \mathbb{R}^B$ to its **pullback** along f , given by

$$f^*(v) = v \circ f.$$

The linear map $f_*: \mathbb{R}^A \rightarrow \mathbb{R}^B$ sends any vector $v \in \mathbb{R}^A$ to its **pushforward** along f , given by

$$(f_*(v))(b) = \sum_{\{a: f(a)=b\}} v(a).$$

Now, suppose we are given an open Markov process

$$\begin{array}{ccc} & (X, H) & \\ i \nearrow & & \nwarrow o \\ S & & T \end{array}$$

together with **inflows** $I: \mathbb{R} \rightarrow \mathbb{R}^S$ and **outflows** $O: \mathbb{R} \rightarrow \mathbb{R}^T$, arbitrary smooth functions of time. We write the value of the inflow at $s \in S$ at time t as $I_s(t)$, and similarly for outflows and other functions of time. We say a function $p: \mathbb{R} \rightarrow \mathbb{R}^X$ obeys the **open master equation** if

$$\frac{dp(t)}{dt} = Hp(t) + i_*(I(t)) - o_*(O(t)).$$

This says that for any state $x \in X$ the time derivative of the probability $p_x(t)$ takes into account not only the usual term from the master equation, but also inflows and outflows.

If the inflows and outflows are constant in time, a solution p of the open master equation that is also constant in time is called a **steady state**. More formally:

Definition 2.6. Given an open Markov process $S \xrightarrow{i} (X, H) \xleftarrow{o} T$ together with $I \in \mathbb{R}^S$ and $O \in \mathbb{R}^T$, a **steady state** with inflows I and outflows O is an element $p \in \mathbb{R}^X$ such that

$$Hp + i_*(I) - o_*(O) = 0.$$

Given $p \in \mathbb{R}^X$ we call $i^*(p) \in \mathbb{R}^S$ and $o^*(p) \in \mathbb{R}^T$ the **input probabilities** and **output probabilities**, respectively.

Definition 2.7. Given an open Markov process $S \xrightarrow{i} (X, H) \xleftarrow{o} T$, we define its **black-boxing** to be the set

$$\blacksquare(S \xrightarrow{i} (X, H) \xleftarrow{o} T) \subseteq \mathbb{R}^S \oplus \mathbb{R}^S \oplus \mathbb{R}^T \oplus \mathbb{R}^T$$

consisting of all 4-tuples $(i^*(p), I, o^*(p), O)$ where $p \in \mathbb{R}^X$ is some steady state with inflows $I \in \mathbb{R}^S$ and outflows $O \in \mathbb{R}^T$.

Thus, black-boxing records the relation between input probabilities, inflows, output probabilities and outflows that holds in steady state. This is the ‘externally observable steady state behavior’ of the open Markov process. It has already been shown [5, 6] that black-boxing can be seen as a functor between categories. Here we go further and describe it as a double functor between double categories, in order to study the effect of black-boxing on morphisms between open Markov processes.

3. MORPHISMS OF OPEN MARKOV PROCESSES

There are various ways to approximate a Markov process by another Markov process on a smaller set, all of which can be considered forms of coarse-graining [8]. A common approach is to take a Markov process H on a finite set X and a surjection $p: X \rightarrow X'$ and create a Markov process on X' . In general this requires a choice of ‘stochastic section’ for p , defined as follows:

Definition 3.1. *Given a function $p: X \rightarrow X'$ between finite sets, a **stochastic section** for p is a stochastic operator $s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$ such that $p_*s = 1_{X'}$.*

It is easy to check that a stochastic section for p exists if and only if p is a surjection. In Lemma 3.9 we show that given a Markov process H on X and a surjection $p: X \rightarrow X'$, any stochastic section $s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$ gives a Markov process on X' , namely

$$H' = p_*Hs.$$

Experts call the matrix corresponding to p_* the **collector matrix**, and they call s the **distributor matrix** [8]. The names help clarify what is going on. The collector matrix, coming from the surjection $p: X \rightarrow X'$, typically maps many states of X to each state of X' . The distributor matrix, the stochastic section $s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$, typically maps each state in X' to a linear combination of many states in X . Thus, $H' = p_*Hs$ distributes each state of X' , applies H , and then collects the results.

In general H' depends on the choice of s , but sometimes it does not:

Definition 3.2. *We say a Markov process H on X is **lumpable** with respect to a surjection $p: X \rightarrow X'$ if the operator p_*Hs is independent of the choice of stochastic section $s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$.*

This concept is not new [8]. While our definition may be new, in Thm. 3.10 we show that it is equivalent to the traditional one, and also to an even simpler one: H is lumpable with respect to p if and only if $p_*H = H'p_*$. This equation has the advantage of making sense even when p is not a surjection. Thus, we can use it to define a more general concept of morphism between Markov processes:

Definition 3.3. *Given Markov processes (X, H) and (X', H') , a **morphism of Markov processes** $p: (X, H) \rightarrow (X', H')$ is a map $p: X \rightarrow X'$ such that $p_*H = H'p_*$.*

There is a category Mark with Markov processes as objects and the morphisms as defined above, where composition is the usual composition of functions. But what is the meaning of such a morphism? Using Lemma 3.7 one can check that for any Markov processes (X, H) and (X', H') , and any map $p: X \rightarrow X'$, we have

$$p_*H = H'p_* \iff p_* \exp(tH) = \exp(tH')p_* \text{ for all } t \geq 0.$$

Thus, p is a morphism of Markov processes if evolving a probability distribution on X via $\exp(tH)$ and then pushing it forward along p is the same as pushing it forward and then evolving it via $\exp(tH')$.

We can also define morphisms between *open* Markov processes:

Definition 3.4. A **morphism of open Markov processes** from the open Markov process $S \xrightarrow{i} (X, H) \xleftarrow{o} T$ to the open Markov process $S' \xrightarrow{i'} (X', H') \xleftarrow{o'} T'$ is a triple of functions $f: S \rightarrow S'$, $p: X \rightarrow X'$, $g: T \rightarrow T'$ such that the squares in this diagram are pullbacks:

$$\begin{array}{ccccc} S & \xrightarrow{i_1} & X & \xleftarrow{o_1} & T \\ \downarrow f & & \downarrow p & & \downarrow g \\ S' & \xrightarrow{i'_1} & X' & \xleftarrow{o'_1} & T' \end{array}$$

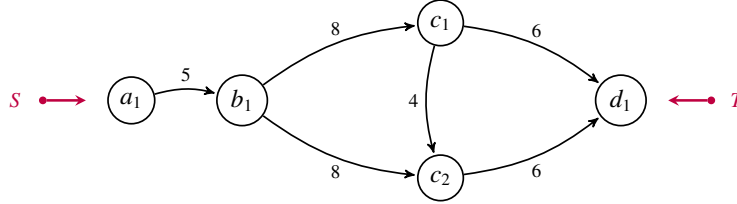
and $p_*H = H'p_*$.

We need the squares to be pullbacks so that in Lemma 5.3 we can black-box morphisms of open Markov processes. In Lemma 4.2 we show that horizontally composing these morphisms preserves this pullback property. But to do this, we need the horizontal arrows in these squares to be injections. This explains the conditions in Defs. 2.4 and 3.4.

We often abbreviate a morphism of open Markov processes as

$$\begin{array}{ccccc} S & \xrightarrow{i_1} & (X, H) & \xleftarrow{o_1} & T \\ \downarrow f & & \downarrow p & & \downarrow g \\ S' & \xrightarrow{i'_1} & (X', H') & \xleftarrow{o'_1} & T' \end{array}$$

As an example, consider the following open Markov process:



This is a way of drawing an open Markov process with state space

$$X = \{a_1, b_1, c_1, c_2, d_1\}$$

and infinitesimal stochastic operator $H: \mathbb{R}^X \rightarrow \mathbb{R}^X$ given by the following matrix:

$$H = \begin{bmatrix} -5 & 0 & 0 & 0 & 0 \\ 5 & -16 & 0 & 0 & 0 \\ 0 & 8 & -10 & 0 & 0 \\ 0 & 8 & 4 & -6 & 0 \\ 0 & 0 & 6 & 6 & 0 \end{bmatrix}.$$

Let $X' = \{a, b, c, d\}$. We can define a surjection $p: X \rightarrow X'$ where each element of X goes to the element of X' named by the same letter. We can choose a stochastic section

$s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$ of p as follows:

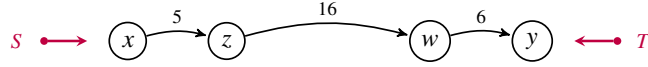
$$s = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1/3 & 0 \\ 0 & 0 & 2/3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

The infinitesimal stochastic matrix $H' = p_* H s$ is given by

$$H' = \begin{bmatrix} -5 & 0 & 0 & 0 \\ 5 & -16 & 0 & 0 \\ 0 & 16 & -6 & 0 \\ 0 & 0 & 6 & 0 \end{bmatrix}.$$

One can check that given any other stochastic section $s': \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$ we have $p_* H s = p_* H s'$, so H is lumpable with respect to p . This verification is made much easier by Thm. 3.10 below.

So far we have described a morphism of Markov processes $p: (X, H) \rightarrow (X', H')$, but together with identity functions on the inputs S and outputs T this defines a morphism of open Markov processes, going from the above open Markov process to one that may be drawn as follows:



In Section 4 we construct a double category $\mathbb{M}\mathbf{ark}$ with open Markov processes as horizontal 1-cells and morphism between these as 2-morphisms. This double category is our main object of study. First, however, we should prove the results mentioned above. For this it is helpful to recall a few standard concepts:

Definition 3.5. A **1-parameter semigroup of operators** is a collection of linear operators $U(t): V \rightarrow V$ on a vector space V , one for each $t \in [0, \infty)$, such that

- (i) $U(0) = 1$ and
- (ii) $U(s+t) = U(s)U(t)$ for all $s, t \in [0, \infty)$. If V is finite-dimensional we say the collection $U(t)$ is **continuous** if $t \mapsto U(t)v$ is continuous for each $v \in V$.

Definition 3.6. Let X be a finite set. A **Markov semigroup** is a continuous 1-parameter semigroup $U(t): \mathbb{R}^X \rightarrow \mathbb{R}^X$ such that $U(t)$ is stochastic for each $t \in [0, \infty)$.

