

# Understanding Causal Primitives Using Modular Probability

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## 1 Introduction

Two widely used approaches to causal modelling are *graphical causal models* and *potential outcomes models*. Graphical causal models, which include Causal

Bayesian Networks and Structural Causal Models, provide a set of *intervention* operations that take probability distributions and a graph and return a modified probability distribution (Pearl, 2009). Potential outcomes models feature *potential outcome variables* that represent the “potential” value that a quantity of interest would take under the right circumstances, a potential that may be realised if the circumstances actually arise, but will otherwise remain only a potential or *counterfactual* value (Rubin, 2005).

One challenge for both of these approaches is understanding how their causal primitives – interventions and potential outcome variables respectively – relate to the causal questions we are interested in. This challenge is related to the distinction, first drawn by (Korzybski, 1933), between “the map” and “the territory”. Causal models, like other models, are “maps” that purport to represent a “territory” that we are interested in understanding. Causal primitives are elements of the maps, and the things to which they refer are parts of the territory. The maps contain all the things that we can talk about unambiguously, so it is challenging to speak clearly about how parts of the maps relate to parts of the territory that fall outside of the maps.

For example, Hernán and Taubman (2008), who observed that many epidemiological papers have been published estimating the “causal effect” of body mass index and argued that, because *actions* affecting body mass index<sup>1</sup> are vaguely defined, potential outcome variables and causal effects themselves become ill-defined. We note that “actions targeting body mass index” are not elements of a potential outcomes model but “things to which potential outcomes should correspond”. The authors claim is that vagueness in the “territory” leads to ambiguity about elements of the “map” – and, as we have suggested, anything we can try to say about the territory is unavoidably vague. This seems like a serious problem.

In a response, Pearl (2018) argues that *interventions* (by which we mean the operation defined by a causal graphical model) are well defined, but may not always be a good model of an action. Pearl further suggests that interventions in graphical models correspond to “virtual interventions” or “ideal, atomic interventions”, and that perhaps carefully chosen interventions can be good models of actions. Shahar (2009), also in response, argued that interventions targeting body mass index applied to correctly specified graphical causal models will necessarily yield no effect on anything else which, together with Pearl’s suggestion, implies perhaps that an “ideal, atomic intervention” on body mass index cannot have any effect on anything else. If this is so, it seems that we are dealing with quite a serious case of vagueness – there is a whole body of literature devoted to estimating a “causal effect” that, it is claimed, is necessarily equal to zero! Authors of the original literature on the effects of BMI might counter that they were estimating something different that wasn’t necessarily zero, but as far as we are concerned such a response would only underscore the problem of ambiguity.

One of the key problems in this whole discussion is how the things we have

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<sup>1</sup>the authors use the term “intervention”, but they do not use it mean a formal operation on a graphical causal model, and we reserve the term for such operations to reduce ambiguity.

called *interventions* – which are elements of causal models – relate to the things we have called *actions*, which live outside of causal models. One way to address this difficulty is to construct a bigger causal model that can contain both “interventions” and “actions”, and we can then speak unambiguously about how one relates to another. This is precisely what we do here.

To do this, we use a novel approach to probability modelling that we find is well suited to building causal models. A typical approach to probability modelling is to construct a probability space  $(\mathbb{P}, \Omega, \mathcal{F})$  that serves as a top level model, along with a collection of random variables defined by measurable functions on this space, such that the particular quantities of interest can be obtained from conditional and marginal distributions on this space. Instead we consider a modelling context  $\mathcal{M}$  that contains a collection of *probability components*, which are Markov kernels with named inputs and outputs. The names correspond to variables in the standard setting. Probability components with the right input and output types can be *connected*, an operation that yields a new probability component. We relate this back to the standard approach by equipping each probability component with a probability space and requiring that all components are the conditional probability distributions on their assigned spaces corresponding to their input and output labels.

Equipped with this foundation, we apply it to a variety of approaches to causal modelling, showing how it can enable understanding of different approaches in a common framework, and how it can represent assertions that were previously made “outside the model”. First, we consider causal decision problems and derive *see-do models*, which reduce to statistical decision problems when augmented with the principle of expected utility. See-do models are a particular kind of probability component that we call a *comb*, which can be thought of as a probability model that needs something to be inserted into the middle. We consider causal graphical models, and show how under a very slight modification to the standard notation they induce see-do models, which allows us to formally connect *interventions* to *actions*. Finally, we consider potential outcomes models and show how we can formalise the typical assertion (which again, lives “outside the model”) that potential outcomes represent counterfactual values. Potential outcomes models as typically used do not contain counterfactual assertions and in fact feature comb and insert components almost but not quite identical to combs and inserts found in causal graphical models.

I’m probably going to have to cut some of the above

## 2 Probability with connectable submodels

Throughout this paper, we will assume all measurable sets  $X$  are finite sets. This is both because it makes explanations simpler and because it is easy to show that submodels exist in this setting (Lemma 2.11). Many of the proofs in this paper can likely be specialised to more general settings due to our use of string diagrams which represent abstract morphisms in Markov categories,

rather than finite Markov kernels specifically.

The standard method of constructing probability models introduces a probability space  $(\mathbb{P}, (\Omega, \mathcal{F}))$  with  $\Omega$  a sample space,  $\mathcal{F}$  a  $\sigma$ -algebra on  $\Omega$  and  $\mathbb{P}$  a probability measure on  $(\Omega, \mathcal{F})$ . Random variables are defined by measurable functions on  $\Omega$  and are given names in sans-serif like  $X$ . A probability distribution  $\mathbb{P}^{XYZ}$  is “the joint distribution of  $X$ ,  $Y$  and  $Z$  under  $\mathbb{P}$ ” where  $X$ ,  $Y$  and  $Z$  are associated with random variables on  $\Omega$  and is given by the pushforward of the function  $\omega \mapsto (X(\omega), Y(\omega), Z(\omega))$ . Unless otherwise stated, a random variable named  $X$  will take values in the space  $X$  (note the serif font).

This approach needs to be extended if we are to apply it to causal modelling. The causal graphical models literature provides some simple examples illustrating this need, while the fact that the potential outcomes approach also benefits from extension requires more explanation, and will be discussed in Section 5.

Consider the “truncated factorisation”, a linchpin operation in causal graphical models. Given a probability  $\mathbb{P}^{XYZ}$  and a graphical model in which  $Z$  blocks all backdoor paths between  $X$  and  $Y$ , the truncated factorisation defines a new probability measure  $\mathbb{P}_x$  as follows (Pearl, 2009, page 24):

$$\mathbb{P}_x^{YZ}(y, z) := \mathbb{P}^{Y|XZ}(y|x, z)\mathbb{P}^Z(z) \quad (1)$$

Without a causal model justifying the claim that  $Z$  blocks backdoor paths between  $X$  and  $Y$ , there is in general no special significance to the expression on the right side of Equation 1, and causal models that can justify such claims are not a feature of the standard approach to probability modelling. At the same time, the notation we have chosen for the left side of Equation 1 suggests that  $\mathbb{P}_x^{YZ}$  is a distribution over the same variables  $Y$  and  $Z$  as the original  $\mathbb{P}^{XYZ}$ . The standard approach to probability modelling *does* offer an account of what it means for variables to be the same, which is that they are represented by the same measurable functions on the probability space.

An immediate issue is that  $\mathbb{P}_x$  is a different probability measure to  $\mathbb{P}$ . However, even if we substitute probability measures, we could perhaps keep the sample space  $\Omega$  and define variables as measurable functions on  $\Omega$ . This is the approach taken in Pearl (2009) (but see Section 2.6).

This approach rules out the possibility of performing some interventions. For example, if  $X = Z$  and  $\mathbb{P}^Z$  is non-deterministic, then no  $\mathbb{P}_x$  exists with the property required in Equation 1. We think that this is probably a useful feature. Consider a variable  $B$  representing a person’s body mass index. It seems reasonable to hold that this variable is by definition equivalent to  $\frac{W}{H^2}$  where  $W$  represents their weight in kilograms and  $H$  represents their height in metres. This rules out the existence of any probability measure that represents the results of an intervention on  $B$  in any model that also contains  $H$  and  $W$  and features the expected causal relationships (and, regardless of causal relationships, it completely rules out the possibility that  $B$ ,  $H$  and  $W$  can all be intervened on). Such interventions can be ruled out by defining the random variables such that  $B = \frac{W}{H^2}$ .

Along the same lines as Dawid (2000), we find that it is often desirable to introduce variables representing the results of choices, and we often don’t

want to attach probability distributions to such variables. We might have  $D$ , representing a choice, and  $\mathbb{P}^{Y|D}$  representing the consequences of this choice, but no  $\mathbb{P}^{Y,D}$  as we have no need of a marginal probability of  $D$ .

As a brief summary, we want a version of “probability theory” that:

- Defines what we mean by a “variable”
- Includes generalised variables that do not have marginal probabilities (for example, to represent choices)
- Operations like Equation 1 are standard rather than special cases

Standard probability theory does the first, but not the second two.

## 2.1 Markov categories

We base our approach on the theory of Markov categories. This has two benefits: firstly, Markov categories have a graphical notation that help present some ideas in an intuitive manner. Secondly, because they are abstract categories that represent models of the flow of information, proofs that use only string diagrams correspond to theorems in many formalisations of probability, not just the finite set case that we focus on here. More comprehensive introductions to Markov categories can be found in Fritz (2020); Cho and Jacobs (2019).

Rather than explain Markov categories in the abstract, we will instead introduce string diagrams with reference to how they represent stochastic maps and finite sets (though see Appendix 9). Given measurable sets  $(X, \mathcal{X})$  and  $(Y, \mathcal{Y})$ , a Markov kernel or stochastic map is a map  $\mathbf{K} : X \times \mathcal{Y} \rightarrow [0, 1]$  such that

- The map  $x \mapsto \mathbf{K}(x, A)$  is  $\mathcal{X}$ -measurable for every  $A \in \mathcal{Y}$
- The map  $A \mapsto \mathbf{K}(x, A)$  is a probability measure for every  $x \in X$

Where  $X$  and  $Y$  are finite sets with the discrete  $\sigma$ -algebra, we can represent a Markov kernel  $\mathbf{K}$  as a  $|X| \times |Y|$  matrix where  $\sum_{y \in Y} \mathbf{K}_x^y = 1$  for every  $x \in X$ . We will give Markov kernels the signature  $\mathbf{K} : X \rightarrow Y$  to indicate that they map from  $X$  to probability distributions on  $Y$ .

Graphically, Markov kernels are drawn as boxes with input and output wires, and probability measures (which are kernels with the domain  $\{*\}$ ) are represented by triangles:

$$\mathbf{K} := \boxed{\mathbf{K}} \quad (2)$$

$$\mathbf{P} := \triangleleft \mathbf{P} \quad (3)$$

Two Markov kernels  $\mathbf{L} : X \rightarrow Y$  and  $\mathbf{M} : Y \rightarrow Z$  have a product  $\mathbf{LM} : X \rightarrow Z$  given by the matrix product  $\mathbf{LM}_x^z = \sum_y \mathbf{L}_x^y \mathbf{M}_y^z$ . Graphically, we write represent by joining wires together:

$$\mathbf{LM} := \boxed{\mathbf{K}} \boxed{\mathbf{M}} \quad (4)$$

The Cartesian product  $X \times Y := \{(x, y) | x \in X, y \in Y\}$ . Given kernels  $\mathbf{K} : W \rightarrow Y$  and  $\mathbf{L} : X \rightarrow Z$ , the tensor product  $\mathbf{K} \otimes \mathbf{L} : W \times X \rightarrow Y \times Z$  is defined by  $(\mathbf{K} \otimes \mathbf{L})_{(w,x)}^{(y,z)} := K_w^y L_x^z$  and represents applying the kernels in parallel to their inputs.

The tensor product is represented by drawing kernels in parallel:

$$\mathbf{K} \otimes \mathbf{L} := \begin{array}{c} W \boxed{\mathbf{K}} Y \\ X \boxed{\mathbf{L}} Z \end{array} \quad (5)$$

We read diagrams from left to right (this is somewhat different to Fritz (2020); Cho and Jacobs (2019); Fong (2013) but in line with Selinger (2010)). A diagram describes products and tensor products of Markov kernels, which are expressed according to the conventions described above. There are a collection of special Markov kernels for which we can replace the generic “box” of a Markov kernel with a diagrammatic elements that are visually suggestive of what these kernels accomplish.

A description of these kernels follows.

The identity map  $\text{id}_X : X \rightarrow X$  defined by  $(\text{id}_X)_x^{x'} = \llbracket x = x' \rrbracket$ , where the Iverson bracket  $\llbracket \cdot \rrbracket$  evaluates to 1 if  $\cdot$  is true and 0 otherwise, is a bare line:

$$\text{id}_X := X \text{---} X \quad (6)$$

We choose a particular 1-element set  $\{*\}$  that acts as the identity in the sense that  $\{*\} \times A = A \times \{*\} = A$  for any set  $A$ . The erase map  $\text{del}_X : X \rightarrow \{*\}$  defined by  $(\text{del}_X)_x^* = 1$  is a Markov kernel that “discards the input” (we will later use it for marginalising joint distributions). It is drawn as a fuse:

$$\text{del}_X := \text{---} * X \quad (7)$$

The copy map  $\text{copy}_X : X \rightarrow X \times X$  defined by  $(\text{copy}_X)_x^{x',x''} = \llbracket x = x' \rrbracket \llbracket x = x'' \rrbracket$  is a Markov kernel that makes two identical copies of the input. It is drawn as a fork:

$$\text{copy}_X := X \text{---} \begin{array}{c} X \\ \swarrow \searrow \\ X \end{array} \quad (8)$$

The swap map  $\text{swap}_{X,Y} : X \times Y \rightarrow Y \times X$  defined by  $(\text{swap}_{X,Y})_{x,y}^{y',x'} = \llbracket x = x' \rrbracket \llbracket y = y' \rrbracket$  swaps two inputs, and is represented by crossing wires:

$$\text{swap}_X := \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \quad (9)$$

Because we anticipate that the graphical notation will be unfamiliar to many, we will also include translations to more familiar notation.

## 2.2 Truncated factorisation with Markov kernels

The Markov kernels introduced in the previous section can be thought of as “conditional probability distributions without variables”. We can use these to represent an operation very similar to Equation 1. Note that  $P^{Y|XZ}$  must be represented by a Markov kernel  $\mathbf{K} : X \times Z \rightarrow Y$  and  $\mathbb{P}^Z$  by a Markov kernel  $\mathbf{L} \in \Delta(Z)$ . Then we can define a Markov kernel  $\mathbf{M} : X \rightarrow X \times Z$  representing  $x \mapsto \mathbb{P}_x^{YZ}(y, z)$  by

The diagram shows a Markov kernel  $\mathbf{M}$  represented as a composition of two kernels. On the left, a triangle labeled  $\mathbf{L}$  has an input wire from the bottom labeled  $X$  and an output wire to the right. This output wire connects to a dot, which then connects to a square labeled  $\mathbf{K}$ . The square  $\mathbf{K}$  has two output wires: one to the top labeled  $Y$  and one to the right labeled  $Z$ . The entire expression is labeled  $\mathbf{M} :=$  on the left and (10) on the right.

There is, however, a key difference between Equation 10 and Equation 1: the Markov kernels in the latter equation describe the distribution of particular variables, while the former equation describes Markov kernels only.

To illustrate why we need variables, consider an arbitrary Markov kernel  $\mathbf{K} : \{*\} \rightarrow \Delta(X \times X)$ . We could draw this:

The diagram shows a Markov kernel  $\mathbf{K}$  represented as a triangle. It has a single input wire from the left and two output wires to the right, both labeled  $X$ . The entire expression is labeled  $\mathbf{K} :=$  on the left and (11) on the right.

We label both wires with the set  $X$ . However, say  $X = \{0, 1\}$ . Then  $\mathbf{K}$  could be the kernel  $\mathbf{K}^{x_1, x_2} = \llbracket x_1 = 0 \rrbracket \llbracket x_2 = 1 \rrbracket$ . In this case, both of its outputs must represent *different* variables, despite taking values in the same set. On the other hand, if  $\mathbf{K}^{x_1, x_2} = 0.5 \llbracket x_1 = x_2 \rrbracket$  then both outputs could represent the same variable, because they are deterministically the same, or they could represent different variables that happen to be equal. We need some way to distinguish the two cases.

We use a definition of variable that almost matches the standard definition we introduced at the beginning of the section. We define variables as Markov kernels rather than functions as it makes the construction slightly simpler.

**Definition 2.1** (Variable). Given a *sample space*  $\Omega$ , a variable  $\mathbf{X}$  is a Markov kernel  $\Omega \rightarrow A$  such that there exists some function  $f_X : \Omega \rightarrow A$  with  $\mathbf{X}_x^a = \llbracket a = f_X(x) \rrbracket$ .

We define the *product* of two variables as follows:

- **Product:** Given variables  $\mathbf{W} : \Omega \rightarrow A$  and  $\mathbf{V} : \Omega \rightarrow B$ , the product is defined as  $(\mathbf{W}, \mathbf{V}) = \text{copy}_\Omega(\mathbf{W} \otimes \mathbf{V})$

The *identity* variable is the erase map  $\mathbf{I} := \text{del}_\Omega$ , with  $(\mathbf{I}, \mathbf{X}) = (\mathbf{X}, \mathbf{I}) = \mathbf{X}$  (up to isomorphism) for any  $\mathbf{X}$ .

We then need a notion of Markov kernels that “maps between variables”. An *indexed Markov kernel* is such a thing.

**Definition 2.2** (Indexed Markov kernel). Given variables  $X : \Omega \rightarrow A$  and  $Y : \Omega \rightarrow B$ , an indexed Markov kernel  $K : X \rightarrow Y$  is a triple  $(K', X, Y)$  where  $K' : A \rightarrow B$  is the *underlying kernel*,  $X$  is the *input index* and  $Y$  is the *output index*. Indexed Markov kernels must satisfy the property of *non-contradiction*:

$$\max_{\omega \in \Omega} (X, Y)_{\omega}^{a', b'} = 0 \implies K_{a'}^{b'} = 0 \quad (12)$$

We will call an indexed Markov kernel a *model* for short.

We define  $\text{Id}_X$  to be the model  $(\text{Id}_X, X, X)$ , and similarly the indexed versions  $\text{del}_X$ ,  $\text{copy}_X$  and  $\text{swap}_{X,Y}$  are obtained by taking the unindexed versions of these maps and attaching the appropriate random variables as indices. Diagrams are the diagrams associated with the underlying kernel, with input and output wires annotated with input and output indices.

For example, if  $K : (A_1, A_2) \rightarrow \Delta(B_1, B_2)$ , for example, we can draw:

$$K := \begin{array}{c} A_1 \\ A_2 \end{array} \dashv \boxed{K} \begin{array}{c} B_1 \\ B_2 \end{array} \quad (13)$$

or

$$K = (A_1, A_2) \dashv \boxed{K[L]} \vdash (B_1, B_2) \quad (14)$$

Non-contradiction means that, if there is no  $\omega \in \Omega$  such that  $f_X(\omega) = a'$  and  $f_Y(\omega) = b'$  then the probability assigned to a simultaneous occurrence of  $a'$  and  $b'$  must be zero.

Non-contradiction implies that for any  $X : \Omega \rightarrow A$ , there is a unique model mapping  $\Omega$  to  $X$  for which the underlying kernel is  $X$  itself. In category theoretic terminology,  $\Omega$  is an *initial object*. One consequence of this is, given a probability measure  $\mathbf{P} : \{*\} \rightarrow \text{Id}_{\Omega}$  (a probability measure “on  $\Omega$ ”),  $\mathbf{P}X$  is the unique measure on  $X$  obtainable by composition with  $\mathbb{P}$ . Crucially,  $\mathbf{P}X$  is the pushforward of  $\mathbf{P}$  by  $X$ , which is the rule for obtaining a probability distribution on  $X$  given a probability distribution “on  $\Omega$ ” in standard probability theory.

A more general version of non-contradiction is desirable

**Lemma 2.3** ( $\Omega$  is an initial object). *For any  $X : \Omega \rightarrow A$ , there is a unique model  $\mathbf{X} : \text{Id}_{\Omega} \rightarrow X$  given by  $\mathbf{X} := (X, \text{Id}_{\Omega}, X)$ .*

*Proof.*  $X$  is a Markov kernel mapping from  $\Omega \rightarrow A$ , so it is a valid underlying kernel for  $\mathbf{X}$ , and  $\mathbf{X}$  has input and output indices matching its signature. We need to show it satisfies non-contradiction.

For any  $\omega \in \Omega$ ,  $a \in A$

$$\max_{\omega \in \Omega} (\text{Id}_{\Omega}, X)_{\omega}^{\omega', a} = \max_{\omega \in \Omega} [\omega = \omega'] [\omega = f_X(a)] \quad (15)$$

$$= [\omega = f_X(a)] \quad (16)$$

$$= \mathbf{X}_{\omega}^a \quad (17)$$



Thus  $\mathbf{X}$  satisfies non-contradiction.

Suppose there were some  $\mathbf{K} : \text{Id}_\Omega \rightarrow \mathbf{X}$  not equal to  $\mathbf{X}$ . Then there must be some  $\omega \in \Omega$ ,  $b \in A$  such that  $\mathbf{K}_\omega^b \neq 0$  and  $f_X(\omega) \neq b$ . Then

$$\max_{\omega \in \Omega} (\text{Id}_\Omega, \mathbf{X})_\omega^{\omega', a} = \max_{\omega \in \Omega} \llbracket \omega = \omega' \rrbracket \llbracket \omega = f_X(b) \rrbracket \quad (18)$$

$$= \llbracket \omega = f_X(b) \rrbracket \quad (19)$$

$$= 0 \quad (20)$$

$$< \mathbf{K}_\omega^b \quad (21)$$

Thus  $\mathbf{K}$  doesn't satisfy non-contradiction.  $\square$

**Corollary 2.4** (Pushforward measure). *Given any indexed probability measure  $\mathbf{P} : \{*\} \rightarrow \text{Id}_\Omega$ , there is a unique probability measure  $\mathbf{P}^X : \{*\} \rightarrow \mathbf{X}$  such that  $\mathbf{P}^X = \mathbf{P}\mathbf{Q}$  for some  $\mathbf{Q} : \text{Id}_\Omega \rightarrow \mathbf{X}$  and it is given by  $(\mathbf{P}^X)^a = \sum_{\omega \in f^{-1}(a)} \mathbf{P}^\omega$ .*

*Proof.* As  $\mathbf{X}$  is the unique model  $\text{Id}_\Omega \rightarrow \mathbf{X}$ , it must be the case that  $\mathbf{P}^X = \mathbf{P}\mathbf{X}$ . Then for any  $a \in A$

$$(\mathbf{P}\mathbf{X})^a = \sum_{\omega \in \Omega} \mathbf{P}^\omega \mathbf{X}_\omega^a \quad (22)$$

$$= \sum_{\omega \in \Omega} \mathbf{P}^\omega \llbracket a = f_X(\omega) \rrbracket \quad (23)$$

$$= \sum_{\omega \in f^{-1}(a)} \mathbf{P}^\omega \quad (24)$$

$\square$

We also show a number of other useful properties.