Lemma 3.7. Let X be a finite set and $U(t): \mathbb{R}^X \rightarrow \mathbb{R}^X$ a Markov semigroup. Then $U(t) = \exp(tH)$ for a unique infinitesimal stochastic operator $H: \mathbb{R}^X \rightarrow \mathbb{R}^X$, which is given by

$$Hv = \left. \frac{d}{dt} U(t)v \right|_{t=0}$$

for all $v \in \mathbb{R}^X$. Conversely, given an infinitesimal stochastic operator H , then $\exp(tH) = U(t)$ is a Markov semigroup.

Proof. This is well-known; for a proof, see for example [2, Thm. 17]. \square

Lemma 3.8. Let $U(t): \mathbb{R}^X \rightarrow \mathbb{R}^X$ be a differentiable family of stochastic operators defined for $t \in [0, \infty)$ and having $U(0) = 1$. Then $\left. \frac{d}{dt} U(t) \right|_{t=0}$ is infinitesimal stochastic.

Proof. Let $H = \left. \frac{d}{dt}U(t) \right|_{t=0} = \lim_{t \rightarrow 0^+} (U(t) - 1)/t$. As $U(t)$ is stochastic, its entries are nonnegative and the column sum of any particular column is 1. Then the column sum of any particular column of $U(t) - 1$ will be 0 with the off-diagonal entries being nonnegative. Thus $U(t) - 1$ is infinitesimal stochastic for all $t \geq 0$, as is $(U(t) - 1)/t$, from which it follows that $\lim_{t \rightarrow 0^+} (U(t) - U(0))/t = H$ is infinitesimal stochastic. \square

Lemma 3.9. *Let $p: X \rightarrow X'$ be a function between finite sets with a stochastic section $s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$, and let $H: \mathbb{R}^X \rightarrow \mathbb{R}^X$ be an infinitesimal stochastic operator. Then $H' = p_* H s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^{X'}$ is also infinitesimal stochastic.*

Proof. Lemma 3.7 implies that $\exp(tH)$ is stochastic for all $t \geq 0$. For any map $p: X \rightarrow X'$ the operator $p_*: \mathbb{R}^X \rightarrow \mathbb{R}^{X'}$ is easily seen to be stochastic, and s is stochastic by assumption. Thus, $U(t) = p_* \exp(tH) s$ is stochastic for all $t \geq 0$. Differentiating, we conclude that

$$\left. \frac{d}{dt}U(t) \right|_{t=0} = \left. \frac{d}{dt} p_* \exp(tH) s \right|_{t=0} = p_* \exp(tH) H s \Big|_{t=0} = p_* H s$$

is infinitesimal stochastic by Lemma 3.8. \square

We can now give some conditions equivalent to lumpability. The third is the most common in the literature [8] and the easiest to check in examples. It makes use of the standard basis vectors $e_j \in \mathbb{R}^X$ associated to the elements j of any finite set X . The surjection $p: X \rightarrow X'$ defines a partition on X where two states $j, j' \in X$ lie in the same block of the partition if and only if $p(j) = p(j')$. The elements of X' correspond to these blocks. The third condition for lumpability says that $p_* H$ has the same effect on two basis vectors e_j and $e_{j'}$ when j and j' are in the same block.

Theorem 3.10. *Let $p: X \rightarrow X'$ be a surjection of finite sets and let H be a Markov process on X . Then the following conditions are equivalent:*

- (i) H is lumpable with respect to p .
- (ii) There exists a linear operator $H': \mathbb{R}^{X'} \rightarrow \mathbb{R}^{X'}$ such that $p_* H = H' p_*$.
- (iii) $p_* H e_j = p_* H e_{j'}$ for all $j, j' \in X$ such that $p(j) = p(j')$.

When these conditions hold there is a unique operator $H': \mathbb{R}^{X'} \rightarrow \mathbb{R}^{X'}$ such that $p_ H = H' p_*$, it is given by $H' = p_* H s$ for any stochastic section s of p , and it is infinitesimal stochastic.*

Proof. (i) \implies (iii). Suppose that H is lumpable with respect to p . Thus, $p_* H s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$ is independent of the choice of stochastic section $s: \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$. Such a stochastic section is simply an arbitrary linear operator that maps each basis vector $e_i \in \mathbb{R}^{X'}$ to a probability distribution on X supported on the set $\{j \in X : p(j) = i\}$. Thus, for any $j, j' \in X$ with $p(j) = p(j') = i$, we can find stochastic sections $s, s': \mathbb{R}^{X'} \rightarrow \mathbb{R}^X$ such that $s(e_i) = e_j$ and $s'(e_i) = e_{j'}$. Since $p_* H s = p_* H s'$, we have

$$p_* H e_j = p_* H s(e_i) = p_* H s'(e_i) = p_* H e_{j'}$$

(iii) \implies (ii). Define $H': \mathbb{R}^{X'} \rightarrow \mathbb{R}^{X'}$ on basis vectors $e_i \in \mathbb{R}^{X'}$ by setting

$$H' e_i = p_* H e_j$$

for any j with $p(j) = i$. Note that H' is well-defined: since p is a surjection such j exists, and since H is lumpable, H' is independent of the choice of such j . Next, note that for any $j \in X$, if we let $p(j) = i$ we have $p_* H e_j = H' e_i = H' p_* e_j$. Since the vectors e_j form a basis for \mathbb{R}^X , it follows that $p_* H = H' p_*$.

(ii) \implies (i). Suppose there exists an operator $H' : \mathbb{R}^{X'} \rightarrow \mathbb{R}^{X'}$ such that $p_*H = H'p_*$. Choose such an operator; then for any stochastic section s for p we have

$$p_*Hs = H'p_*s = H'.$$

It follows that p_*Hs is independent of the stochastic section s , so H is lumpable with respect to p .

Suppose that any, hence all, of conditions (i), (ii), (iii) hold. Suppose that $H' : \mathbb{R}^{X'} \rightarrow \mathbb{R}^{X'}$ is an operator with $p_*H = H'p_*$. Then the argument in the previous paragraph shows that $H' = p_*Hs$ for any stochastic section s of p . Thus H' is unique, and by Lemma 3.9 it is infinitesimal stochastic. \square

4. A DOUBLE CATEGORY OF OPEN MARKOV PROCESSES

In this section we construct a symmetric monoidal double category $\mathbb{M}\mathbf{ark}$ with open Markov processes as horizontal 1-cells and morphisms between these as 2-morphisms. Symmetric monoidal double categories were introduced by Shulman [23] and applied to various examples from engineering by the second author [12]. We refer the reader to those papers for the basic definitions, since they are rather long.

The pieces of the double category $\mathbb{M}\mathbf{ark}$ work as follows:

- (i) An object is a finite set.
- (ii) A vertical 1-morphism $f : S \rightarrow S'$ is a map between finite sets.
- (iii) A horizontal 1-cell is an open Markov process

$$S \xrightarrow{i} (X, H) \xleftarrow{o} T.$$

In other words, it is a pair of injections $S \xrightarrow{i} X \xleftarrow{o} T$ together with a Markov process H on X .

- (iv) A 2-morphism is a morphism of open Markov processes

$$\begin{array}{ccccc} S & \xrightarrow{i_1} & (X, H) & \xleftarrow{o_1} & T \\ \downarrow f & & \downarrow p & & \downarrow g \\ S' & \xrightarrow{i'_1} & (X', H') & \xleftarrow{o'_1} & T' \end{array}$$

In other words, it is a triple of maps f, p, g such that these squares are pullbacks:

$$\begin{array}{ccccc} S & \xrightarrow{i_1} & X & \xleftarrow{o_1} & T \\ \downarrow f & & \downarrow p & & \downarrow g \\ S' & \xrightarrow{i'_1} & X' & \xleftarrow{o'_1} & T', \end{array}$$

and $H'p_* = p_*H$.

Composition of vertical 1-morphisms in $\mathbb{M}\mathbf{ark}$ is straightforward. So is vertical composition of 2-morphisms, since we can paste two pullback squares and get a new pullback

square. Composition of horizontal 1-cells is a bit more subtle. Given open Markov processes

$$S \xrightarrow{i_1} (X, H) \xleftarrow{o_1} T$$

and

$$T \xrightarrow{i_2} (Y, G) \xleftarrow{o_2} U$$

we first compose their underlying cospans using a pushout:

$$\begin{array}{ccccc}
 & & X +_T Y & & \\
 & j \nearrow & & \nwarrow k & \\
 & X & & Y & \\
 i_1 \nearrow & & & & \nwarrow o_2 \\
 S & & T & & U \\
 & \nwarrow o_1 & & \nearrow i_2 &
 \end{array}$$

Since monomorphisms are stable under pushout in a topos, the legs of this new cospan are again injections, as required. We then define the composite open Markov process to be

$$S \xrightarrow{j i_1} (X +_T Y, H \odot G) \xleftarrow{k o_2} U \quad (1)$$

where

$$H \odot G = j_* H j^* + k_* G k^*.$$

Here we use both pullbacks and pushforwards along the maps j and k , as defined in Def. 2.5. To check that $H \odot G$ is a Markov process on $X +_T Y$ we need to check that $j_* H j^*$ and $k_* G k^*$, and thus their sum, are infinitesimal stochastic:

Lemma 4.1. *Suppose that $f: X \rightarrow Y$ is any map between finite sets. If $H: \mathbb{R}^X \rightarrow \mathbb{R}^X$ is infinitesimal stochastic, then $f_* H f^*: \mathbb{R}^Y \rightarrow \mathbb{R}^Y$ is infinitesimal stochastic.*

Proof. Using Def. 2.5, we see that the matrix elements of f^* and f_* are given by

$$(f^*)_{ji} = (f_*)_{ij} = \begin{cases} 1 & f(j) = i \\ 0 & \text{otherwise} \end{cases}$$

for all $i \in Y, j \in X$. Thus, $f_* H f^*$ has matrix entries

$$(f_* H f^*)_{i'i'} = \sum_{j, j': f(j)=i, f(j')=i'} H_{jj'}.$$

To show that $f_* H f^*$ is infinitesimal stochastic we need to show that its off-diagonal entries are nonnegative and its columns sum to zero. By the above formula, these follow from the same facts for H . \square

Horizontal composition of 2-morphisms is even subtler:

Lemma 4.2. *Suppose that we have horizontally composable 2-morphisms as follows:*

$$\begin{array}{ccccc}
 S & \xrightarrow{i_1} & (X, H) & \xleftarrow{o_1} & T & & T & \xrightarrow{i_2} & (Y, G) & \xleftarrow{o_2} & U \\
 \downarrow f & & \downarrow p & & \downarrow g & & \downarrow g & & \downarrow q & & \downarrow h \\
 S' & \xrightarrow{i'_1} & (X', H') & \xleftarrow{o'_1} & T' & & T' & \xrightarrow{i'_2} & (Y', G') & \xleftarrow{o'_2} & U'
 \end{array}$$

By assumption the top and bottom faces are pushouts, the two left-hand vertical faces are pullbacks, and the arrows o'_1 and i'_2 are monic. In an adhesive category, this implies that the two right-hand vertical faces are pullbacks as well. One of these is the square in question.