The following proofs are not done with string diagrams because we'd need a more general version of non-contradiction to do it

**Lemma 2.5** (Output copies of the same variable are identical). *For any  $\mathbf{K} : \mathbf{X} \rightarrow (\mathbf{Y}, \mathbf{Y}, \mathbf{Z})$ , there exists some  $\mathbf{L} : \mathbf{X} \rightarrow (\mathbf{Y}, \mathbf{Z})$  such that*

$$\mathbf{K}_x'^{y, y', z} = \llbracket y = y' \rrbracket \mathbf{L}_x'^{y, z} \quad (25)$$

*Proof.* For any  $\omega, x, y, y', z$ :

$$(\mathbf{X}, \mathbf{Y}, \mathbf{Y}, \mathbf{Z})_\omega^{x, y, y', z} = \llbracket f_Y(\omega) = y \rrbracket \llbracket f_Y(\omega) = y' \rrbracket (\mathbf{X}, \mathbf{Z})_\omega^{x, z} \quad (26)$$

$$= \llbracket y = y' \rrbracket \llbracket f_Y(\omega) = y \rrbracket (\mathbf{X}, \mathbf{Z})_\omega^{x, z} \quad (27)$$

Therefore, by non-contradiction, for any  $x, y, y', z$ ,  $y \neq y' \implies \mathbf{K}_x'^{y, y', z} = 0$ . Define  $\mathbf{L}$  by  $\mathbf{L}_x'^{y, z} := \mathbf{K}_x'^{y, y, z}$ . Then

$$\mathbf{K}_x'^{y, y', z} = \llbracket y = y' \rrbracket \mathbf{L}_x'^{y, z} \quad (28)$$

$\square$

**Lemma 2.6** (Copies shared between input and output are identical). *For any  $\mathbf{K} : (\mathbf{X}, \mathbf{Y}) \rightarrow (\mathbf{X}, \mathbf{Z})$ , there exists some  $\mathbf{L} : (\mathbf{X}, \mathbf{Y}) \rightarrow \mathbf{Z}$  such*

$$\mathbf{K}_{x,y}^{!x',z} = \llbracket x = x' \rrbracket \mathbf{L}_{!x,y}^z \quad (29)$$

*Proof.* For any  $\omega, x, y, y', z$ :

$$(\mathbf{X}, \mathbf{Y}, \mathbf{Y}, \mathbf{Z})_{\omega}^{x,y,y',z} = \llbracket f_{\mathbf{Y}}(\omega) = y \rrbracket \llbracket f_{\mathbf{Y}}(\omega) = y' \rrbracket (\mathbf{X}, \mathbf{Z})_{\omega}^{x,z} \quad (30)$$

$$= \llbracket y = y' \rrbracket \llbracket f_{\mathbf{Y}}(\omega) = y \rrbracket (\mathbf{X}, \mathbf{Z})_{\omega}^{x,z} \quad (31)$$

Therefore, by non-contradiction, for any  $x, y, y', z, x \neq x' \implies \mathbf{K}_{x,y}^{!x',z} = 0$ . Define  $\mathbf{L}$  by  $\mathbf{L}_{x,y}^{!x',z} := \mathbf{K}_{x,y}^{!x,y}$ . Then

$$\mathbf{K}_{x,y}^{!x',z} = \llbracket x = x' \rrbracket \mathbf{L}_{x,y}^z \quad (32)$$

□

**Lemma 2.7** (No duplicated inputs). *There is no model  $\mathbf{K} : (\mathbf{X}, \mathbf{X}, \mathbf{Y}) \rightarrow \mathbf{Z}$  for any  $\mathbf{X} \neq *$ .*

*Proof.* Suppose such a  $\mathbf{K}$  exists. By the definition of a Markov kernel, for any  $x, x', y$  where  $x \neq x'$

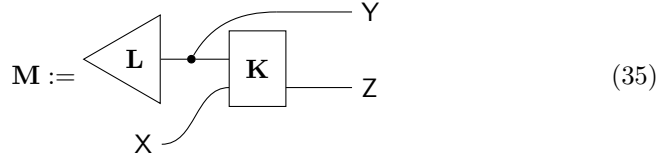
$$\sum_{z \in \mathbf{Z}} \mathbf{K}_{x,x',y}^z = 1 \quad (33)$$

$$\implies \exists z \in \mathbf{Z} : \mathbf{K}_{x,x',y}^z > 0 \quad (34)$$

But non contradiction requires that  $\mathbf{K}_{x,x',y}^z = 0$  wherever  $x \neq x'$ . □

### 2.3 Truncated factorisation a third time

At this point, we can represent Equation 1 using models. Suppose  $P^{\mathbf{Y}|\mathbf{XZ}}$  is a model  $\mathbf{K} : (\mathbf{X}, \mathbf{Z}) \rightarrow \mathbf{Y}$  and  $\mathbb{P}^{\mathbf{Z}}$  an model  $\mathbf{L} : \{*\} \rightarrow \mathbf{Z}$ . Then we can define an model  $\mathbf{M} : \mathbf{X} \rightarrow \mathbf{X}, \mathbf{Z}$  representing  $x \mapsto \mathbb{P}_x^{\mathbf{YZ}}(y, z)$  by



If it exists. Equation 35 is almost identical to Equation 10, except it now specifies which variables each measure applies to, not just which sets they take values in. Like Equation 1, there is no guarantee that any model satisfying Equation 35 exists. Depending on the definition of  $\mathbf{X}$  and  $\mathbf{Z}$ , the rule of non-contradiction might rule out the existence of any such morphism even if  $\mathbf{K}$  and  $\mathbf{L}$  both exist. To return to a familiar example, consider  $\mathbf{Z} = (\mathbf{H}, \mathbf{W})$ , representing

a person’s height and weight, and  $X = B$ , representing a person’s body mass index. If we define random variables such that  $f_B = \frac{f_W}{f_H^2}$ , then  $\mathbf{M}$  above cannot exist.

It seems to be desirable that we rule out models that violate the definitions of random variables. However, it does leave us in the annoying place of needing to qualify definitions like Equation 35 with “if it exists”. As far as we can tell, this is simply something we have to deal with. Any definition of an intervention in the standard framework of causal graphical models also requires such a qualification.

We could carefully construct the sample space and select all named variables are carefully chosen such that any model that does not violate Lemmas 2.5 to 2.7 exists. For example, the sample space could be a tensor product of the codomains of all named variables, and each named variable a corresponding projection. We use the example of body mass index to suggest that this isn’t always desirable – even if we could *define* interventions on body mass index, it is hard to understand what exactly we are trying to model with an “intervention” that involves redefining a quantity of interest.

We really do want to rule out some models, and if there’s a benefit to saying “let’s assume this model is useful” instead of “let’s assume this model exists” it’s not apparent to us. Thus we don’t construct the sample space to ensure as many models as possible exist by default, though this is an option available to anyone using the theory.

## 2.4 Submodels

We do not yet have a notion of *marginal probability* or *conditional probability*. In the paragraph above, the terms  $P^{Y|XZ}$  and  $P^Z$  are external to the theory we have postulated so far. In particular, the idea that  $P^{Y|XZ}$  and  $P^Z$  are both parts of a larger model  $P$  is not something we can yet express. We will use the term *submodels* to refer to marginals and conditionals of a larger model.

**Definition 2.8** (Marginalising model). For any variable  $X : \Omega \rightarrow A$ , a model  $\mathbf{K} : Y \rightarrow Z$  *marginalises over*  $X$  if there exists some  $W$  such that  $Y = (X, W)$  and  $\mathbf{K} = \text{del}_X \otimes \text{Id}_W$ .

Note that any model  $\mathbf{M} : Y \rightarrow Z$  that marginalises over  $*$  is equal to  $\text{del}_* \otimes \text{Id}_Y = \text{Id}_Y$ .

**Definition 2.9** (Marginal submodel). Given any  $\mathbf{K} : X \rightarrow Y$ , any  $\mathbf{L} : X \rightarrow Z$  and any variable  $A$ ,  $\mathbf{L}$  is a *marginal submodel* of  $\mathbf{K}$  if there is some model  $\mathbf{M} : Y \rightarrow Z$  that marginalises over  $A$  such that  $\mathbf{L} = \mathbf{KM}$ .

Because  $\mathbf{KId}_Y = \mathbf{K}$ , and  $\text{Id}_Y$  is the model that marginalises over  $*$ ,  $\mathbf{K}$  is always a marginal of itself.

**Definition 2.10** (Conditional submodel). Given  $\mathbf{K} : X \rightarrow Y$  and  $\mathbf{L} : W, X \rightarrow Z$ ,  $\mathbf{L}$  is a conditional submodel of  $\mathbf{K}$  if there are marginal submodels  $\mathbf{K}^1 : X \rightarrow W$ ,

$\mathbf{K}^2 : X \rightarrow (W, Z)$  of  $\mathbf{K}$  such that

$$\mathbf{K}^2 = X \text{ --- } \bullet \text{ --- } \boxed{\mathbf{K}^1} \text{ --- } \bullet \text{ --- } \boxed{\mathbf{L}} \text{ --- } Z \quad (36)$$

$W$

$$(\mathbf{K}^2)_x^{w,z} = (\mathbf{K}^1)_x^w \mathbf{L}_{w,x}^z \quad (37)$$

The erase map  $\text{del}_X : X \rightarrow *$  is a marginal of  $\mathbf{K}$  and letting  $\mathbf{K}^1 = \text{del}_X$ , then any other marginal  $\mathbf{K}^2$  satisfies Equation 36. So every marginal submodel of  $\mathbf{K}$  is also a conditional submodel.

Marginal submodels are unique by definition, while conditional submodels are not unique. Because all marginal submodels are also conditional submodels, we will simply use “submodel” to refer to the latter.

**Lemma 2.11** (Submodel existence). *For any model  $\mathbf{K} : W \rightarrow (X, Y)$  (where variables take values in finite sets), there exists a submodel  $\mathbf{L} : (X, W) \rightarrow Y$ .*

*Proof.* Consider any Markov kernel  $\mathbf{L} : (X, W) \rightarrow \Delta(Y)$  with the property

$$\mathbf{L}_{xw}^y = \frac{\mathbf{K}_w^{xy}}{\sum_{x \in X} \mathbf{K}_w^{xy}} \quad \forall w, y : \text{the denominator is positive} \quad (38)$$

Note that in general there are many Markov kernels  $\mathbf{L}$  that satisfy this.

Then define  $\mathbf{K}^1 : W \rightarrow X$ , obtained by marginalising  $\mathbf{K}$  over  $Y$ . Then

$$\mathbf{M}_w^x \mathbf{L}_{xw}^y = \sum_{x \in X} \mathbf{K}_w^{xy} \frac{\mathbf{K}_w^{xy}}{\sum_{x \in X} \mathbf{K}_w^{xy}} \quad \text{if } \mathbf{K}_w^{xy} > 0 \quad (39)$$

$$= \mathbf{K}_w^{xy} \quad \text{if } \mathbf{K}_w^{xy} > 0 \quad (40)$$

$$= 0 \quad \text{otherwise} \quad (41)$$

$$= \mathbf{K}_w^{xy} \quad \text{otherwise} \quad (42)$$

□

It is the existence of submodels that makes this theory more complex when sets may be uncountably infinite. While submodels are known to exist in the case that the domain of  $\mathbf{K}$  is  $\{*\}$  and the codomain a standard measurable set (this being equivalent to the existence of regular conditional probabilities Cho and Jacobs (2019)), this does not necessarily guarantee the existence of submodels for models where the domain is also an uncountable set.

With the definition of submodels in hand, we can introduce a more familiar notation. If  $\mathbf{L} : X \rightarrow Y$  is a submodel of  $\mathbf{K}$ , we may write  $\mathbf{L} \in \mathbf{K}^{Y|X}$ . We can also write  $\mathbf{L} \equiv \mathbf{K}^{Y|X;\mathbf{L}}$  and  $\mathbf{L}_x^y \equiv \mathbf{K}^{Y|X;\mathbf{L}}(y|x)$ . Note that  $\mathbf{L}$  might be a submodel of other models, and other kernels might be submodels of  $\mathbf{K}$  with the same signature. This notation isn’t *entirely* standard, as we use  $\mathbf{K}^{Y|X}$  to

refer to a set and not a single model. The non-uniqueness of submodels is more problematic for causal models than for standard probabilistic models, as we will see in Section 4.