To show that $(p +_g q)_*(H \odot G) = (H' \odot G')(p +_g q)_*$, we again use the above cube. Because its two right-hand vertical faces commute, we have

$$(p +_g q)_*j_* = j'_*p_* \quad \text{and} \quad (p +_g q)_*k_* = k'_*q_*$$

so using the definition of $H \odot G$ we obtain

$$\begin{aligned} (p +_g q)_*(H \odot G) &= (p +_g q)_*(j_*Hj_*^* + k_*Gk_*^*) \\ &= (p +_g q)_*j_*Hj_*^* + (p +_g q)_*k_*Gk_*^* \\ &= j'_*p_*Hj_*^* + k'_*q_*Gk_*^*. \end{aligned}$$

By assumption we have

$$p_*H = H'p_* \quad \text{and} \quad q_*G = G'q_*$$

so we can go a step further, obtaining

$$(p +_g q)_*(H \odot G) = j'_*H'p_*j_*^* + k'_*G'q_*k_*^*.$$

Because the two right-hand vertical faces of the cube are pullbacks, Lemma 4.3 implies that

$$p_*j_*^* = j'^*(p +_g q)_* \quad \text{and} \quad q_*k_*^* = k'^*(p +_g q)_*.$$

Using these, we obtain

$$\begin{aligned} (p +_g q)_*(H \odot G) &= j'_*H'j'^*(p +_g q)_* + k'_*G'k'^*(p +_g q)_* \\ &= (j'_*H'j'^* + k'_*G'k'^*)(p +_g q)_* \\ &= (H' \odot G')(p +_g q)_* \end{aligned}$$

completing the proof. \square

The following lemma is reminiscent of the Beck–Chevalley condition for adjoint functors:

Lemma 4.3. *Given a pullback square in FinSet :*

$$\begin{array}{ccc} A & \xrightarrow{f} & B \\ g \downarrow & & \downarrow h \\ C & \xrightarrow{k} & D \end{array}$$

the following square of linear operators commutes:

$$\begin{array}{ccc} \mathbb{R}^A & \xleftarrow{f^*} & \mathbb{R}^B \\ g_* \downarrow & & \downarrow h_* \\ \mathbb{R}^C & \xleftarrow{k^*} & \mathbb{R}^D \end{array}$$

Proof. Choose $v \in \mathbb{R}^B$ and $c \in C$. Then

$$(g_*f^*(v))(c) = \sum_{a:g(a)=c} v(f(a)),$$

$$(k^*h_*(v))(c) = \sum_{b:h(b)=k(c)} v(b),$$

so to show $g_*f^* = k^*h_*$ it suffices to show that f restricts to a bijection

$$f: \{a \in A : g(a) = c\} \xrightarrow{\sim} \{b \in B : h(b) = k(c)\}.$$

On the one hand, if $a \in A$ has $g(a) = c$ then $b = f(a)$ has $h(b) = h(f(a)) = k(g(a)) = k(c)$, so the above map is well-defined. On the other hand, if $b \in B$ has $h(b) = k(c)$, then by the definition of pullback there exists a unique $a \in A$ such that $f(a) = b$ and $g(a) = c$, so the above map is a bijection. \square

Theorem 4.4. *There exists a double category $\mathbb{M}\mathbf{ark}$ as defined above.*

Proof. Let $\mathbb{M}\mathbf{ark}_0$, the ‘category of objects’, consist of finite sets and functions. Let $\mathbb{M}\mathbf{ark}_1$ the ‘category of arrows’, consist of open Markov processes and morphisms between these:

$$\begin{array}{ccccc} S & \xrightarrow{i_1} & (X, H) & \xleftarrow{o_1} & T \\ \downarrow f & & \downarrow p & & \downarrow g \\ S' & \xrightarrow{i'_1} & (X', H') & \xleftarrow{o'_1} & T' \end{array}$$

To make $\mathbb{M}\mathbf{ark}$ into a double category we need to specify the identity-assigning functor

$$u: \mathbb{M}\mathbf{ark}_0 \rightarrow \mathbb{M}\mathbf{ark}_1,$$

the source and target functors

$$s, t: \mathbb{M}\mathbf{ark}_1 \rightarrow \mathbb{M}\mathbf{ark}_0,$$

and the composition functor

$$\odot: \mathbb{M}\mathbf{ark}_1 \times_{\mathbb{M}\mathbf{ark}_0} \mathbb{M}\mathbf{ark}_1 \rightarrow \mathbb{M}\mathbf{ark}_1.$$

These are given as follows.

For a finite set S , $u(S)$ is given by

$$S \xrightarrow{1_S} (S, 0_S) \xleftarrow{1_S} S$$

where 0_S is the zero operator from \mathbb{R}^S to \mathbb{R}^S . For a map $f: S \rightarrow S'$ between finite sets, $u(f)$ is given by

$$\begin{array}{ccccc} S & \longrightarrow & (S, 0_S) & \longleftarrow & S \\ \downarrow f & & \downarrow f & & \downarrow f \\ S' & \longrightarrow & (S', 0_{S'}) & \longleftarrow & S' \end{array}$$

The source and target functors s and t map a Markov process $S \xrightarrow{i} (X, H) \xleftarrow{o} T$ to S and T , respectively, and they map a morphism of open Markov processes

$$\begin{array}{ccccc} S & \xrightarrow{i_1} & (X, H) & \xleftarrow{o_1} & T \\ \downarrow f & & \downarrow p & & \downarrow g \\ S' & \xrightarrow{i'_1} & (X', H') & \xleftarrow{o'_1} & T' \end{array}$$

to $f: S \rightarrow S'$ and $g: T \rightarrow T'$, respectively. The composition functor \odot maps the pair of open Markov processes

$$S \xrightarrow{i_1} (X, H) \xleftarrow{o_1} T \quad T \xrightarrow{i_2} (Y, G) \xleftarrow{o_2} U$$

to their composite

$$S \xrightarrow{j_{i_1}} (X +_T Y, H \odot G) \xleftarrow{k_{o_2}} U$$

defined as in Eq. (1), and it maps the pair of morphisms of open Markov processes

$$\begin{array}{ccccc} S & \xrightarrow{i_1} & (X, H) & \xleftarrow{o_1} & T & T & \xrightarrow{i_2} & (Y, G) & \xleftarrow{o_2} & U \\ \downarrow f & & \downarrow p & & \downarrow g & \downarrow g & & \downarrow q & & \downarrow h \\ S' & \xrightarrow{i'_1} & (X', H') & \xleftarrow{o'_1} & T' & T' & \xrightarrow{i'_2} & (Y', G') & \xleftarrow{o'_2} & U' \end{array}$$

to their horizontal composite as defined as in Lemma 4.2.

It is easy to check that u , s and t are functors. To prove that \odot is a functor, the main thing we need to check is the interchange law. Suppose we have four morphisms of open Markov processes as follows:

$$\begin{array}{ccccc} S & \longrightarrow & (X, H) & \longleftarrow & T & T & \longrightarrow & (Y, G) & \longleftarrow & U \\ \downarrow f & & \downarrow p & & \downarrow g & \downarrow g & & \downarrow q & & \downarrow h \\ S' & \longrightarrow & (X', H') & \longleftarrow & T' & T' & \longrightarrow & (Y', G') & \longleftarrow & U' \\ \\ S' & \longrightarrow & (X', H') & \longleftarrow & T' & T' & \longrightarrow & (Y', G') & \longleftarrow & U' \\ \downarrow f' & & \downarrow p' & & \downarrow g' & \downarrow g' & & \downarrow q' & & \downarrow h' \\ S'' & \longrightarrow & (X'', H'') & \longleftarrow & T'' & T'' & \longrightarrow & (Y'', G'') & \longleftarrow & U'' \end{array}$$

Composing horizontally gives

$$\begin{array}{ccccc}
 S & \longrightarrow & (X +_T Y, H \odot G) & \longleftarrow & U \\
 \downarrow f & & \downarrow p +_g q & & \downarrow h \\
 S' & \longrightarrow & (X' +_{T'} Y', H' \odot G') & \longleftarrow & U'
 \end{array}$$

$$\begin{array}{ccccc}
 S' & \longrightarrow & (X' +_{T'} Y', H' \odot G') & \longleftarrow & U' \\
 \downarrow f' & & \downarrow p' +_{g'} q' & & \downarrow h' \\
 S'' & \longrightarrow & (X'' +_{T''} Y'', H'' \odot G'') & \longleftarrow & U''
 \end{array}$$

and then composing vertically gives

$$\begin{array}{ccccc}
 S & \longrightarrow & (X +_T Y, H \odot G) & \longleftarrow & U \\
 \downarrow f' \circ f & & \downarrow (p' +_{g'} q') \circ (p +_g q) & & \downarrow h' \circ h \\
 S'' & \longrightarrow & (X'' +_{T''} Y'', H'' \odot G'') & \longleftarrow & U''
 \end{array}$$

Composing vertically gives

$$\begin{array}{ccccc}
 S & \longrightarrow & (X, H) & \longleftarrow & T \\
 \downarrow f' \circ f & & \downarrow p' \circ p & & \downarrow g' \circ g \\
 S'' & \longrightarrow & (X'', H'') & \longleftarrow & T''
 \end{array}
 \quad
 \begin{array}{ccccc}
 T & \longrightarrow & (Y, G) & \longleftarrow & U \\
 \downarrow g' \circ g & & \downarrow q' \circ q & & \downarrow h' \circ h \\
 T'' & \longrightarrow & (Y'', G'') & \longleftarrow & U''
 \end{array}$$

and then composing horizontally gives

$$\begin{array}{ccccc}
 S & \longrightarrow & (X +_T Y, H \odot G) & \longleftarrow & U \\
 \downarrow f' \circ f & & \downarrow (p' \circ p) +_{(g' \circ g)} (q' \circ q) & & \downarrow h' \circ h \\
 S'' & \longrightarrow & (X'' +_{T''} Y'', H'' \odot G'') & \longleftarrow & U''
 \end{array}$$

The only apparent difference between the two results is the map in the middle: one has $(p' +_{g'} q') \circ (p +_g q)$ while the other has $(p' \circ p) +_{(g' \circ g)} (q' \circ q)$. But these are in fact the same map, so the interchange law holds.

The functors u , s , t and \circ obey the necessary relations

$$s \circ u = 1 = t \circ u,$$

and the relations saying that the source and target of a composite behave as they should. Lastly, we have three natural isomorphisms: the associator, left unitor, and right unitor, which arise from the corresponding natural isomorphisms for the double category of finite sets, functions, cospans of finite sets, and maps of cospans. The triangle and pentagon equations hold in \mathbf{Mark} because they do in this simpler double category [12]. \square

Next we give \mathbf{Mark} a symmetric monoidal structure. We call the tensor product ‘addition’. Given objects $S, S' \in \mathbf{Mark}_0$ we define their sum $S + S'$ using a chosen coproduct in \mathbf{FinSet} . The unit for this tensor product in \mathbf{Mark}_0 is the empty set. We can similarly define the sum of morphisms in \mathbf{Mark}_0 , since given maps $f: S \rightarrow T$ and $f': S' \rightarrow T'$ there is a natural map $f + f': S + S' \rightarrow T + T'$. Given two objects in \mathbf{Mark}_1 :

$$S_1 \xrightarrow{i_1} (X_1, H_1) \xleftarrow{o_1} T_1 \quad S_2 \xrightarrow{i_2} (X_2, H_2) \xleftarrow{o_2} T_2$$

we define their sum to be

$$S_1 + S_2 \xrightarrow{i_1 + i_2} (X_1 + X_2, H_1 \oplus H_2) \xleftarrow{o_1 + o_2} T_1 + T_2$$

where $H_1 \oplus H_2: \mathbb{R}^{X_1 + X_2} \rightarrow \mathbb{R}^{X_1 + X_2}$ is the direct sum of the operators H_1 and H_2 . The unit for this tensor product in \mathbf{Mark}_1 is $\emptyset \rightarrow (\emptyset, 0_\emptyset) \leftarrow \emptyset$ where $0_\emptyset: \mathbb{R}^\emptyset \rightarrow \mathbb{R}^\emptyset$ is the zero operator. Finally, given two morphisms in \mathbf{Mark}_1 :

$$\begin{array}{ccc} S_1 \xrightarrow{i_1} (X_1, H_1) \xleftarrow{o_1} T_1 & & S_2 \xrightarrow{i_2} (X_2, H_2) \xleftarrow{o_2} T_2 \\ \downarrow f_1 & p_1 \downarrow & \downarrow f_2 \\ S'_1 \xrightarrow{i'_1} (X'_1, H'_1) \xleftarrow{o'_1} T'_1 & & S'_2 \xrightarrow{i'_2} (X'_2, H'_2) \xleftarrow{o'_2} T'_2 \\ \downarrow g_1 & & \downarrow g_2 \end{array}$$

we define their sum to be

$$\begin{array}{ccc} S_1 + S_2 \xrightarrow{i_1 + i_2} (X_1 + X_2, H_1 \oplus H_2) \xleftarrow{o_1 + o_2} T_1 + T_2 & & \\ \downarrow f_1 + f_2 & p_1 + p_2 \downarrow & \downarrow g_1 + g_2 \\ S'_1 + S'_2 \xrightarrow{i'_1 + i'_2} (X'_1 + X'_2, H'_1 \oplus H'_2) \xleftarrow{o'_1 + o'_2} T'_1 + T'_2 & & \end{array}$$

We complete the description of \mathbf{Mark} as a symmetric monoidal double category in the proof of this theorem:

Theorem 4.5. *The double category \mathbf{Mark} can be given a symmetric monoidal structure with the above properties.*

Proof. First we complete the description of \mathbf{Mark}_0 and \mathbf{Mark}_1 as symmetric monoidal categories. The symmetric monoidal category \mathbf{Mark}_0 is just the category of finite sets with a chosen coproduct of each pair of finite sets providing the symmetric monoidal structure. We have described the tensor product in \mathbf{Mark}_1 , which we call ‘addition’, so now we need to introduce the associator, unitors, and braiding, and check that they make \mathbf{Mark}_1 into a symmetric monoidal category.

Given three objects in $\mathbb{M}\mathbf{ark}_1$

$$S_1 \longrightarrow (X_1, H_1) \longleftarrow T_1 \quad S_2 \longrightarrow (X_2, H_2) \longleftarrow T_2 \quad S_3 \longrightarrow (X_3, H_3) \longleftarrow T_3$$

tensoring the first two and then the third results in

$$(S_1 + S_2) + S_3 \longrightarrow ((X_1 + X_2) + X_3, (H_1 \oplus H_2) \oplus H_3) \longleftarrow (T_1 + T_2) + T_3$$

whereas tensoring the last two and then the first results in

$$S_1 + (S_2 + S_3) \longrightarrow (X_1 + (X_2 + X_3), H_1 \oplus (H_2 \oplus H_3)) \longleftarrow T_1 + (T_2 + T_3).$$

The associator for $\mathbb{M}\mathbf{ark}_1$ is then given as follows:

$$\begin{array}{ccc} (S_1 + S_2) + S_3 \longrightarrow ((X_1 + X_2) + X_3, (H_1 \oplus H_2) \oplus H_3) \longleftarrow (T_1 + T_2) + T_3 & & \\ \downarrow a & & \downarrow a \\ S_1 + (S_2 + S_3) \longrightarrow (X_1 + (X_2 + X_3), H_1 \oplus (H_2 \oplus H_3)) \longleftarrow T_1 + (T_2 + T_3) & & \downarrow a \end{array}$$

where a is the associator in $(\mathbf{FinSet}, +)$. If we abbreviate an object $S \rightarrow (X, H) \leftarrow T$ of $\mathbb{M}\mathbf{ark}_1$ as (X, H) , and denote the associator for $\mathbb{M}\mathbf{ark}_1$ as α , the pentagon identity says that this diagram commutes:

$$\begin{array}{ccc} & ((X_1, H_1) \oplus (X_2, H_2)) \oplus ((X_3, H_3) \oplus (X_4, H_4)) & \\ & \nearrow \alpha & \searrow \alpha \\ ((X_1, H_1) \oplus (X_2, H_2)) \oplus (X_3, H_3) \oplus (X_4, H_4) & & (X_1, H_1) \oplus ((X_2, H_2) \oplus ((X_3, H_3) \oplus (X_4, H_4))) \\ \downarrow \alpha \oplus 1_{(X_4, H_4)} & & \uparrow 1_{(X_1, H_1)} \oplus \alpha \\ ((X_1, H_1) \oplus ((X_2, H_2) \oplus (X_3, H_3))) \oplus (X_4, H_4) & \xrightarrow{\alpha} & (X_1, H_1) \oplus (((X_2, H_2) \oplus (X_3, H_3)) \oplus (X_4, H_4)) \end{array}$$

which is clearly true. Recall that the monoidal unit for $\mathbb{M}\mathbf{ark}_1$ is given by $\emptyset \rightarrow (\emptyset, 0_\emptyset) \leftarrow \emptyset$. The left and right unitors for $\mathbb{M}\mathbf{ark}_1$, denoted λ and ρ , are given respectively by the following 2-morphisms:

$$\begin{array}{ccc} \emptyset + S \longrightarrow (\emptyset + X, 0_\emptyset \oplus H) \longleftarrow \emptyset + T & & S + \emptyset \longrightarrow (X + \emptyset, H \oplus 0_\emptyset) \longleftarrow T + \emptyset \\ \downarrow \ell & & \downarrow r \\ S \longrightarrow (X, H) \longleftarrow T & & S \longrightarrow (X, H) \longleftarrow T \end{array}$$

where ℓ and r are the left and right unitors in \mathbf{FinSet} . The left and right unitors and associator for $\mathbb{M}\mathbf{ark}_1$ satisfy the triangle identity:

$$\begin{array}{ccc} & (X, H) \oplus (Y, G) & \\ & \nearrow \rho \oplus 1 & \nwarrow 1 \oplus \lambda \\ ((X, H) \oplus (\emptyset, 0_\emptyset)) \oplus (Y, G) & \xrightarrow{\alpha} & (X, H) \oplus ((\emptyset, 0_\emptyset) \oplus (Y, G)). \end{array}$$

The braiding in $\mathbb{M}\mathbf{ark}_1$ is given as follows:

$$\begin{array}{ccccc}
S_1 + S_2 & \longrightarrow & (X_1, H_1) \oplus (X_2, H_2) & \longleftarrow & T_1 + T_2 \\
\downarrow b_{S_1, S_2} & & \downarrow b_{X_1, X_2} & & \downarrow b_{T_1, T_2} \\
S_2 + S_1 & \longrightarrow & (X_2, H_2) \oplus (X_1, H_1) & \longleftarrow & T_2 + T_1
\end{array}$$

where b is the braiding in $(\mathbf{FinSet}, +)$. It is easy to check that the braiding in $\mathbb{M}\mathbf{ark}_1$ is its own inverse and obeys the hexagon identity, making $\mathbb{M}\mathbf{ark}_1$ into a symmetric monoidal category.

The source and target functors $s, t: \mathbb{M}\mathbf{ark}_1 \rightarrow \mathbb{M}\mathbf{ark}_0$ are strict symmetric monoidal functors, as required. To make $\mathbb{M}\mathbf{ark}$ into a symmetric monoidal double category we must also give it two other pieces of structure. One, called χ , says how the composition of horizontal 1-cells interacts with the tensor product in the category of arrows. The other, called μ , says how the identity-assigning functor u relates the tensor product in the category of objects to the tensor product in the category of arrows. We now define these two isomorphisms.