If  $\mathbf{K}^{Y|X} = \mathbf{L}^{Y|X}$  then we mean set equality.

## 2.5 Conditional independence

We define conditional independence in the following manner:

For a *probability distribution*  $\mathbf{P} : \{*\} \rightarrow \Delta(Y)$  and some  $A, B, C \in Y$ , we say  $A$  is independent of  $B$  given  $C$ , written  $A \perp\!\!\!\perp_{\mathbf{P}} B|C$ , if there are submodels  $\mathbf{P}^{ABC;J}, \mathbf{P}^{C;K}, \mathbf{P}^{A|C;L}, \mathbf{P}^{B|C;M}$  such that

$$\mathbf{P}^{ABC;J} = \begin{array}{c} \text{---} \triangleleft \text{---} \\ \text{---} \mathbf{K} \text{---} \\ \text{---} \end{array} \begin{array}{c} \text{---} \mathbf{L} \text{---} A \\ \text{---} C \\ \text{---} \mathbf{M} \text{---} B \end{array} \quad (43)$$

For an arbitrary model  $\mathbf{N} : X \rightarrow \Delta(Y)$  and some  $A, B, C \in (X, Y)$ , we say  $A$  is independent of  $B$  given  $C$ , written  $A \perp\!\!\!\perp_{\mathbf{N}} B|C$ , if there is some  $\mathbf{O} : \{*\} \rightarrow \Delta(X)$  such that  $O^x > 0$  for all  $x \in X$  and  $A \perp\!\!\!\perp_{\mathbf{O}\mathbf{N}} B|C$ .

This definition is inapplicable in the case where sets may be uncountably infinite, as no such  $\mathbf{O}$  can exist in this case. There may well be definitions of conditional independence that generalise better, and we refer to the discussions in Fritz (2020) and Constantinou and Dawid (2017) for some discussion of alternative definitions. One advantage of this definition is that it matches the version given by Cho and Jacobs (2019) which they showed coincides with the standard notion of conditional independence and so we don't have to show this in our particular case.

A particular case of interest is when a kernel  $\mathbf{K} : (X, W) \rightarrow \Delta(Y)$  can, for some  $\mathbf{L} : W \rightarrow \Delta(Y)$ , be written:

$$\mathbf{K} = \begin{array}{c} X \text{---} \boxed{\mathbf{L}} \text{---} Y \\ W \text{---} * \end{array} \quad (44)$$

Then  $Y \perp\!\!\!\perp_{\mathbf{K}} W|X$ .

## 2.6 Variables or vague variables?

Recall our definition of variables: functions from a sample space  $\Omega$  to some codomain set. We also recall a concern raised in our introduction: if actions affecting a measure of interest are vague, then potential outcome random variables *might* be ill-defined. Consider: how can it be that the degree to which we specify actions sometimes, but not always, allows a random variable to be well-defined? These concerns seem to be of different types – on the one hand,

we have the problem of whether my instructions are clear enough for you to follow them and produce the same results, and on the other hand the problem of whether an abstract sample space has the appropriate properties for a certain type of function to exist.

Consider also the definition of *variable* found in Pearl (2009):

By a *variable* we will mean an attribute, measurement or inquiry that may take on one of several possible outcomes, or values, from a specified domain. If we have beliefs (i.e., probabilities) attached to the possible values that a variable may attain, we will call that variable a random variable.

This is claimed to be identical to our definition of a variable – i.e. a measurable function on the sample space. However, we feel that a much closer match is the definition of a *qualitative statistical random variable* given by Menger (2003); roughly speaking, a qualitative statistical random variable is a vague function (our term) whose codomain is well-specified but whose domain is not. Menger offers examples of vague functions that take as arguments acts of measurement, or people in Chicago; in a very similar manner, Pearl’s definition offers examples of arguments that a variable may take, but does not offer examples of sample spaces that may form their domains.

We offer the following rough idea of how vague random variables can be thought about. A vague random variable like “X represents whether this coin lands on heads or tails” can be considered an instruction for whoever is reading to construct a concrete random variable whose domain is related to the set of observations that they might receive. These domains necessarily differ between individuals, and we postulate the existence of a “reality” that offers everyone observations that are sometimes similar in some respects. A vague random variable can be well-defined if the concrete random variables that everyone constructs allow everyone to agree on the result when they are given observations that are appropriately related.

This might seem an excessively pedantic way to describe a coin-flipping experiment. However, we think there that a story like this this may be important in causal models. At the start of this section we asked “how can the degree to which we specify actions sometimes, but not always, allows a random variable to be well-defined?” Our rough model of vague variables offers a solution to this question: sufficiently specific actions are sometimes enough to allow all parties to agree on the values once observations have taken place. We hypothesise that this question arises with variables representing consequences of actions because when it comes to taking actions there is an asymmetry that is extremely hard to avoid: I know more about what I am doing and why I am doing it than you do.

While we believe that this is a potentially fruitful line of inquiry, we won’t develop it here and will satisfy ourselves with a theory based on concrete variables.

### 3 Decision theoretic causal inference

Lattimore and Rohde (2019a) and Lattimore and Rohde (2019b) describe a novel approach to causal inference: rather than consider “one” causal model, they consider a pair of models; an observational and interventional model that share parameters.

We will use the theory of probability set out previously to see how such a model can arise if we are given a decision problem with some data. Our aim is ultimately to represent “causal effects” and “the consequences of my actions” in the same model, so that we can discuss issues like possible non-correspondence between causal effects and consequences in formal mathematical language rather than in English. Understanding how we can model decision problems is a first step, because while decision models don’t feature any notion of “causal effect”, consequences of actions are primitives. We will go on to consider how to combine decision models with models that define causal effects.

We suppose we have a decision problem of the following type: we will be given an observation that takes values in  $X$  and in response to this we can select any decision or stochastic mixture of decisions from  $D$ .  $X$  is the variable representing the question “what will we observe?” and  $D$  the question “what decision will we choose?”. We can consider a number of different strategies for selecting a decision, each of which corresponds to a Markov variable map  $S_\alpha : X \rightarrow \Delta(D)$ . The variable  $Y$  represents “what will we see when all is said and done?”, and it takes values in  $Y$ . After considering the available strategies, we want to select the strategy for which we expect to see the best ultimate outcome.

We will represent our uncertain answers to the questions  $X$ ,  $D$  and  $Y$  with probability distributions. We will allow for multiple probability distributions to be entertained as an answer; let hypotheses  $H$  represent the question “which model best captures this problem?”, taking values in  $H$ . Then for each strategy  $S_\alpha$ , our forecast will be represented by a joint probability  $P_\alpha \equiv P_\alpha^{XDY|H;P_\alpha} : H \rightarrow \Delta(X, D, Y)$ . Because observations come before we execute our strategy, we might assume that they will be unchanged by any choice of strategy:  $P_\alpha^{X|H} = P_\beta^{X|H}$  for all  $\alpha, \beta$ . We expect to choose a decision precisely in line with the strategy under consideration:  $P_\alpha^{D|X} = S_\alpha$ . Finally, our answer to  $Y$  will be the same under any strategy supposing we have the same observation, decision and hypothesis:  $P_\alpha^{Y|HD} = P_\beta^{Y|HD}$  for all  $\alpha, \beta$ .

Under these assumptions, there exists  $T[XY|HD] \in \mathcal{M}$  with  $X \perp\!\!\!\perp_T D|H$  such that for all  $\alpha$ ,

$$P_\alpha[XDY|H] \stackrel{krn}{=} T[X|H] \Rightarrow S_\alpha[D|X] \Rightarrow T[Y|XHD] \quad (45)$$

The proof is given in Appendix 6. Note that  $T[X|H]$  exists by virtue of the fact  $X \perp\!\!\!\perp_T D|H$ . While this independence is what enables Equation 45, in general  $X \not\perp\!\!\!\perp_{P_\alpha} D|H$ , so  $T$  cannot be a disintegration of  $P_\alpha$ . Modular probability allows us to specify  $T$ , which we call a *see-do model*, as a partial forecast to be

completed with a strategy  $\mathbf{S}_\alpha$  while also being able to use consistent names for variables that represent the same things (observations, decisions, consequences, hypotheses) whether their distributions are given by  $\mathbf{P}_\alpha$ ,  $\mathbf{T}$ , which are mutually incompatible conditional probabilities.

### 3.1 See-do models and classical statistics

A *statistical model* (or *statistical experiment*) is a collection of probability distributions indexed by some set  $\Theta$ . We can observe that  $\{\mathbf{T}[X|H]_h\}_{h \in H}$  is a collection of probability distributions indexed by  $H$ .

In statistical decision theory, as introduced by Wald (1950), we are given a statistical experiment  $\{\mathbb{P}_\theta \in \Delta(X)\}_\Theta$ , a decision set  $D$  and a loss  $l : \Theta \times D \rightarrow \mathbb{R}$ . A strategy  $\mathbf{S}_\alpha : X \rightarrow \Delta(D)$  is evaluated according to the risk functional  $R(\theta, \mathbf{S}_\alpha) = \sum_{x \in X} \sum_{d \in D} \mathbb{P}_\theta^x(\mathbf{S}_\alpha)_x^d l(h, d)$ .

Suppose we have a see-do model  $\mathbf{T}[XY|HD]$  with  $Y \perp\!\!\!\perp_{\mathbf{T}} X|HD$ , and suppose that the random variable  $Y$  is a “reverse utility” function taking values in  $\mathbb{R}$  for which low values are considered desirable. Then, defining a loss  $l : H \times D \rightarrow \mathbb{R}$  by  $l(h, d) = \sum_{y \in \mathbb{R}} y \mathbf{T}[Y|HD]_{h,d}^y$ , we have

$$\mathbb{E}_{\mathbf{P}_\alpha[XDY|H]}[Y] = \sum_{x \in X} \sum_{d \in D} \sum_{y \in Y} y (\mathbf{T}[X|H] \Rightarrow \mathbf{S}_\alpha[D|X] \Rightarrow \mathbf{T}[Y|XHD])_h^{x dy} \quad (46)$$

$$= \sum_{x \in X} \sum_{d \in D} \sum_{y \in Y} \mathbf{T}[X|H]_h^x \mathbf{S}_\alpha[D|X]_x^d \mathbf{T}[Y|HD]_{h,d}^y \quad (47)$$

$$= \sum_{x \in X} \sum_{d \in D} \mathbf{T}[X|H]_h^x (\mathbf{S}_\alpha)_x^d l(h, d) \quad (48)$$

$$= R(h, \mathbf{S}_\alpha) \quad (49)$$

That is, if we are given a see-do model where we interpret  $\mathbf{T}[X|H]$  as a statistical experiment and  $Y$  as a reversed utility, the expectation of the utility under the strategy forecast given in equation 45 is the risk of that strategy under hypothesis  $h$ .

### 3.2 Combs

The see-do model  $\mathbf{T}[XY|HD]$  is known as a *comb*. This structure was introduced by Chiribella et al. (2008) in the context of quantum circuit architecture, and Jacobs et al. (2019) adapted the concept to causal modelling.

A comb is a Markov kernel with a “hole” in it. We combine the see-do model with a strategy by putting the strategy “in the middle” of the see-do model (Equation 45), rather than attaching it to one end. While it is not a well-formed diagram in the language described in this paper, we can visualise combs as Markov kernels with holes:



$$\text{T}[XY|HD] = \begin{array}{c} H - \bullet - [T] - \bullet - X \\ \quad \quad \quad | \quad \quad \quad | \\ \quad \quad \quad D - [T] - Y \end{array} \quad (50)$$

$$= \text{H} \begin{array}{|c|} \hline \text{T} \\ \hline \end{array} \begin{array}{|c|} \hline \text{X D} \\ \hline \end{array} \text{Y} \quad (51)$$

We can take any strategy  $\mathbf{S}_\alpha[D|X]$  and drop it into the “hole” in 51 (as described in Equation 45) to get a forecast of the outcome of that strategy.

Dawid (2020) has described his decision theoretic approach to causal inference:

A fundamental feature of the DT approach is its consideration of the relationships between the various probability distributions that govern different regimes of interest. As a very simple example, suppose that we have a binary treatment variable  $T$ , and a response variable  $Y$ . We consider three different regimes [...] the first two regimes may be described as interventional, and the last as observational.

## 4 Causal Bayesian Networks

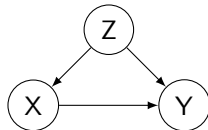
In the presentation of Pearl (2009), a Causal Bayesian Network posits an observational probability distribution such as  $P(X, Y)$ , and a set of interventional distributions, for example  $\{\mathbb{P}_h(X, Y | do(X = x))\}_{x \in X, h \in H}$ . Here we use notation similar to typical notation used for Causal Bayesian Networks and don't intend for these to necessarily be elements of any modelling context. For simplicity, we will consider a Causal Bayesian Network with only hard interventions on a single variable, e.g. interventions only of the form  $do(X = x)$ .

First we will offer some commentary

We can consider this an instance of a see-do model. To do so consistently within a modelling context  $\mathcal{M}$ , we need to distinguish observation and intervention variables - let the former retain the labels  $X, Y$  and call the latter  $X', Y'$ . Let  $D = \{do(X = x)\}_{x \in X}$ . Then a Causal Bayesian Network can be considered a see-do model  $\mathbf{T}[XYX'Y'|\mathbf{HD}]$  by identifying  $\mathbf{T}[XY|\mathbf{H}]_h := \mathbb{P}_h(X, Y)$  and  $\mathbf{T}[X'Y'|\mathbf{HD}]_{h, do(X=x)} := P_h(X, Y|do(X = x))$ .

We need to rename the consequence variables because otherwise we would have  $\mathbf{T}[XYXY|\mathbf{HD}]$  and the two X's and the two Y's would be deterministically equal by the “identical labels” rule

We can say a bit more about Causal Bayesian Networks. Suppose we have the network



Then, letting  $\mathbf{T}[XYZ|H]$  be the observational “see” model and  $\mathbf{T}[X'Y'Z'|HD]$  be the interventional “do” model with  $D$  the set of interventions  $\{do(X = x)\}_{x \in X}$  where we write  $x := do(X = x)$  for short, then we know by the backdoor adjustment rule that  $\mathbf{T}[X'Y'Z'|HD]_{hx}^{x'yz} \stackrel{krn}{=} \mathbf{T}[Z|H]_h^z \delta[x]^{x'} \mathbf{T}[Y|XZH]_{hx'z}^y$ .

Let  $\mathbf{U}[ZY|XH] = \mathbf{T}[Z|H] \Rightarrow \mathbf{T}[Y|XZH]$ , call  $\mathbf{T}[X|H]$  the “observational strategy” and  $\mathbf{D}_x[X|D]_x^{x'} \stackrel{krn}{=} \delta[x]^{x'}$  the interventional strategies for all  $x \in X$ . Then we have

$$\mathbf{T}[XYZ|H] = \mathbf{U}[Z|H] \Rightarrow \mathbf{T}[X|H] \Rightarrow \mathbf{U}[Y|XHZ] \quad (52)$$

$$\mathbf{T}[X'Y'Z'|HD] \stackrel{krn}{=} \mathbf{U}[Z|H] \Rightarrow \mathbf{D}[X|D] \Rightarrow \mathbf{U}[Y|XHZ] \quad (53)$$

So this simple example of a Causal Bayesian network is a “nested comb” where the outer comb  $\mathbf{T}[XYZX'Y'Z'|HD]$  is the “see” and “do” models, which are themselves generated by the inner comb  $\mathbf{U}[ZY|XH]$  with different choices  $\mathbf{T}[X|H]$  and  $\mathbf{D}[X|D]$  for the insert.

This is a simple example, but Jacobs et al. (2019) has used an “inner comb” representation of a general class of Causal Bayesian Networks to prove a sufficient identification condition which is itself slightly more general than the identification condition given by Tian and Pearl (2002).

## 5 Potential outcomes with and without counterfactuals

Potential outcomes is a widely used approach to causal modelling characterised by its use of “potential outcome” random variables. Potential outcome random variables are typically noted for being given counterfactual interpretations. For example, suppose we have something we want to model, call it TYT (“The Y Thing”), which we represent with a variable  $Y$ . Suppose we want to know how TYT behaves under different regimes 0 and 1 under which we want to know about TYT, and we use a variable  $W$  to indicate which regime holds at a given point in time. A potential outcomes model will introduce the two additional “potential outcome” variables  $(Y(0), Y(1))$ . What these variables represent can be given a counterfactual interpretation like “ $Y(0)$  represents what TYT would be under regime 0, whether or not regime 0 is the actual regime” and similarly “ $Y(1)$  represents what TYT would be under regime 1, whether or not regime 1 is the actual regime”. Note that we say “what TYT would be” rather than “what  $Y$  would be” as “what would  $Y$  be if  $W$  was 0 if  $W$  was actually 1” is not a question we can ask of random variables, but it is one that might make sense for the things we use random variables to model.

This is a key point, so it is worth restating: the assumption that potential outcome variables agree with “the value TYT would take” under fixed regimes regardless of the “actual” value of the regime seems to be a critical assumption that distinguishes potential outcome variables from arbitrary random variables

that happen to take values in the same space as  $Y$ . However, this assumption can only be stated by making reference to the informally defined “TYT” and the informal distinction between the supposed and the actual value of the regime.

The potential outcomes framework features other critical assumptions that relate potential outcome variables to things that are only informally defined. For example, Rubin (2005) defines the *Stable Unit Treatment Value Assumption* (SUTVA) as:

SUTVA (stable unit treatment value assumption) [...] comprises two subassumptions. First, it assumes that there is no interference between units (Cox 1958); that is, neither  $Y_i(1)$  nor  $Y_i(0)$  is affected by what action any other unit received. Second, it assumes that there are no hidden versions of treatments; no matter how unit  $i$  received treatment 1, the outcome that would be observed would be  $Y_i(1)$  and similarly for treatment 0

“Versions of treatments” do not appear within typical potential outcomes models, so this is also an assumption about how “the thing we are trying to model” behaves rather than an assumption stated within the model.

Given informal assumptions like this, one may be motivated to “formalize” them. More specifically, one might be motivated to ask whether there is some larger class of models that, under conditions corresponding to the informal conditions above yield regular potential outcome models?

I have a vague intuition here that you always need some kind of assumption like “my model is faithful to the real thing”, but if you are stating fairly specific conditions in English you should also be able to state them mathematically. Among other reasons, this is useful because it’s easier for other people to know what you mean when you state them.

The approach we have introduced here, motivated by decision problems, has in the past been considered a means of avoiding counterfactual statements, which has been considered a positive by some (Dawid, 2000) and a negative by others:

[...] Dawid, in our opinion, incorrectly concludes that an approach to causal inference based on “decision analysis” and free of counterfactuals is completely satisfactory for addressing the problem of inference about the effects of causes. (Robins and Greenland, 2000)

It may be surprising to some, then, that we can use see-do models to formally state these key assumptions associated with potential outcomes models. Furthermore, we will argue that potential outcomes are typically a strategy to motivate inductive assumptions in see-do models, and we will show that the counterfactual interpretation is unnecessary for this purpose.

## 5.1 Potential outcomes in see-do models

A basic property of potential outcomes models is the relation between variables representing actual outcomes and variables representing potential outcomes, which was stated informally in the opening paragraph of this section.

In the following definition,  $Y(W) = (Y(w))_{w \in W}$ .

**Definition 5.1** (Potential outcomes). Given a Markov kernel space  $(\mathbf{K}, E, F)$ , a collection of variables  $\{Y, Y(W), W\}$  where  $Y$  and  $Y(W)$  are random variables and  $W$  could be either a state or a random variable is a *potential outcome submodel* if  $\mathbf{K}[Y|WY(W)]$  exists and  $\mathbf{K}[Y|WY(W)]_{ij_1j_2 \dots j_{|W|}} = \delta[j_i]$ .

How this will change: a potential outcomes model is a comb  $\mathbf{K}[Y(W)|H] \Rightarrow \mathbf{K}[Y|WY(W)]$ .

We allow  $X$  to be a state or a random variable to cover the cases where potential outcomes models feature as submodels of observation models (in which case  $X$  is a random variable) or as submodels of consequence models (in which case  $X$  may be a state variable).

As an aside that we could define stochastic potential outcomes if we allow the variables  $Y(x)$  to take values in  $\Delta(Y)$  rather than in  $Y$ , and then require  $\mathbf{K}[Y|XY(X)]_{ij_1j_2 \dots j_{|X|}} = j_i$  (where  $j_i$  is an element of  $\Delta(Y)$ ). This is more complex to work with and rarely seen in practice, but it is worth noting that Definition 5.1 can be generalised to cover models where  $Y(x)$  describes the value  $Y$  would take if  $X$  were  $x$  *with uncertainty*.

An arbitrary see-do model featuring potential outcome submodels does not necessarily allow for the formal statement of the counterfactual interpretation of potential outcomes. Here we use TYT (“the actual thing”) and “regime” to refer to the things we are actually trying to model. We require that  $Y \stackrel{a.s.}{=} Y(w)$  conditioned on  $W = w$ . If we add an interpretation to this model saying  $Y$  represents TYT and  $W$  represents the regime, then we have “for all  $w$ ,  $Y(w)$  is equal to  $Y$  which represents TYT under the regime  $w$ ”. However, this does not guarantee that our model has anything that reasonably represents “what TYT would be equal to under supposed regime  $w$  if the regime is actually  $w'$ ”.

We propose *parallel potential outcome submodels* as a means of formalising statements about what how TYT behaves under “supposed” and “actual” regimes:

**Definition 5.2** (Parallel potential outcomes). Given a Markov kernel space  $(\mathbf{K}, E, F)$ , a collection of variables  $\{Y_i, Y(W), W_i\}$ ,  $i \in [n]$ , where  $Y_i$  and  $Y(W)$  are random variables and  $W_i$  could be either a state or random variables is a *parallel potential outcome submodel* if  $\mathbf{K}[Y_i|W_iY(W)]$  exists and  $\mathbf{K}[Y_i|W_iY(W)]_{kj_1j_2 \dots j_{|W|}} = \delta[j_k]$ .

How this will change: a parallel potential outcomes model is a comb  $\mathbf{K}[Y(W)|H] \Rightarrow \mathbf{K}[Y_i|W_iY(W)]$ .

A parallel potential outcomes model features a sequence of  $n$  “parallel” outcome variables  $Y_i$  and  $n$  “regime proposals”  $W_i$ , with the property that if the

regime proposal  $W_i = w_i$  then the corresponding outcome  $Y_i \stackrel{a.s.}{=} Y(w_i)$ . We can identify a particular index, say  $n = 1$ , with the actual world and the rest of the indices with supposed worlds. Thus  $Y_1$  represents the value of TYT in the actual world and  $Y_i$   $i \neq 1$  represents TYT under a supposed regime  $W_i$ . Given such an interpretation, the fact that  $Y_i \stackrel{a.s.}{=} Y(w_i)$  can be interpreted as assuming “for all  $w$ , if the supposed regime  $W_i$  is  $w$  then the corresponding outcome will be almost surely equal to  $Y(w)$ , regardless of the value of the actual regime  $W_1$ ”, which is our original counterfactual assumption.