Given horizontal 1-cells

$$\begin{array}{ll}
S_1 \longrightarrow (X_1, H_1) \longleftarrow T_1 & T_1 \longrightarrow (Y_1, G_1) \longleftarrow U_1 \\
S_2 \longrightarrow (X_2, H_2) \longleftarrow T_2 & T_2 \longrightarrow (Y_2, G_2) \longleftarrow U_2
\end{array}$$

the horizontal composites of the top two and the bottom two are given, respectively, by

$$S_1 \rightarrow (X_1 +_{T_1} Y_1, H_1 \odot G_1) \leftarrow U_1 \quad S_2 \rightarrow (X_2 +_{T_2} Y_2, H_2 \odot G_2) \leftarrow U_2$$

‘Adding’ the left two and right two, respectively, we obtain

$$S_1 + S_2 \rightarrow (X_1 + X_2, H_1 \oplus H_2) \leftarrow T_1 + T_2 \quad T_1 + T_2 \rightarrow (Y_1 + Y_2, G_1 \oplus G_2) \leftarrow U_1 + U_2$$

Thus the sum of the horizontal composites is

$$S_1 + S_2 \longrightarrow ((X_1 +_{T_1} Y_1) + (X_2 +_{T_2} Y_2), (H_1 \odot G_1) \oplus (H_2 \odot G_2)) \longleftarrow U_1 + U_2$$

while the horizontal composite of the sums is

$$S_1 + S_2 \longrightarrow ((X_1 + X_2) +_{T_1 + T_2} (Y_1 + Y_2), (H_1 \oplus H_2) \odot (G_1 \oplus G_2)) \longleftarrow U_1 + U_2.$$

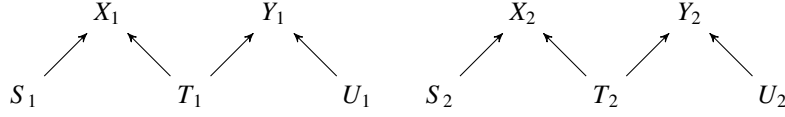
The required globular 2-isomorphism χ between these is

$$\begin{array}{ccccc}
S_1 + S_2 & \longrightarrow & ((X_1, H_1) \odot (Y_1, G_1)) \oplus ((X_2, H_2) \odot (Y_2, G_2)) & \longleftarrow & U_1 + U_2 \\
\downarrow 1_{S_1 + S_2} & & \downarrow \hat{\chi} & & \downarrow 1_{U_1 + U_2} \\
S_1 + S_2 & \longrightarrow & ((X_1, H_1) \oplus (X_2, H_2)) \odot ((Y_1, G_1) \oplus (Y_2, G_2)) & \longleftarrow & U_1 + U_2
\end{array}$$

where $\hat{\chi}$ is the bijection

$$\hat{\chi}: (X_1 +_{T_1} Y_1) + (X_2 +_{T_2} Y_2) \rightarrow (X_1 + X_2) +_{T_1 + T_2} (Y_1 + Y_2)$$

obtained from taking the colimit of the diagram



in two different ways. We call χ ‘globular’ because its source and target 1-morphisms are identities.

For the other globular 2-isomorphism, if S and T are finite sets, then $u(S + T)$ is given by

$$S + T \xrightarrow{1_{S+T}} (S + T, 0_{S+T}) \xleftarrow{1_{S+T}} S + T$$

while $u(S) \oplus u(T)$ is given by

$$S + T \xrightarrow{1_S + 1_T} (S + T, 0_S \oplus 0_T) \xleftarrow{1_S + 1_T} S + T$$

so there is a globular 2-isomorphism μ between these, namely the identity 2-morphism. All the commutative diagrams in the definition of symmetric monoidal double category [23] can be checked in a straightforward way. \square

5. BLACK-BOXING FOR OPEN MARKOV PROCESSES

The general idea of ‘black-boxing’ is to take a system and forget everything except the relation between its inputs and outputs, as if we had placed it in a black box and were unable to see its inner workings. Previous work of Pollard and the first author [6] constructed a black-boxing functor $\blacksquare: \text{Dynam} \rightarrow \text{SemiAlgRel}$ where Dynam is a category of finite sets and ‘open dynamical systems’ and SemiAlgRel is a category of finite-dimensional real vector spaces and relations defined by polynomials and inequalities. When we black-box such an open dynamical system, we obtain the relation between inputs and outputs that holds in steady state.

A special case of an open dynamical system is an open Markov process as defined in this paper. Thus, we could restrict the black-boxing functor $\blacksquare: \text{Dynam} \rightarrow \text{SemiAlgRel}$ to a category Mark with finite sets as objects and open Markov processes as morphisms. Since the steady state behavior of a Markov process is *linear*, we would get a functor $\blacksquare: \text{Mark} \rightarrow \text{LinRel}$ where LinRel is the category of finite-dimensional real vector spaces and *linear* relations [3]. However, we will go further and define black-boxing on the double category $\mathbb{M}\text{ark}$. This will exhibit the relation between black-boxing and morphisms between open Markov processes.

To do this, we promote LinRel to a double category $\mathbb{L}\text{inRel}$ with:

- (i) finite-dimensional real vector spaces U, V, W, \dots as objects,
- (ii) linear maps $f: V \rightarrow W$ as vertical 1-morphisms from V to W ,
- (iii) linear relations $R \subseteq V \oplus W$ as horizontal 1-cells from V to W ,
- (iv) squares

$$\begin{array}{ccc}
 V_1 & \xrightarrow{R \subseteq V_1 \oplus V_2} & V_2 \\
 \downarrow f & & \downarrow g \\
 W_1 & \xrightarrow{S \subseteq W_1 \oplus W_2} & W_2
 \end{array}$$

obeying $(f \oplus g)R \subseteq S$ as 2-morphisms.

The last item deserves some explanation. A preorder is a category such that for any pair of objects x, y there exists at most one morphism $\alpha: x \rightarrow y$. When such a morphism exists we usually write $x \leq y$. Similarly there is a kind of double category for which given any ‘frame’

$$\begin{array}{ccc} A & \xrightarrow{M} & B \\ f \downarrow & & \downarrow g \\ C & \xrightarrow{N} & D \end{array}$$

there exists at most one 2-morphism

$$\begin{array}{ccc} A & \xrightarrow{M} & B \\ f \downarrow & \Downarrow \alpha & \downarrow g \\ C & \xrightarrow{N} & D \end{array}$$

filling this frame. For lack of a better term let us call this a **degenerate** double category. Item (iv) implies that $\mathbb{L}\mathbf{inRel}$ will be degenerate in this sense.

In $\mathbb{L}\mathbf{inRel}$, composition of vertical 1-morphisms is the usual composition of linear maps, while composition of horizontal 1-cells is the usual composition of linear relations. Since composition of linear relations obeys the associative and unit laws strictly, $\mathbb{L}\mathbf{inRel}$ will be a *strict* double category. Since $\mathbb{L}\mathbf{inRel}$ is degenerate, there is at most one way to define the vertical composite of 2-morphisms

$$\begin{array}{ccc} U_1 & \xrightarrow{R \subseteq U_1 \oplus U_2} & U_2 \\ f \downarrow & \Downarrow \alpha & \downarrow g \\ V_1 & \xrightarrow{S \subseteq V_1 \oplus V_2} & V_2 \\ f' \downarrow & \Downarrow \beta & \downarrow g' \\ W_1 & \xrightarrow{T \subseteq W_1 \oplus W_2} & W_2 \end{array} = \begin{array}{ccc} U_1 & \xrightarrow{R \subseteq U_1 \oplus U_2} & U_2 \\ f'f \downarrow & \Downarrow \beta\alpha & \downarrow g'g \\ W_1 & \xrightarrow{T \subseteq W_1 \oplus W_2} & W_2 \end{array}$$

so we need merely check that a 2-morphism $\beta\alpha$ filling the frame at right exists. This amounts to noting that

$$(f \oplus g)R \subseteq S, (f' \oplus g')S \subseteq T \implies (f' \oplus g')(f \oplus g)R \subseteq T.$$

Similarly, there is at most one way to define the horizontal composite of 2-morphisms

$$\begin{array}{ccc}
 V_1 & \xrightarrow{R \subseteq V_1 \oplus V_2} & V_2 & \xrightarrow{R' \subseteq V_2 \oplus V_3} & V_3 \\
 \downarrow f & & \downarrow g & & \downarrow h \\
 W_1 & \xrightarrow{S \subseteq W_1 \oplus W_2} & W_2 & \xrightarrow{S' \subseteq W_2 \oplus W_3} & W_3
 \end{array}
 \quad \Downarrow \alpha
 \quad =
 \quad
 \begin{array}{ccc}
 V_1 & \xrightarrow{R'R \subseteq V_1 \oplus V_3} & V_3 \\
 \downarrow f & & \downarrow h \\
 W_1 & \xrightarrow{S'S \subseteq W_1 \oplus W_3} & W_3
 \end{array}
 \quad \Downarrow \alpha' \circ \alpha$$

so we need merely check that a filler $\alpha' \circ \alpha$ exists, which amounts to noting that

$$(f \oplus g)R \subseteq S, (g \oplus h)R' \subseteq S' \implies (f \oplus h)(R'R) \subseteq S'S.$$

Theorem 5.1. *There exists a strict double category $\mathbb{L}\mathbf{inRel}$ with the above properties.*

Proof. The category of objects $\mathbb{L}\mathbf{inRel}_0$ has finite-dimensional real vector spaces as objects and linear maps as morphisms. The category of arrows $\mathbb{L}\mathbf{inRel}_1$ has linear relations as objects and squares

$$\begin{array}{ccc}
 V_1 & \xrightarrow{R \subseteq V_1 \oplus V_2} & V_2 \\
 \downarrow f & & \downarrow g \\
 W_1 & \xrightarrow{S \subseteq W_1 \oplus W_2} & W_2
 \end{array}$$

with $(f \oplus g)R \subseteq S$ as morphisms. The source and target functors $s, t: \mathbb{L}\mathbf{inRel}_1 \rightarrow \mathbb{L}\mathbf{inRel}_0$ are clear. The identity-assigning functor $u: \mathbb{L}\mathbf{inRel}_0 \rightarrow \mathbb{L}\mathbf{inRel}_1$ sends a finite-dimensional real vector space V to the identity map 1_V and a linear map $f: V \rightarrow W$ to the unique 2-morphism

$$\begin{array}{ccc}
 V & \xrightarrow{1_V} & V \\
 \downarrow f & & \downarrow f \\
 W & \xrightarrow{1_W} & W.
 \end{array}$$

The composition functor $\odot: \mathbb{L}\mathbf{inRel}_1 \times_{\mathbb{L}\mathbf{inRel}_0} \mathbb{L}\mathbf{inRel}_1 \rightarrow \mathbb{L}\mathbf{inRel}_1$ acts on objects by the usual composition of linear relations, and it acts on 2-morphisms by horizontal composition as described above. These functors can be shown to obey all the axioms of a double category. In particular, because $\mathbb{L}\mathbf{inRel}$ is degenerate, all the required equations between 2-morphisms, such as the interchange law, hold automatically. \square

Next we make $\mathbb{L}\mathbf{inRel}$ into a symmetric monoidal double category. To do this, we first give $\mathbb{L}\mathbf{inRel}_0$ the structure of a symmetric monoidal category. We do this using a specific choice of direct sum for each pair of finite-dimensional real vector spaces as the tensor product, and a specific 0-dimensional vector space as the unit object. Then we give $\mathbb{L}\mathbf{inRel}_1$ a symmetric monoidal structure as follows. Given linear relations $R_1 \subseteq V_1 \oplus W_1$ and $R_2 \subseteq V_2 \oplus W_2$, we define their direct sum by

$$R_1 \oplus R_2 = \{(v_1, v_2, w_1, w_2) : (v_1, w_1) \in R_1, (v_2, w_2) \in R_2\} \subseteq V_1 \oplus V_2 \oplus W_1 \oplus W_2.$$

Given two 2-morphisms in $\mathbb{L}\mathbf{inRel}_1$:

$$\begin{array}{ccc} V_1 & \xrightarrow{R \subseteq V_1 \oplus V_2} & V_2 \\ \downarrow f & \Downarrow \alpha & \downarrow g \\ W_1 & \xrightarrow{S \subseteq W_1 \oplus W_2} & W_2 \end{array} \quad \begin{array}{ccc} V'_1 & \xrightarrow{R' \subseteq V'_1 \oplus V'_2} & V'_2 \\ \downarrow f' & \Downarrow \alpha' & \downarrow g' \\ W'_1 & \xrightarrow{S' \subseteq W'_1 \oplus W'_2} & W'_2 \end{array}$$

there is at most one way to define their direct sum

$$\begin{array}{ccc} V_1 \oplus V'_1 & \xrightarrow{R \oplus R' \subseteq V_1 \oplus V'_1 \oplus V_2 \oplus V'_2} & V_2 \oplus V'_2 \\ \downarrow f \oplus f' & \Downarrow \alpha \oplus \alpha' & \downarrow g \oplus g' \\ W_1 \oplus W'_1 & \xrightarrow{S \oplus S' \subseteq W_1 \oplus W'_1 \oplus W_2 \oplus W'_2} & W_2 \oplus W'_2 \end{array}$$

because $\mathbb{L}\mathbf{inRel}$ is degenerate. To show that $\alpha \oplus \alpha'$ exists, we need merely note that

$$(f \oplus g)R \subseteq S, (f' \oplus g')R' \subseteq S' \implies (f \oplus f' \oplus g \oplus g')(R \oplus R') \subseteq S \oplus S'.$$

Theorem 5.2. *The double category $\mathbb{L}\mathbf{inRel}$ can be given the structure of a symmetric monoidal double category with the above properties.*

Proof. We have described $\mathbb{L}\mathbf{inRel}_0$ and $\mathbb{L}\mathbf{inRel}_1$ as symmetric monoidal categories. The source and target functors $s, t: \mathbb{L}\mathbf{inRel}_1 \rightarrow \mathbb{L}\mathbf{inRel}_0$ are strict symmetric monoidal functors. The required globular 2-isomorphisms χ and μ are defined as follows. Given four horizontal 1-cells

$$\begin{aligned} R_1 &\subseteq U_1 \oplus V_1, & R_2 &\subseteq V_1 \oplus W_1, \\ S_1 &\subseteq U_2 \oplus V_2, & S_2 &\subseteq V_2 \oplus W_2, \end{aligned}$$

the globular 2-isomorphism $\chi: (R_2 \oplus S_2)(R_1 \oplus S_1) \Rightarrow (R_2 R_1) \oplus (S_2 S_1)$ is the identity 2-morphism

$$\begin{array}{ccc} U_1 \oplus U_2 & \xrightarrow{(R_2 \oplus S_2)(R_1 \oplus S_1)} & W_1 \oplus W_2 \\ \downarrow 1 & & \downarrow 1 \\ U_1 \oplus U_2 & \xrightarrow{(R_2 R_1) \oplus (S_2 S_1)} & W_1 \oplus W_2. \end{array}$$

The globular 2-isomorphism $\mu: u(V \oplus W) \Rightarrow u(V) \oplus u(W)$ is the identity 2-morphism

$$\begin{array}{ccc} V \oplus W & \xrightarrow{1_{V \oplus W}} & V \oplus W \\ \downarrow 1 & & \downarrow 1 \\ V \oplus W & \xrightarrow{1_V \oplus 1_W} & V \oplus W. \end{array}$$

All the commutative diagrams in the definition of symmetric monoidal double category [23] can be checked straightforwardly. In particular, all diagrams of 2-morphisms commute automatically because $\mathbb{L}\mathbf{inRel}$ is degenerate. \square

This sets the stage for defining the symmetric monoidal double functor $\blacksquare: \mathbf{Mark} \rightarrow \mathbb{L}\mathbf{inRel}$. We start as follows:

- (i) On objects: for a finite set S , we define $\blacksquare(S)$ to be the vector space $\mathbb{R}^S \oplus \mathbb{R}^S$.
- (ii) On horizontal 1-cells: for an open Markov process $S \xrightarrow{i} (X, H) \xleftarrow{o} T$, we define its black-boxing as in Def. 2.7:

$$\blacksquare(S \xrightarrow{i} (X, H) \xleftarrow{o} T) =$$

$$\{(i^*(v), I, o^*(v), O) : v \in \mathbb{R}^X, I \in \mathbb{R}^S, O \in \mathbb{R}^T \text{ and } H(v) + i_*(I) - o_*(O) = 0\}.$$

- (iii) On vertical 1-morphisms: for a map $f: S \rightarrow S'$, we define $\blacksquare(f): \mathbb{R}^S \oplus \mathbb{R}^S \rightarrow \mathbb{R}^{S'} \oplus \mathbb{R}^{S'}$ to be the linear map $f_* \oplus f_*$.

What remains to be done is define how \blacksquare acts on 2-morphisms of \mathbf{Mark} . This describes the relation between steady state input and output concentrations and flows of a coarse-grained open Markov process in terms of the corresponding relation for the original process:

Lemma 5.3. *Given a 2-morphism*

$$\begin{array}{ccccc} S & \xrightarrow{i} & (X, H) & \xleftarrow{o} & T \\ \downarrow f & & \downarrow p & & \downarrow g \\ S' & \xrightarrow{i'} & (X', H') & \xleftarrow{o'} & T' \end{array}$$

in \mathbf{Mark} , there exists a unique 2-morphism

$$\begin{array}{ccc} \blacksquare(S) & \xrightarrow{\blacksquare(S \xrightarrow{i} (X, H) \xleftarrow{o} T)} & \blacksquare(T) \\ \downarrow \blacksquare(f) & & \downarrow \blacksquare(g) \\ \blacksquare(S') & \xrightarrow{\blacksquare(S' \xrightarrow{i'} (X', H') \xleftarrow{o'} T')} & \blacksquare(T') \end{array}$$

in $\mathbb{L}\mathbf{inRel}$.

Proof. Since $\mathbb{L}\mathbf{inRel}$ is degenerate, if there exists a 2-morphism of the claimed kind it is automatically unique. To prove that such a 2-morphism exists, it suffices to prove

$$(i^*(v), I, o^*(v), O) \in V \implies (f_* i^*(v), f_*(I), g_* o^*(v), g_*(O)) \in W$$

where

$$V = \blacksquare(S \xrightarrow{i} (X, H) \xleftarrow{o} T) =$$

$$\{(i^*(v), I, o^*(v), O) : v \in \mathbb{R}^X, I \in \mathbb{R}^S, O \in \mathbb{R}^T \text{ and } H(v) + i_*(I) - o_*(O) = 0\}$$

and

$$W = \blacksquare(S' \xrightarrow{i'} (X', H') \xleftarrow{o'} T') =$$

$$\{(i'^*(v'), I', o'^*(v'), O') : v' \in \mathbb{R}^{X'}, I' \in \mathbb{R}^{S'}, O' \in \mathbb{R}^{T'} \text{ and } H'(v') + i'_*(I') - o'_*(O') = 0\}.$$

To do this, assume $(i^*(v), I, o^*(v), O) \in V$, which implies that

$$H(v) + i_*(I) - o_*(O) = 0. \quad (2)$$

Since the commuting squares in α are pullbacks, Lemma 4.3 implies that

$$f_*i^* = i'^*p_*, \quad g_*o^* = o'^*p_*.$$

Thus

$$(f_*i^*(v), f_*(I), g_*o^*(v), g_*(O)) = (i'^*p_*(v), f_*(I), o'^*p_*(v), g_*(O))$$

and this is an element of W as desired if

$$H'p_*(v) + i'_*f_*(I) - o'_*g_*(O) = 0. \quad (3)$$

To prove Eq. (3), note that

$$\begin{aligned} H'p_*(v) + i'_*f_*(I) - o'_*g_*(O) &= p_*H(v) + p_*i_*(I) - p_*o_*(O) \\ &= p_*(H(v) + i_*(I) - o_*(O)) \end{aligned}$$

where in the first step we use the fact that the squares in α commute, together with the fact that $H'p_* = p_*H$. Thus, Eq. (2) implies Eq. (3). \square

The following result is a special case of a result by Pollard and the first author on black-boxing open dynamical systems [6]. To make this paper self-contained we adapt the proof to the case at hand:

Lemma 5.4. *The black-boxing of a composite of two open Markov processes equals the composite of their black-boxings.*

Proof. Consider composable open Markov processes

$$S \xrightarrow{i} (X, H) \xleftarrow{o} T, \quad T \xrightarrow{i'} (Y, G) \xleftarrow{o'} U.$$

To compose these, we first form the pushout

$$\begin{array}{ccccc} & & X +_T Y & & \\ & j \nearrow & & \nwarrow k & \\ & X & & Y & \\ i \nearrow & & & & \nwarrow o' \\ S & & T & & U \\ & \nwarrow o & \nearrow i' & & \end{array}$$

Then their composite is

$$S \xrightarrow{ji} (X +_T Y, H \odot G) \xleftarrow{ko'} U$$

where

$$H \odot G = j_*Hj^* + k_*Gk^*.$$

To prove that \blacksquare preserves composition, we first show that

$$\blacksquare(X +_T Y, H \odot G) \subseteq \blacksquare(Y, G) \blacksquare(X, H)$$

Thus, given

$$(i^*(v), I, o^*(v), O) \in \blacksquare(X, H), \quad (i'^*(v'), I', o'^*(v'), O') \in \blacksquare(Y, G)$$

with

$$o^*(v) = i'^*(v'), \quad O = O'$$

we need to prove that

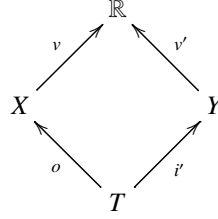
$$(i^*(v), I, o'^*(v'), O') \in \blacksquare(X +_T Y, H \odot G).$$

To do this, it suffices to find probabilities $w \in \mathbb{R}^{X+T Y}$ such that

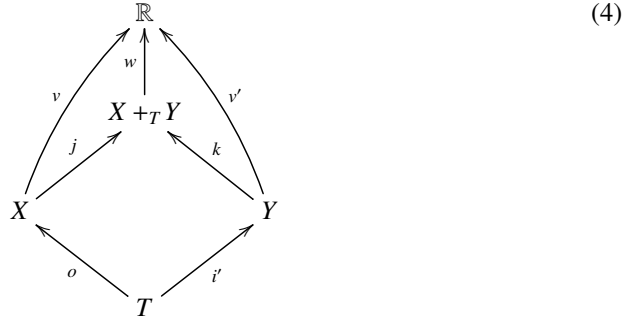
$$(i^*(v), I, o'^*(v'), O') = ((ji)^*(w), I, (ko')^*(w), O')$$

and w is a steady state of $(X +_T Y, H \odot G)$ with inflows I and outflows O' .