We do not intend to defend this as the only way that counterfactuals can be modeled, or even that it is appropriate to capture the idea of counterfactuals at all. It is simply a way that we can model the counterfactual assumption typically associated with potential outcomes. We will show that parallel potential outcome submodels correspond precisely to *extendably exchangeable* and *deterministically reproducible* submodels of Markov kernel spaces.

## 5.2 Parallel potential outcomes representation theorem

Exchangeable sequences of random variables are sequences whose joint distribution is unchanged by permutation. Independent and identically distributed random variables are one example: if  $X_1$  is the result of the first flip of a coin that we know to be fair and  $X_2$  is the second flip then  $\mathbb{P}[X_1 X_2] = \mathbb{P}[X_2 X_1]$ . There are also many examples of exchangeable sequences that are not mutually independent and identically distributed – for example, if we want to use random variables  $Y_1$  and  $Y_2$  to model our subjective uncertainty regarding two flips of a coin of unknown fairness, we regard our initial uncertainty for each flip to be equal  $\mathbb{P}[Y_1] = \mathbb{P}[Y_2]$  and we regard our state of knowledge of the second flip after observing only the first will be the same as our state of knowledge of the first flip after observing only the second  $\mathbb{P}[Y_2|Y_1] = \mathbb{P}[Y_1|Y_2]$ , then our model of subjective uncertainty is exchangeable.

De Finetti’s representation theorem establishes the fact that any infinite exchangeable sequence  $Y_1, Y_2, \dots$  can be modeled by the product of a *prior* probability  $\mathbb{P}[J]$  with  $J$  taking values in the set of marginal probabilities  $\Delta(Y)$  and a conditionally independent and identically distributed Markov kernel  $\mathbb{P}[Y_A|J]_j^{y_A} = \prod_{i \in A} \mathbb{P}[Y_i|J]_j^{y_i}$ .

We extend the idea of exchangeable sequences to cover both random variables and state variables, and we show that a similar representation theorem holds for potential outcomes. De Finetti’s original theorem introduced the variable  $J$  that took values in the set of marginal distributions over a single observation; the set of potential outcome variables plays an analogous role taking values in the set of functions from propositions to outcomes.

The representation theorem for potential outcomes is somewhat simpler than De Finetti’s original theorem due to the fact that potential outcomes are usually assumed to be *deterministically reproducible*; in the parallel potential outcomes model, this means that for  $j \neq i$ , if  $W_j$  and  $W_i$  are equal then  $Y_j$  and  $Y_i$  will be almost surely equal. This assumption of determinism means that we can avoid appeal to a law of large numbers in the proof of our theorem.

An interesting question is whether there is a similar representation theorem for potential outcomes without the assumption of deterministic reproducibility. I'm reasonably confident that this is a straightforward corollary of the representation theorem proved in my thesis. However, this requires maths not introduced in this draft of the paper.

Extendably exchangeable sequences can be permuted without changing their conditional probabilities, and can be extended to arbitrarily long sequences while maintaining this property. We consider here sequences that are exchangeable conditional on some variable; this corresponds to regular exchangeability if the conditioning variable is  $*$  where  $*_i = 1$ .

**Definition 5.3** (Exchangeability). Given a Markov kernel space  $(\mathbf{K}, E, F)$ , a sequence of variables  $((D_i, Y_i))_{i \in [n]}$  with  $Y_i$  random variables is *exchangeable* conditional on  $Z$  if, defining  $Y_{[n]} = (Y_i)_{i \in [n]}$  and  $D_{[n]} = (D_i)_{i \in [n]}$ ,  $\mathbf{K}[Y_{[n]}|D_{[n]}Z]$  exists and for any bijection  $\pi : [n] \rightarrow [n]$   $\mathbf{K}[Y_{\pi([n])}|D_{\pi([n])}Z] = \mathbf{K}[Y_{[n]}|D_{[n]}Z]$ .

**Definition 5.4** (Extension). Given a Markov kernel space  $(\mathbf{K}, E, F)$ ,  $(\mathbf{K}', E', F')$  is an *extension* of  $(\mathbf{K}, E, F)$  if there is some random variable  $X$  and some state variable  $U$  such that  $\mathbf{K}'[X|U]$  exists and  $\mathbf{K}'[X|U] = \mathbf{K}$ .

If  $(\mathbf{K}', E', F')$  is an extension of  $(\mathbf{K}, E, F)$  we can identify any random variable  $Y$  on  $(\mathbf{K}, E, F)$  with  $Y \circ X$  on  $(\mathbf{K}', E', F')$  and any state variable  $D$  with  $D \circ U$  on  $(\mathbf{K}', E', F')$  and under this identification  $\mathbf{K}'[Y \circ X|D \circ U]$  exists iff  $\mathbf{K}[Y|D]$  exists and  $\mathbf{K}'[Y \circ X|D \circ U] = \mathbf{K}[Y|D]$ . To avoid proliferation of notation, if we propose  $(\mathbf{K}, E, F)$  and later an extension  $(\mathbf{K}', E', F')$ , we will redefine  $\mathbf{K} := \mathbf{K}'$  and  $Y := Y \circ X$  and  $D := D \circ U$ .

I think this is a very standard thing to do – propose some  $X$  and  $\mathbb{P}(X)$  then introduce some random variable  $Y$  and  $\mathbb{P}(XY)$  as if the sample space contained both  $X$  and  $Y$  all along.

**Definition 5.5** (Extendably exchangeable). Given a Markov kernel space  $(\mathbf{K}, E, F)$ , a sequence of variables  $((D_i, Y_i))_{i \in [n]}$  and a state variable  $Z$  with  $Y_i$  random variables is *extendably exchangeable* if there exists an extension of  $\mathbf{K}$  with respect to which  $((D_i, Y_i))_{i \in \mathbb{N}}$  is exchangeable conditional on  $Z$ .

Here that we identify  $Z$  and  $((D_i, Y_i))_{i \in [n]}$  defined on the extension with the original variables defined on  $(\mathbf{K}, E, F)$  while  $((D_i, Y_i))_{i \in \mathbb{N} \setminus [n]}$  may be defined only on the extension.

Deterministically reproducible sequences have the property that repeating the same decision gets the same response with probability 1. This could be a model of an experiment that exhibits no variation in results (e.g. every time I put green paint on the page, the page appears green), or an assumption about collections of “what-ifs” (e.g. if I went for a walk an hour ago, just as I actually did, then I definitely would have stubbed my toe, just like I actually did). Incidentally, many consider that this assumption is false concerning what-if questions about things that exhibit quantum behaviour.

**Definition 5.6** (Deterministically reproducible). Given a Markov kernel space  $(\mathbf{K}, E, F)$ , a sequence of variables  $((D_i, Y_i))_{i \in [n]}$  with  $Y_i$  random variables is *deterministically reproducible* conditional on  $Z$  if  $n \geq 2$ ,  $\mathbf{K}[Y_{[n]}|D_{[n]}Z]$  exists and  $\mathbf{K}[Y_{\{i,j\}}|D_{\{i,j\}}Z]_{kk}^{lm} = \mathbb{I}[l = m]\mathbf{K}[Y_i|D_iZ]_k^l$  for all  $i, j, k, l, m$ .

**Theorem 5.7** (Potential outcomes representation). *Given a Markov kernel space  $(\mathbf{K}, E, F)$  along with a sequence of variables  $((D_i, Y_i))_{i \in [n]}$  with  $n \geq 2$  and a conditioning variable  $Z$ ,  $(\mathbf{K}, E, F)$  can be extended with a set of variables  $Y(D) := (Y(i))_{i \in D}$  such that  $\{Y_i, Y(D), D_i\}$  is a parallel potential outcome submodel if and only if  $((D_i, Y_i))_{i \in [n]}$  is extendably exchangeable and deterministically reproducible conditional on  $Z$ .*

*Proof.* If: Because  $((D_i, Y_i))_{i \in [n]}$  is extendably exchangeable, we can without loss of generality assume  $n \geq |D|$ .

Let  $e = (e_i)_{i \in [|D|]}$ . Introduce the variable  $Y(i)$  for  $i \in D$  such that  $\mathbf{K}[Y(D)|D_{[D]}Z]_{ez} = \mathbf{K}[Y_D|D_DZ]_{ez}$  and introduce  $X_i$ ,  $i \in D$  such that  $\mathbf{K}[X_i|D_iZY(D)]_{e_i z j_1 \dots j_{|D|}}^{x_i} = \delta[j_{e_i}]^{x_i}$ . Clearly  $\{X_{[n]}, D_{[n]}, Y(D)\}$  is a parallel potential outcome submodel. We aim to show that  $\mathbf{K}[Y_{[n]}|D_{[n]}Z] = \mathbf{K}[X_{[n]}|D_{[n]}Z]$ .

Let  $y := (y_i)_{i \in [D]} \in Y^{|D|}$ ,  $d := (d_i)_{i \in [n]} \in D^{[n]}$ ,  $x := (x_i)_{i \in [n]} \in Y^{[n]}$ .

$$\mathbf{K}[X_n|D_nZ]_{dz}^x = \sum_{y \in Y^{|D|}} \mathbf{K}[X_{[n]}|D_nZY(D)]_{dzy}^x \mathbf{K}[Y(D)|D_{[n]}Z]_{dz}^y \quad (54)$$

$$= \sum_{y \in Y^{|D|}} \prod_{i \in [n]} \delta[y_{d_i}]^{x_i} \mathbf{K}[Y(D)|D_nZ]_{dz}^y \quad (55)$$

Wherever  $d_i = d_j := \alpha$ , every term in the above expression will contain the product  $\delta[\alpha]^{x_i} \delta[\alpha]^{x_j}$ . If  $x_i \neq x_j$ , this will always be zero. By deterministic reproducibility,  $d_i = d_j$  and  $x_i \neq x_j$  implies  $\mathbf{K}[Y_{[n]}|D_{[n]}Z]_{dz}^{z^x} = 0$  also. We need to check for equality for sequences  $x$  and  $d$  such that wherever  $d_i = d_j$ ,  $x_i = x_j$ . In this case,  $\delta[\alpha]^{x_i} \delta[\alpha]^{x_j} = \delta[\alpha]^{x_i}$ . Let  $Q_d \subset [n] := \{i \nmid \exists i \in [n] : j < i \text{ \& } d_j = d_i\}$ , i.e.  $Q$  is the set of all indices such that  $d_i$  is the first time this value appears in  $d$ . Note that  $Q_d$  is of size at most  $|D|$ . Let  $Q_d^C = [n] \setminus Q_d$ , let  $R_d \subset D : \{d_i | i \in Q_d\}$  i.e. all the elements of  $D$  that appear at least once in the sequence  $d$  and let  $R_d^C = D \setminus R_d$ .