Since $o^*(v) = i'^*(v')$, this diagram commutes:



so by the universal property of the pushout there is a unique map $w: X +_T Y \rightarrow \mathbb{R}$ such that this commutes:



This simply says that because the functions v and v' agree on the ‘overlap’ of our two open Markov processes, we can find a function w that restricts to v on X and v' on Y .

We now prove that w is a steady state of the composite open Markov process with inflows I and outflows O' :

$$(H \odot G)(w) + (ji)_*(I) - (ko')_*(O') = 0. \quad (5)$$

To do this we use the fact that v is a steady state of $S \xrightarrow{i} (X, H) \xleftarrow{o} T$ with inflows I and outflows O :

$$H(v) + i_*(I) - o_*(O) = 0 \quad (6)$$

and v' is a steady state of $T \xrightarrow{i'} (Y, G) \xleftarrow{o'} U$ with inflows I' and outflows O' :

$$G(v') + i'_*(I') - o'_*(O') = 0. \quad (7)$$

We push Eq. (6) forward along j , push Eq. (7) forward along k , and sum them:

$$j_*(H(v)) + (ji)_*(I) - (jo)_*(O) + k_*(G(v')) + (ki')_*(I') - (ko')_*(O') = 0.$$

Since $O = I'$ and $jo = ki'$, two terms cancel, leaving us with

$$j_*(H(v)) + (ji)_*(I) + k_*(G(v')) - (ko')_*(O') = 0.$$

Next we combine the terms involving the infinitesimal stochastic operators H and G , with the help of Eq. (4) and the definition of $H \odot G$:

$$\begin{aligned} j_*(H(v)) + k_*(G(v')) &= (j_*Hj^* + k_*Gk^*)(w) \\ &= (H \odot G)(w). \end{aligned} \quad (8)$$

This leaves us with

$$(H \odot G)(w) + (ji)_*(I) - (ko')_*(O') = 0$$

which is Eq. (5), precisely what we needed to show.

To finish showing that \blacksquare is a functor, we need to show that

$$\blacksquare(X +_T Y, H \odot G) \subseteq \blacksquare(Y, G) \blacksquare(X, H).$$

So, suppose we have

$$((ji)^*(w), I, (ko')^*(w), O') \in \blacksquare(X +_T Y, H \odot G).$$

We need to show

$$((ji)^*(w), I, (ko')^*(w), O') = (i^*(v), I, o'^*(v'), O') \quad (9)$$

where

$$(i^*(v), I, o^*(v), O) \in \blacksquare(X, H), \quad (i'^*(v'), I', o'^*(v'), O') \in \blacksquare(Y, G)$$

and

$$o^*(v) = i'^*(v'), \quad O = I'.$$

To do this, we begin by choosing

$$v = j^*(w), \quad v' = k^*(w).$$

This ensures that Eq. (9) holds, and since $jo = ki'$, it also ensures that

$$o^*(v) = (jo)^*(w) = (ki')^*(w) = i'^*(v').$$

To finish the job, we need to find an element $O = I' \in \mathbb{R}^T$ such that v is a steady state of (X, H) with inflows I and outflows O and v' is a steady state of (Y, G) with inflows I' and outflows O' . Of course, we are given the fact that w is a steady state of $(X +_T Y, H \odot G)$ with inflows I and outflows O' .

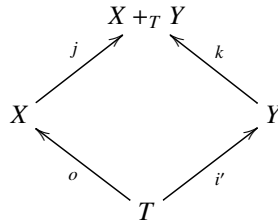
In short, we are given Eq. (5), and we seek $O = I'$ such that Eqs. (6) and (7) hold. Thanks to our choices of v and v' , we can use Eq. (8) and rewrite Eq. (5) as

$$j_*(H(v) + i_*(I)) + k_*(G(v') - o'_*(O')) = 0. \quad (10)$$

Eqs. (6) and (7) say that

$$\begin{aligned} H(v) + i_*(I) - o_*(O) &= 0 \\ G(v') + i'_*(I') - o'_*(O') &= 0. \end{aligned} \quad (11)$$

Now we use the fact that



is a pushout. Applying the ‘free vector space on a finite set’ functor, which preserves colimits, this implies that

$$\begin{array}{ccccc}
 & & \mathbb{R}^{X+TY} & & \\
 & \nearrow^{j_*} & & \nwarrow_{k_*} & \\
 \mathbb{R}^X & & & & \mathbb{R}^Y \\
 & \nwarrow_{o_*} & & \nearrow_{i'_*} & \\
 & & \mathbb{R}^T & &
 \end{array}$$

is a pushout in the category of vector spaces. Since a pushout is formed by taking first a coproduct and then a coequalizer, this implies that

$$\mathbb{R}^T \begin{array}{c} \xrightarrow{(o_*, 0)} \\ \xrightarrow{(0, i'_*)} \end{array} \mathbb{R}^X \oplus \mathbb{R}^Y \xrightarrow{j_* + k_*} \mathbb{R}^{X+TY}$$

is a coequalizer. Thus, the kernel of $j_* + k_*$ is the image of $(o_*, 0) - (0, i'_*)$. Eq. (10) says precisely that

$$(H(v) + i_*(I), G(v') - o'_*(O')) \in \ker(j_* + k_*).$$

Thus, it is in the image of $o_* - i'_*$. In other words, there exists some element $O = I' \in \mathbb{R}^T$ such that

$$(H(v) + i_*(I), G(v') - o'_*(O')) = (o_*(O), -i'_*(I')).$$

This says that Eqs. (6) and (7) hold, as desired. \square

This is the main result of this paper:

Theorem 5.5. *There exists a symmetric monoidal double functor $\blacksquare: \mathbf{Mark} \rightarrow \mathbf{LinRel}$ with the following behavior:*

- (i) *Objects:* \blacksquare sends any finite set S to the vector space $\mathbb{R}^S \oplus \mathbb{R}^S$.
- (ii) *Vertical 1-morphisms:* \blacksquare sends any map $f: S \rightarrow S'$ to the linear map $f_* \oplus f_*: \mathbb{R}^S \oplus \mathbb{R}^S \rightarrow \mathbb{R}^{S'} \oplus \mathbb{R}^{S'}$.
- (iii) *Horizontal 1-cells:* \blacksquare sends any open Markov process $S \xrightarrow{i} (X, H) \xleftarrow{o} T$ to the linear relation given in Def. 2.7:

$$\blacksquare(S \xrightarrow{i} (X, H) \xleftarrow{o} T) =$$

$$\{(i^*(v), I, o^*(v), O) : H(v) + i_*(I) - o_*(O) = 0 \text{ for some } I \in \mathbb{R}^S, v \in \mathbb{R}^X, O \in \mathbb{R}^T\}.$$

- (iv) *2-Morphisms:* \blacksquare sends any morphism of open Markov processes

$$\begin{array}{ccccc}
 S & \xrightarrow{i} & (X, H) & \xleftarrow{o} & T \\
 \downarrow f & & \downarrow p & & \downarrow g \\
 S' & \xrightarrow{i'} & (X', H') & \xleftarrow{o'} & T'
 \end{array}$$

to the 2-morphism in $\mathbb{L}\mathbf{inRel}$ given in Lemma 5.3:

$$\begin{array}{ccc}
 \blacksquare(S) & \xrightarrow{\blacksquare(S \xrightarrow{f} (X, H) \xleftarrow{e} T)} & \blacksquare(T) \\
 \blacksquare(f) \downarrow & & \downarrow \blacksquare(g) \\
 \blacksquare(S') & \xrightarrow{\blacksquare(S' \xrightarrow{f'} (X', H') \xleftarrow{e'} T')} & \blacksquare(T').
 \end{array}$$

Proof. First we must define functors $\blacksquare_0: \mathbb{M}\mathbf{ark}_0 \rightarrow \mathbb{L}\mathbf{inRel}_0$ and $\blacksquare_1: \mathbb{M}\mathbf{ark}_1 \rightarrow \mathbb{L}\mathbf{inRel}_1$. The functor \blacksquare_0 is defined on finite sets and maps between these as described in (i) and (ii) of the theorem statement, while \blacksquare_1 is defined on open Markov processes and morphisms between these as described in (iii) and (iv). Lemma 5.3 shows that \blacksquare_1 is well-defined on morphisms between open Markov processes; given this is it easy to check that \blacksquare_1 is a functor. One can verify that \blacksquare_0 and \blacksquare_1 combine to define a double functor $\blacksquare: \mathbb{M}\mathbf{ark} \rightarrow \mathbb{L}\mathbf{inRel}$: the hard part is checking that horizontal composition of open Markov processes is preserved, but this was shown in Lemma 5.4. Horizontal composition of 2-morphisms is automatically preserved because $\mathbb{L}\mathbf{inRel}$ is degenerate.

To make \blacksquare into a symmetric monoidal double functor we need to make \blacksquare_0 and \blacksquare_1 into symmetric monoidal functors, which we do using these extra structures:

- an isomorphism in $\mathbb{L}\mathbf{inRel}_0$ between $\{0\}$ and $\blacksquare(\emptyset)$,
- a natural isomorphism between $\blacksquare(S) \oplus \blacksquare(S')$ and $\blacksquare(S + S')$ for any two objects $S, S' \in \mathbb{M}\mathbf{ark}_0$,
- an isomorphism in $\mathbb{L}\mathbf{inRel}_1$ between the unique linear relation $\{0\} \rightarrow \{0\}$ and $\blacksquare(\emptyset \rightarrow (\emptyset, 0_\emptyset) \leftarrow \emptyset)$, and
- a natural isomorphism between

$$\blacksquare((S \rightarrow (X, H) \leftarrow T) \oplus (S' \rightarrow (X', H') \leftarrow T'))$$

and

$$\blacksquare(S + S' \rightarrow (X, H) \oplus (X', H') \leftarrow T + T')$$

for any two objects $S \rightarrow (X, H) \leftarrow T, S' \rightarrow (X', H') \leftarrow T'$ of $\mathbb{M}\mathbf{ark}_1$.

There is an evident choice for each of these extra structures, and it is straightforward to check that they not only make \blacksquare_0 and \blacksquare_1 into symmetric monoidal functors but also meet the extra requirements for a symmetric monoidal double functor listed in Shulman's paper [23]. In particular, all diagrams of 2-morphisms commute automatically because $\mathbb{L}\mathbf{inRel}$ is degenerate. \square

6. A BICATEGORY OF OPEN MARKOV PROCESSES

In Thm. 4.5, we constructed a symmetric monoidal double category $\mathbb{M}\mathbf{ark}$ with

- finite sets as objects,
- functions as vertical 1-morphisms,
- open Markov processes as horizontal 1-cells, and
- morphisms of open Markov processes as 2-morphisms.

Using the following result of Shulman [23], we can obtain a symmetric monoidal bicategory $\mathbb{M}\mathbf{ark}$ with

- finite sets as objects,
- open Markov processes as morphisms,

(iii) morphisms of open Markov processes as 2-morphisms.

To do this, we need to check that the symmetric monoidal double category \mathbf{Mark} is ‘isofibrant’—a concept we explain in the proof of Lemma 6.3. The bicategory \mathbf{Mark} then arises as the ‘horizontal bicategory’ of the double category \mathbf{Mark} .

Definition 6.1. *Let \mathbb{D} be a double category. Then the **horizontal bicategory** of \mathbb{D} , which we denote as $H(\mathbb{D})$, is the bicategory with*

- (i) objects of \mathbb{D} as objects,
- (ii) horizontal 1-cells of \mathbb{D} as 1-morphisms,
- (iii) globular 2-morphisms of \mathbb{D} (i.e., 2-morphisms with identities as their source and target) as 2-morphisms,

and vertical and horizontal composition, identities, associators and unitors arising from those in \mathbb{D} .

Theorem 6.2 (Shulman). *Let \mathbb{D} be an isofibrant symmetric monoidal double category. Then $H(\mathbb{D})$ is a symmetric monoidal bicategory, where $H(\mathbb{D})$ is the horizontal bicategory of \mathbb{D} .*

Lemma 6.3. *The symmetric monoidal double category \mathbf{Mark} is isofibrant.*

Proof. To show that \mathbf{Mark} is isofibrant, we need to show that every vertical 1-isomorphism has both a companion and a conjoint. Given a vertical 1-isomorphism $f: S \rightarrow S'$, meaning a bijection between finite sets, then a companion of f is given by the horizontal 1-cell:

$$S \xrightarrow{f} (S', 0_{S'}) \xleftarrow{1_{S'}} S'$$

together with two 2-morphisms

$$\begin{array}{ccc} S \longrightarrow (S', 0_{S'}) \longleftarrow S' & & S \longrightarrow (S, 0_S) \longleftarrow S \\ \downarrow f & \downarrow 1_{S'} & \downarrow 1_{S'} \\ S' \longrightarrow (S', 0_{S'}) \longleftarrow S' & & S \longrightarrow (S', 0_{S'}) \longleftarrow S' \end{array} \quad \begin{array}{ccc} S \longrightarrow (S, 0_S) \longleftarrow S & & S \longrightarrow (S, 0_S) \longleftarrow S \\ \downarrow 1_S & \downarrow f & \downarrow f \\ S \longrightarrow (S', 0_{S'}) \longleftarrow S' & & S \longrightarrow (S', 0_{S'}) \longleftarrow S' \end{array}$$

such that vertical composition gives

$$\begin{array}{ccc} S \longrightarrow (S, 0_S) \longleftarrow S & & S \longrightarrow (S, 0_S) \longleftarrow S \\ \downarrow & \downarrow f & \downarrow \\ S \longrightarrow (S', 0_{S'}) \longleftarrow S' & & S \longrightarrow (S', 0_{S'}) \longleftarrow S' \\ \downarrow f & & \downarrow f \\ S' \longrightarrow (S', 0_{S'}) \longleftarrow S' & = & S' \longrightarrow (S', 0_{S'}) \longleftarrow S' \end{array}$$

and horizontal composition gives

$$\begin{array}{ccccc}
 S & \longrightarrow & (S, 0_S) & \longleftarrow & S \xrightarrow{f} (S', 0_{S'}) \longleftarrow S' \\
 \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
 S & \xrightarrow{f} & (S', 0_{S'}) & \longleftarrow & S' & \longrightarrow & (S', 0_{S'}) & \longleftarrow & S' \\
 \end{array} = \begin{array}{ccccc}
 S & \xrightarrow{f} & (S', 0_{S'}) & \longleftarrow & S' \\
 \downarrow & & \downarrow & & \downarrow \\
 S & \xrightarrow{f} & (S', 0_{S'}) & \longleftarrow & S'
 \end{array}$$

All unlabeled arrows are identities. A conjoint of $f: S \rightarrow S'$ is given by the horizontal 1-cell

$$S' \xrightarrow{1_{S'}} (S', 0_{S'}) \xleftarrow{f} S$$

together with two 2-morphisms

$$\begin{array}{ccc}
 S' \xrightarrow{1_{S'}} (S', 0_{S'}) \xleftarrow{f} S & & S \xrightarrow{1_S} (S, 0_S) \xleftarrow{1_S} S \\
 \downarrow 1_{S'} & & \downarrow f \\
 S' \xrightarrow{1_{S'}} (S', 0_{S'}) \xleftarrow{1_{S'}} S' & & S' \xrightarrow{1_{S'}} (S', 0_{S'}) \xleftarrow{f} S \\
 \downarrow 1_{S'} & & \downarrow f \\
 S' \xrightarrow{1_{S'}} (S', 0_{S'}) \xleftarrow{1_{S'}} S' & & S' \xrightarrow{1_{S'}} (S', 0_{S'}) \xleftarrow{f} S
 \end{array}$$

that satisfy equations analogous to the two above. \square

Theorem 6.4. *Mark is a symmetric monoidal bicategory.*

Proof. This follows immediately from Thm. [23]: **Mark** is an isofibrant symmetric monoidal double category, so we obtain the symmetric monoidal bicategory **Mark** as the horizontal bicategory of **Mark**. \square

We can also obtain a symmetric monoidal bicategory **LinRel** from the symmetric monoidal double category **LinRel** using this fact:

Lemma 6.5. *The symmetric monoidal double category LinRel is isofibrant.*

Proof. Let $f: X \rightarrow Y$ be a linear isomorphism between finite-dimensional real vector spaces. Define \hat{f} to be the linear relation given by the linear isomorphism f and define 2-morphisms in **LinRel**

$$\begin{array}{ccc}
 X & \xrightarrow{\hat{f}} & Y \\
 \downarrow f & & \downarrow 1 \\
 Y & \xrightarrow{1} & Y \\
 \end{array} \quad \alpha_f \Downarrow
 \quad
 \begin{array}{ccc}
 X & \xrightarrow{1} & X \\
 \downarrow 1 & & \downarrow f \\
 X & \xrightarrow{\hat{f}} & Y \\
 \end{array}$$

where α_f and ${}_f\alpha$, the unique fillers of their frames, are identities. These two 2-morphisms and \hat{f} satisfy the required equations, and the conjoint of f is given by reversing the direction of \hat{f} , which is just $f^{-1}: Y \rightarrow X$. It follows that **LinRel** is isofibrant. \square

Theorem 6.6. *There exists a symmetric monoidal bicategory LinRel with*

- (i) finite-dimensional real vector spaces as objects,
- (ii) linear relations $R \subseteq V \oplus W$ as morphisms from V to W ,
- (iii) inclusions $R \subseteq S$ between linear relations $R, S \subseteq V \oplus W$ as 2-morphisms.

Proof. Apply Shulman’s result, Thm. 6.2, to the isofibrant symmetric monoidal double category $\mathbb{L}\mathbf{inRel}$ to obtain the symmetric monoidal bicategory \mathbf{LinRel} as the horizontal edge bicategory of $\mathbb{L}\mathbf{inRel}$. \square

Thus we have symmetric monoidal bicategories \mathbf{Mark} and \mathbf{LinRel} , both of which come from discarding the vertical 1-morphisms of the symmetric monoidal double categories $\mathbb{M}\mathbf{ark}$ and $\mathbb{L}\mathbf{inRel}$, respectively. Morally, we should be able to do something similar to the symmetric monoidal double functor $\mathbf{\blacksquare} : \mathbf{Mark} \rightarrow \mathbf{LinRel}$ to obtain a symmetric monoidal functor of bicategories $\mathbf{\blacksquare} : \mathbf{Mark} \rightarrow \mathbf{LinRel}$.

Conjecture 6.7. *There exists a symmetric monoidal functor $\mathbf{\blacksquare} : \mathbf{Mark} \rightarrow \mathbf{LinRel}$ that maps:*

- (i) any finite set S to the finite-dimensional real vector space $\mathbf{\blacksquare}(S) = \mathbb{R}^S \oplus \mathbb{R}^S$,
- (ii) any open Markov process $S \xrightarrow{i} (X, H) \xleftarrow{o} T$ to the linear relation from $\mathbf{\blacksquare}(S)$ to $\mathbf{\blacksquare}(T)$ given by the linear subspace

$$\mathbf{\blacksquare}(S \xrightarrow{i} (X, H) \xleftarrow{o} T) = \{(i^*(v), I, o^*(v), O) : H(v) + i_*(I) - o_*(O) = 0\} \subseteq \mathbb{R}^S \oplus \mathbb{R}^S \oplus \mathbb{R}^T \oplus \mathbb{R}^T,$$

- (iii) any morphism of open Markov processes

$$\begin{array}{ccccc} S & \xrightarrow{i_1} & (X, H) & \xleftarrow{o_1} & T \\ \downarrow 1_S & & \downarrow p & & \downarrow 1_T \\ S & \xrightarrow{i'_1} & (X', H') & \xleftarrow{o'_1} & T \end{array}$$

to the inclusion

$$\mathbf{\blacksquare}(X, H) \subseteq \mathbf{\blacksquare}(X', H').$$

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