Let  $y' = (y_i)_{i \in Q_d^C}$ ,  $x_{Q_d} = (x_i)_{i \in Q_d}$ ,  $Y(R_d) = (Y_d)_{d \in R_d}$  and  $Y(S_d) = (Y_d)_{d \in S_d}$ .

$$\mathbf{K}[X_{[n]}|D_{[n]}Z]_{dz}^x = \sum_{y \in Y^{[D]}} \prod_{i \in Q_d} \delta[y_{d_i}]^{x_i} \mathbf{K}[Y(D)|D_{[n]}Z]_{dz}^y \quad (56)$$

$$= \sum_{y' \in Y^{[R_d^C]}} \mathbf{K}[Y(R_d)Y(R_d^C)|D_{Q_d}D_{Q_d^C}Z]_{d_{Q_d}d_{Q_d^C}z}^{x_{Q_d}y'} \quad (57)$$

$$= \sum_{y' \in Y^{[R_d^C]}} \mathbf{K}[Y_{R_d}Y_{R_d^C}|D_{Q_d}D_{Q_d^C}Z]_{dz}^{x_{Q_d}y'} \quad (58)$$

$$= \sum_{y' \in Y^{[R_d^C]}} \mathbf{K}[Y_{[n]}|D_{[n]}Z]_{dz}^{x_{Q_d}y'} \quad (\text{using exchangeability}) \quad (59)$$

Note that

Only if: We aim to show that the sequences  $Y_{[n]}$  and  $D_{[n]}$  in a parallel potential outcomes submodel are exchangeable and deterministically reproducible.  $\square$

## 6 Appendix:see-do model representation

### Modularise the treatment of probability

**Theorem 6.1** (See-do model representation). *Suppose we have a decision problem that provides us with an observation  $x \in X$ , and in response to this we can select any decision or stochastic mixture of decisions from a set  $D$ ; that is we can choose a “strategy” as any Markov kernel  $\mathbf{S} : X \rightarrow \Delta(D)$ . We have a utility function  $u : Y \rightarrow \mathbb{R}$  that models preferences over the potential consequences of our choice. Furthermore, suppose that we maintain a denumerable set of hypotheses  $H$ , and under each hypothesis  $h \in H$  we model the result of choosing some strategy  $\mathbf{S}$  as a joint probability over observations, decisions and consequences  $\mathbb{P}_{h,\mathbf{S}} \in \Delta(X \times D \times Y)$ .*

*Define  $X, Y$  and  $D$  such that  $X_{xdy} = x$ ,  $Y_{xdy} = y$  and  $D_{xdy} = d$ . Then making the following additional assumptions:*

1. *Holding the hypothesis  $h$  fixed the observations as have the same distribution under any strategy:  $\mathbb{P}_{h,\mathbf{S}}[X] = \mathbb{P}_{h,\mathbf{S}'}[X]$  for all  $h, \mathbf{S}, \mathbf{S}'$  (observations are given “before” our strategy has any effect)*
2. *The chosen strategy is a version of the conditional probability of decisions given observations:  $\mathbf{S} = \mathbb{P}_{h,\mathbf{S}}[D|X]$*
3. *There exists some strategy  $\mathbf{S}$  that is strictly positive*
4. *For any  $h \in H$  and any two strategies  $\mathbf{Q}$  and  $\mathbf{S}$ , we can find versions of each disintegration such that  $\mathbb{P}_{h,\mathbf{Q}}[Y|DX] = \mathbb{P}_{h,\mathbf{S}}[Y|DX]$  (our strategy tells*



us nothing about the consequences that we don't already know from the observations and decisions)

Then there exists a unique see-do model  $(\mathbf{T}, \mathbf{H}', \mathbf{D}', \mathbf{X}', \mathbf{Y}')$  such that  $\mathbb{P}_{h,\mathbf{S}}[\mathbf{XDY}]^{ijk} = \mathbf{T}[\mathbf{X}'|\mathbf{H}']_h^i \mathbf{S}_i^j \mathbf{T}[\mathbf{Y}'|\mathbf{X}'\mathbf{H}'\mathbf{D}']_{ijk}^k$ .

*Proof.* Consider some probability  $\mathbb{P} \in \Delta(X \times D \times Y)$ . By the definition of disintegration (section ??), we can write

$$\mathbb{P}[\mathbf{XDY}]^{ijk} = \mathbb{P}[\mathbf{X}]^i \mathbb{P}[\mathbf{D}|\mathbf{X}]_i^j \mathbb{P}[\mathbf{Y}|\mathbf{XD}]_{ij}^k \quad (60)$$

Fix some  $h \in H$  and some strictly positive strategy  $\mathbf{S}$  and define  $\mathbf{T} : H \times D \rightarrow \Delta(X \times Y)$  by

$$\mathbf{T}_{hj}^{kl} = \mathbb{P}_{h,\mathbf{S}}[\mathbf{X}]^k \mathbb{P}_{h,\mathbf{S}}[\mathbf{Y}|\mathbf{XD}]_{kj}^l \quad (61)$$

Note that because  $\mathbf{S}$  is strictly positive and by assumption  $\mathbf{S} = \mathbb{P}_{h,\mathbf{S}}[\mathbf{D}|\mathbf{X}]$ ,  $\mathbb{P}_{h,\mathbf{S}}[\mathbf{D}]$  is also strictly positive. Therefore  $\mathbb{P}_{h,\mathbf{S}}[\mathbf{Y}|\mathbf{D}]$  is unique and therefore  $\mathbf{T}$  is also unique.

Define  $\mathbf{X}'$  and  $\mathbf{Y}'$  by  $\mathbf{X}'_{xy} = x$  and  $\mathbf{Y}'_{xy} = y$ . Define  $\mathbf{H}'$  and  $\mathbf{D}'$  by  $\mathbf{H}'_{hd} = h$  and  $\mathbf{D}'_{hd} = d$ .

We then have

$$\mathbf{T}[\mathbf{X}'|\mathbf{H}'\mathbf{D}']_{hj}^k = \mathbf{T}\mathbf{X}'_{hj}^k \quad (62)$$

$$= \sum_l \mathbf{T}_{hj}^{kl} \quad (63)$$

$$= \mathbb{P}_{h,\mathbf{S}}[\mathbf{X}]^k \quad (64)$$

$$= \mathbf{T}[\mathbf{X}'|\mathbf{H}'\mathbf{D}']_{hj'}^k \quad (65)$$

Thus  $\mathbf{X}' \perp\!\!\!\perp_{\mathbf{T}} \mathbf{D}'|\mathbf{H}'$  and so  $\mathbf{T}[\mathbf{X}'|\mathbf{H}']$  exists (section 2.5) and  $(\mathbf{T}, \mathbf{H}', \mathbf{D}', \mathbf{X}', \mathbf{Y}')$  is a see-do model.

Applying Equation 60 to  $\mathbb{P}_{h,\mathbf{S}}$ :

$$\mathbb{P}_{h,\mathbf{S}}[\mathbf{XDY}]^{ijk} = \mathbb{P}_{h,\mathbf{S}}[\mathbf{X}]^i \mathbb{P}_{h,\mathbf{S}}[\mathbf{D}|\mathbf{X}]_i^j \mathbb{P}_{h,\mathbf{S}}[\mathbf{Y}|\mathbf{XD}]_{ij}^k \quad (66)$$

$$= \mathbb{P}_{h,\mathbf{S}}[\mathbf{X}]^i \mathbb{P}_{h,\mathbf{S}}[\mathbf{Y}|\mathbf{XD}]_{ij}^k \quad (67)$$

$$= \mathbb{P}_{h,\mathbf{S}}[\mathbf{D}|\mathbf{X}]_i^j \mathbf{T}[\mathbf{X}'\mathbf{Y}'|\mathbf{H}'\mathbf{D}']_{hj}^{ik} \quad (68)$$

$$= \mathbf{S}_i^j \mathbf{T}[\mathbf{X}'\mathbf{Y}'|\mathbf{H}'\mathbf{D}']_{hj}^{ik} \quad (69)$$

$$= \mathbf{S}_i^j \mathbf{T}[\mathbf{X}'|\mathbf{H}'\mathbf{D}']_{hj}^i \mathbf{T}[\mathbf{Y}'|\mathbf{X}'\mathbf{H}'\mathbf{D}']_{ihj}^k \quad (70)$$

$$= \mathbf{T}[\mathbf{X}'|\mathbf{H}']_h^i \mathbf{S}_i^j \mathbf{T}[\mathbf{Y}'|\mathbf{X}'\mathbf{H}'\mathbf{D}']_{ihj}^k \quad (71)$$

Consider some arbitrary alternative strategy  $\mathbf{Q}$ . By assumption

$$\mathbb{P}_{h,\mathbf{S}}[\mathbf{X}]^i = \mathbb{P}_{h,\mathbf{Q}}[\mathbf{X}]^i \quad (72)$$

$$\mathbb{P}_{h,\mathbf{S}}[\mathbf{Y}|\mathbf{XD}]_{ij}^k = \mathbb{P}_{h,\mathbf{Q}}[\mathbf{Y}|\mathbf{XD}]_{ij}^k \text{ for some version of } \mathbb{P}_{h,\mathbf{Q}}[\mathbf{Y}|\mathbf{XD}] \quad (73)$$

It follows that, for some version of  $\mathbb{P}_{h,\mathbf{Q}}[\mathbf{Y}|\mathbf{XD}]$ ,

$$\mathbf{T}_{hj}^{kl} = \mathbb{P}_{h,\mathbf{Q}}[\mathbf{X}]^k \mathbb{P}_{h,\mathbf{Q}}[\mathbf{Y}|\mathbf{XD}]_{kj}^l \quad (74)$$

Then by substitution of  $\mathbf{Q}$  for  $\mathbf{S}$  in Equation 66 and working through the same steps

$$\mathbb{P}_{h,\mathbf{S}}[\mathbf{XDY}]^{ijk} = \mathbf{T}[\mathbf{X}'|\mathbf{H}']_h^i \mathbf{Q}_i^j \mathbf{T}[\mathbf{Y}'|\mathbf{X}'\mathbf{H}'\mathbf{D}']_{ij}^k \quad (75)$$

As  $\mathbf{Q}$  was arbitrary, this holds for all strategies.  $\square$

## 7 Appendix: Connection is associative

This will be proven with string diagrams, and consequently generalises to the operation defined by Equation ?? in other Markov kernel categories.

Define

$$\mathbf{l}_{K..} := \mathbf{l}_K \setminus \mathbf{l}_L \setminus \mathbf{l}_J \quad (76)$$

$$\mathbf{l}_{KL.} := \mathbf{l}_K \cap \mathbf{l}_L \setminus \mathbf{l}_J \quad (77)$$

$$\mathbf{l}_{K.J} := \mathbf{l}_K \cap \mathbf{l}_J \setminus \mathbf{l}_L \quad (78)$$

$$\mathbf{l}_{KLJ} := \mathbf{l}_K \cap \mathbf{l}_L \cap \mathbf{l}_J \quad (79)$$

$$\mathbf{l}_{L.} := \mathbf{l}_L \setminus \mathbf{l}_K \setminus \mathbf{l}_J \quad (80)$$

$$\mathbf{l}_{LJ} := \mathbf{l}_L \cap \mathbf{l}_J \setminus \mathbf{l}_K \quad (81)$$

$$\mathbf{l}_{..J} := \mathbf{l}_J \setminus \mathbf{l}_K \setminus \mathbf{l}_L \quad (82)$$

$$\mathbf{o}_{K..} := \mathbf{o}_K \setminus \mathbf{l}_N \setminus \mathbf{l}_J \quad (83)$$

$$\mathbf{o}_{KL.} := \mathbf{o}_K \cap \mathbf{l}_L \setminus \mathbf{l}_J \quad (84)$$

$$\mathbf{o}_{K.J} := \mathbf{o}_K \cap \mathbf{l}_J \setminus \mathbf{l}_L \quad (85)$$

$$\mathbf{o}_{KLJ} := \mathbf{o}_K \cap \mathbf{l}_L \cap \mathbf{l}_J \quad (86)$$

$$\mathbf{o}_{L.} := \mathbf{o}_L \setminus \mathbf{l}_J \quad (87)$$

$$\mathbf{o}_{LJ} := \mathbf{o}_L \cap \mathbf{l}_J \quad (88)$$

Also define

$$(\mathbf{P}, \mathbf{l}_P, \mathbf{o}_P) := \mathbf{K} \rightrightarrows \mathbf{L} \quad (89)$$

$$(\mathbf{Q}, \mathbf{l}_Q, \mathbf{o}_Q) := \mathbf{L} \rightrightarrows \mathbf{J} \quad (90)$$

Then

$$(\mathbf{K} \Rightarrow \mathbf{L}) \Rightarrow \mathbf{J} = \mathbf{P} \Rightarrow \mathbf{J} \quad (91)$$

$$= \begin{array}{c} \text{Diagram: } \mathbf{P} \Rightarrow \mathbf{J} \\ \text{Inputs: } l_{P.}, l_{P.J}, l_{.J} \\ \text{Outputs: } o_{P.}, o_{P.J}, o_J \\ \text{Box } \mathbf{P} \text{ connects } l_{P.} \text{ to } o_{P.} \text{ and } l_{P.J} \text{ to } o_{P.J}. \\ \text{Box } \mathbf{J} \text{ connects } l_{.J} \text{ to } o_J. \end{array} \quad (92)$$

$$= \begin{array}{c} \text{Diagram: } \mathbf{K} \Rightarrow \mathbf{L} \Rightarrow \mathbf{J} \\ \text{Inputs: } l_{K..}, l_{KL.}, l_{.L.}, l_{K.J}, l_{KLJ}, l_{.LJ}, l_{..J} \\ \text{Outputs: } o_{K..}, o_{KL.}, o_{K.J}, o_{KLJ}, o_{L.}, o_{LJ}, o_J \\ \text{Box } \mathbf{K} \text{ connects } l_{K..} \text{ to } o_{K..} \text{ and } l_{KL.} \text{ to } o_{KL.}. \\ \text{Box } \mathbf{L} \text{ connects } l_{.L.} \text{ to } o_{L.} \text{ and } l_{K.J} \text{ to } o_{K.J}. \\ \text{Box } \mathbf{J} \text{ connects } l_{KLJ} \text{ to } o_{KLJ} \text{ and } l_{.LJ} \text{ to } o_{LJ}. \\ \text{Box } \mathbf{J} \text{ also connects } l_{..J} \text{ to } o_J. \end{array} \quad (93)$$

$$\stackrel{\text{perm}}{=} \begin{array}{c} \text{Diagram: } \mathbf{K} \Rightarrow \mathbf{L} \Rightarrow \mathbf{J} \text{ (permuted)} \\ \text{Inputs: } l_{K..}, l_{KL.}, l_{K.J}, l_{KLJ}, l_{.L.}, l_{.LJ}, l_{..J} \\ \text{Outputs: } o_{K..}, o_{KL.}, o_{K.J}, o_{KLJ}, o_{L.}, o_{LJ}, o_J \\ \text{Box } \mathbf{K} \text{ connects } l_{K..} \text{ to } o_{K..} \text{ and } l_{KL.} \text{ to } o_{KL.}. \\ \text{Box } \mathbf{L} \text{ connects } l_{K.J} \text{ to } o_{K.J} \text{ and } l_{KLJ} \text{ to } o_{KLJ}. \\ \text{Box } \mathbf{J} \text{ connects } l_{.L.} \text{ to } o_{L.} \text{ and } l_{.LJ} \text{ to } o_{LJ}. \\ \text{Box } \mathbf{J} \text{ also connects } l_{..J} \text{ to } o_J. \end{array} \quad (94)$$

$$= \begin{array}{c} \text{Diagram: } \mathbf{K} \Rightarrow \mathbf{Q} \\ \text{Inputs: } l_{K.}, l_{KQ}, l_{.Q} \\ \text{Outputs: } o_{K.}, o_{KQ}, o_Q \\ \text{Box } \mathbf{K} \text{ connects } l_{K.} \text{ to } o_{K.} \text{ and } l_{KQ} \text{ to } o_{KQ}. \\ \text{Box } \mathbf{Q} \text{ connects } l_{.Q} \text{ to } o_Q. \end{array} \quad (95)$$

$$= \mathbf{K} \Rightarrow (\mathbf{L} \Rightarrow \mathbf{J}) \quad (96)$$

## 8 Appendix: String Diagram Examples

Recall the definition of *connection*:

**Definition 8.1** (Connection).

$$\mathbf{K} \Rightarrow \mathbf{L} := \begin{array}{c} \text{Diagram: } \mathbf{K} \Rightarrow \mathbf{L} \\ \text{Inputs: } l_{F.}, l_{FS}, l_{.S} \\ \text{Outputs: } o_{F.}, o_{FS}, o_S \\ \text{Box } \mathbf{K} \text{ connects } l_{F.} \text{ to } o_{F.} \text{ and } l_{FS} \text{ to } o_{FS}. \\ \text{Box } \mathbf{L} \text{ connects } l_{.S} \text{ to } o_S. \end{array} \quad (97)$$

$$:= \mathbf{J} \quad (98)$$

$$\mathbf{J}_{yqr}^{zxw} = \mathbf{K}_{yq}^{zx} \mathbf{L}_{xqr}^w \quad (99)$$

Equation 97 can be broken down to the product of four Markov kernels, each

of which is itself a tensor product of a number of other Markov kernels:

$$(\mathbf{J}, (\mathbf{l}_{F\cdot}, \mathbf{l}_{FS}, \mathbf{l}_S), (\mathbf{O}_{F\cdot}, \mathbf{O}_{FS}, \mathbf{O}_S)) = \left[ \begin{array}{c} \mathbf{l}_{F\cdot} \\ \mathbf{l}_{FS} \\ \mathbf{l}_S \end{array} \right] \left[ \begin{array}{c} \boxed{\mathbf{K}} \\ \hline \hline \end{array} \right] \left[ \begin{array}{c} \hline \hline \end{array} \right] \left[ \begin{array}{c} \mathbf{O}_{FS} \\ \mathbf{O}_{F\cdot} \\ \mathbf{O}_S \end{array} \right] \quad (100)$$

$$(101)$$

## 9 Markov variable maps and variables form a Markov category

In the following, given *arbitrary measurable sets*  $(X, \mathcal{X})$  and  $(Y, \mathcal{Y})$ , a Markov kernel is a function  $\mathbf{K} : X \times \mathcal{Y} \rightarrow [0, 1]$  such that

- For every  $A \in \mathcal{Y}$ , the function  $x \mapsto \mathbf{K}(x, A)$  is  $\mathcal{X}$ -measurable
- For every  $x \in X$ , the function  $A \mapsto \mathbf{K}(x, A)$  is a probability measure on  $(Y, \mathcal{Y})$

Note that this is a more general definition than the one used in the main paper; the version in the main paper is the restriction of this definition to finite sets.

The *delta function*  $\delta : X \rightarrow \Delta(\mathcal{X})$  is the Markov kernel defined by

$$\delta(x, A) = \begin{cases} 1 & x \in A \\ 0 & \text{otherwise} \end{cases} \quad (102)$$

Fritz (2020) defines Markov categories in the following way:

**Definition 9.1.** A Markov category  $C$  is a symmetric monoidal category in which every object  $X \in C$  is equipped with a commutative comonoid structure given by a comultiplication  $\text{copy}_X : X \rightarrow X \otimes X$  and a counit  $\text{del}_X : X \rightarrow I$ , depicted in string diagrams as

$$\text{del}_X := \text{---} * \text{copy}_X \quad := \text{---} \bullet \text{---} \quad (103)$$

and satisfying the commutative comonoid equations

$$\begin{array}{c} \text{---} \bullet \text{---} \text{---} \bullet \text{---} \\ \text{---} \bullet \text{---} \text{---} \bullet \text{---} \end{array} = \begin{array}{c} \text{---} \bullet \text{---} \text{---} \bullet \text{---} \\ \text{---} \bullet \text{---} \text{---} \bullet \text{---} \end{array} \quad (104)$$

$$\begin{array}{c} \text{---} \bullet \text{---} * \\ \text{---} \bullet \text{---} * \end{array} = \text{---} = \begin{array}{c} * \\ \text{---} \bullet \text{---} \end{array} \quad (105)$$

$$(106)$$

as well as compatibility with the monoidal structure

$$X \otimes Y \xrightarrow{\quad} * \quad X \xrightarrow{\quad} * \\ = \quad X \xrightarrow{\quad} * \quad (107)$$

$$(108)$$

and the naturality of  $del$ , which means that

$$(109)$$

for every morphism  $f$ .

The category of labeled Markov kernels is the category consisting of labeled measurable sets as objects and labeled Markov kernels as morphisms. Given  $\mathbf{K} : \mathsf{X} \rightarrow \Delta(\mathsf{Y})$  and  $\mathbf{L} : \mathsf{Y} \rightarrow \Delta(\mathsf{Z})$ , sequential composition is given by

$$\mathbf{KL} : \mathsf{X} \rightarrow \Delta(\mathsf{Z}) \quad (110)$$

$$\text{defined by } (\mathbf{KL})(x, A) = \int_{\mathsf{Y}} \mathbf{L}(y, A) \mathbf{K}(x, dy) \quad (111)$$

For  $\mathbf{K} : \mathsf{X} \rightarrow \Delta(\mathsf{Y})$  and  $\mathbf{L} : \mathsf{W} \rightarrow \Delta(\mathsf{Z})$ , parallel composition is given by

$$\mathbf{K} \otimes \mathbf{L} : (\mathsf{X}, \mathsf{W}) \rightarrow \Delta(\mathsf{Y}, \mathsf{Z}) \quad (112)$$

$$\text{defined by } \mathbf{K} \otimes \mathbf{L}(x, w, A \times B) = \mathbf{K}(x, A) \mathbf{L}(w, B) \quad (113)$$

The identity map is

$$\text{Id}_{\mathsf{X}} : \mathsf{X} \rightarrow \Delta(\mathsf{X}) \quad (114)$$

$$\text{defined by } (\text{Id}_{\mathsf{X}})(x, A) = \delta(x, A) \quad (115)$$

We take an arbitrary single element labeled set  $I = (*, \{*\})$  to be the unit, which we note satisfies  $I \otimes X = X \otimes I = X$  by Lemma ??.

The swap map is given by

$$\text{swap}_{\mathbf{X}, \mathbf{Y}} : (\mathbf{X}, \mathbf{Y}) \rightarrow \Delta(\mathbf{Y}, \mathbf{X}) \quad (116)$$

$$\text{defined by } (\text{swap}_{\mathbf{X}, \mathbf{Y}})(x, y, A \times B) = \delta(x, B)\delta(y, A) \quad (117)$$

And we use the standard associativity isomorphisms for Cartesian products such that  $(A \times B) \times C \cong A \times (B \times C)$ , which in turn implies  $(\mathbf{X}, (\mathbf{Y}, \mathbf{Z})) \cong ((\mathbf{X}, \mathbf{Y}), \mathbf{Z})$ .

The copy map is given by

$$\text{copy}_{\mathbf{X}} : \mathbf{X} \rightarrow \Delta(\mathbf{X}, \mathbf{X}) \quad (118)$$

$$\text{defined by } (\text{copy}_{\mathbf{X}})(x, A \times B) = \delta_x(A)\delta_x(B) \quad (119)$$

and the erase map by

$$\text{del}_{\mathbf{X}} : \mathbf{X} \rightarrow \Delta(*) \quad (120)$$

$$\text{defined by } (\text{del}_{\mathbf{X}})(x, A) = \delta(*, A) \quad (121)$$

$$(122)$$

Note that the category formed by taking the underlying unlabeled sets and the underlying unlabeled morphisms is identical to the category of measurable sets and Markov kernels described in Fong (2013); Cho and Jacobs (2019); Fritz (2020).

**Theorem 9.2** (The category of labeled Markov kernels and labeled measurable sets is a Markov category). *The category described above is a Markov category.*

*Proof.*

I'm not sure how to formally argue that it is monoidal and symmetric as the relevant texts I've checked all gloss over the functors with respect to which the relevant isomorphisms should be natural, but labels with products were intentionally made to act just like sets with cartesian products which are symmetric monoidal

Equations 104 to 109 are known to be satisfied for the underlying unlabeled Markov kernels. We need to show is that they hold given our stricter criterion of labeled Markov kernel equality; that the underlying kernels *and the label sets* match. It is sufficient to check the label sets only.

□

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## Appendix: