

# Thesis Proposal Review: How Hard is a Causal Inference Problem

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February 4, 2020

## 1 Introduction: Consequences of Decisions

This thesis is concerned with understanding a particular kind of decision problem: we are given a set of feasible decisions and a set of observed data, we know the potential consequences these decisions may have and we know how desirable these consequences are. We wish to develop strategies for selecting decisions that are likely to lead to favourable consequences. For example, the decisions may be a set of possible medical treatments, consequences are states of health and data are from published medical trials; we also assume that some states of health are known to be more desirable than others.

This general kind of problem seems to me to be a reasonable description of a type of problem that people often face (allowing that it may be somewhat simplified). But I need not rely only on an appeal to intuition to argue that this is an important class of problem, as decision problems of this type have a long and extensive history of study: Von Neumann and Morgenstern (1944) considers the problem of choosing between consequences directly with some means of evaluating their desirability, Weirich (2016) discusses decision problems featuring decisions, consequences and desirability but no explicit consideration of data. Wald (1950) considers the problem of selecting a favourable decision given a set of data and a desirability function, though he eschews explicitly considering consequences, and Savage (1972) develops Wald's theory to also include consequences of decisions, yielding a class of decision problems very similar to those discussed here. Many of the solutions presented by these authors have "entered the water supply" - in particular, the expected utility theory of Von Neumann and Morgenstern (1944) underpins an enormous amount of the work on decision problems of any type, and the risk functionals of Wald (1950) are fundamental to much of statistics and machine learning. Even theories that reject the particulars proposed by these authors build on the foundations laid by them - in short, the type of problem studied here is widely accepted to be a very important class of problem.

This type of problem has particular practical relevance to the field of *causal inference*. A Google Scholar search for "causal inference" found, in the top five results:

- Holland (1986) and Frangakis and Rubin (2002) discuss causal inference as the project of relating *treatments* to *responses* via *observations*. If we postulate an implicit desirability of responses, we have a decision problem of the type outlined
- Morgan and Winship (2014) provide in their opening paragraph three examples of causal problems. Two of them have clear interpretations as decision problems where decisions involve funding of charter schools and engaging in or encouraging college study, while the third is perhaps more concerned with *responsibility* and *remedy*:
  - Do charter schools increase test scores?
  - Does obtaining a college degree increase an individual’s labor market earnings?
  - Did the use of a butterfly ballot in some Florida counties in the 2000 presidential election cost Al Gore votes?
- Pearl (2009a) begins with four examples of causal questions. The first appears to be part of a decision problem, while the second to fourth are questions of responsibility and remedy:
  - What is the efficacy of a given drug in a given population?
  - Whether data can prove an employer guilty of hiring discrimination?
  - What fraction of past crimes could have been avoided by a given policy?
  - What was the cause of death of a given individual, in a specific incident?
- Robins et al. (2000) is again concerned with estimating responses to treatments via observations

From this informal survey we have six out of ten example problems that correspond directly to the type of decision problem studied here. While decision problems are a substantial class of causal inference problems, we find that questions of responsibility also figure prominently. While the approach built in this thesis may have eventual applications to questions of responsibility and other causal questions, we take the attitude that in the worst case it will only be applicable to decision problems and this is a large and important enough class of problems that a clearer understanding of just these problems will still be very valuable.

One key difference between CSDT and existing popular approaches to causal inference is that we stipulate that *the set of decisions is a feature of the problem*, and does not depend in any way on how we choose to analyse the problem. Existing approaches provide “standard” objects (e.g. counterfactual random variables) or operations (e.g. intervening on the value of some random variable) which, if they are to be interpreted as decisions, impose some presuppositions

on the nature of the decisions available. Even if these presuppositions correspond to very common regularities of decision problems, we take the view that such regularities should be included as assumptions rather than be part of the language used to express the problem.

This difference is illustrated by the question of *external validity*. Given a randomised controlled trial (RCT), under ideal conditions existing causal inference approaches agree that certain causal effects can be consistently estimated. However, as reported by Deaton and Cartwright (2018):

Trials, as is widely noted, often take place in artificial environments which raises well recognized problems for extrapolation. For instance, with respect to economic development, Drèze (J. Drèze, personal communications, November 8, 2017) notes, based on extensive experience in India, that when a foreign agency comes in with its heavy boots and deep pockets to administer a treatment, whether through a local NGO or government or whatever, there tends to be a lot going on other than the treatment. There is also the suspicion that a treatment that works does so because of the presence of the treators, often from abroad, and may not do so with the people who will work it in practice.

Here, Drèze is describing the problem of determining the consequences of the “treatment in practice”, and why these may differ from the “causal effects of treatment in the trial” - the question of external validity is, loosely, the question of how informative the latter are about the former. The usual approach of causal inference is to determine conditions under which the latter can be estimated and then, maybe, consider some additional assumptions that might allow for the latter estimate to inform the former. CSDT inverts the priority of these questions: the question of treatment in practice is primary and the question of causal effects in the trial may be a subproblem of interest under particular conditions.

Bareinboim and Pearl (2012) have claimed to have a complete solution to the problem of “[identifying] conditions under which causal information learned from experiments can be reused in a different environment where only passive observations can be collected”, a claim made with more force in Pearl (2018). A complete solution to the transportability of causal information is *not* a claim of a complete solution to the problem of determining the effects of “treatment in practice” or the problem of making decisions with causal information. These latter problems ask when causal effects are informative about the consequences of decisions in the given problem, a question that doesn’t even make sense without our insistence that decisions are a feature of the problem.

Key features (/aims - not all are realised yet) of CSDT are:

- Conceptual clarity:
  - CSDT separates of those aspects of a problem that are fixed by non-causal considerations (objectives, feasible decisions) and causal assumptions

- Unification and extension of existing approaches to causal inference for decision problems
  - Faithful translation from any existing approach to CSDT (including the derivation of key results)
  - Exact and approximate comparison of arbitrary causal theories
  - Quantification of the *difficulty* of a causal problem
  - Necessary conditions for key results
  - Novel approaches/assumptions for causal inference

the following seems like a reasonable point, but not sure where to put it right now

The core features of CSDT are that it is a new approach to causality that is strictly more capable of representing decision problems than existing approaches, and that it allows for novel and fundamental questions to be asked. However, a secondary feature of CSDT is that its statements can be clearly resolved to statements in the underlying theory of probability. This may also be true of some counterfactual approaches, but I don't think it is true of interventional graphical models. For example, Causal Bayesian Networks feature an elementary operation notated  $P(\cdot|do(X_k = a))$  where  $X_k$  is a random variable on some implicit sample space  $E$ . We can ask: what does  $P(\cdot|do(X_k = a))$  mean in more elementary terms?  $do(X_k = a)$  itself *looks* like a function, and the conventional interpretation of  $X_k = a$  is the preimage of  $a$  under  $X_k$ . Thus,  $do()$  appears to be a function typed like a measure on  $\mathcal{E}$  with the domain being the sigma algebra generated by all statements  $X_i = a$  for all  $X_i$  associated with some graph  $\mathcal{G}$ , which we will denote  $\sigma(\bigotimes_{i \in \mathcal{G}} X_i)$ . We might surmise that the “conditional probability”  $P(\cdot|do(X_k = \cdot))$  might then be the conditional probability on  $\sigma(\bigotimes_{i \in \mathcal{G}} X_i)$ . However, CBNs in general support models where  $P(\cdot|do(X_k = \cdot))$  is not equal to  $P(\cdot|A)$  for any  $A \in \sigma(\bigotimes_{i \in \mathcal{G}} X_i)$ , so our attempt to parse this notation by “conventional reading” has failed.

In fact, the situation is even more dire: we may view  $do(X_k = a)$  as a relation between probability measures on  $E$  which is not, in general, functional – an interpretation compatible with the definitions in Pearl (2009b). If  $do()$  were functional, we could define  $P(\cdot|(X_k = a))$  to be the element of  $\Delta(\mathcal{E})$  related to  $P$  by  $(X_k = a)$ . However, because  $do(X_k = a)$  is not functional, “conditioning” on  $do(X_k = \cdot)$  is ambiguous - does  $P(\cdot|do(X_k = a))$  refer to the set of probability measures related to  $P$ ? A distinguished member of this set? In contrast to regular conditioning, where a similar ambiguity prevails but the ambient measure guarantees that disagreement can only happen on sets of measure zero,  $P(\cdot|do(X_k = a))$  can under different interpretations assign different measures to the same set. Causal Bayesian Network notational conventions suggest interpretations that do not make sense, and their meaning may be ambiguous even if we dig more deeply into the matter.

## 2 Definitions and key notation

We use three notations for working with probability theory. The “elementary” notation makes use of regular symbolic conventions (functions, products, sums, integrals, unions etc.) along with the expectation operator  $\mathbb{E}$ . This is the most flexible notation which comes at the cost of being verbose and difficult to read. Secondly, we use a semi-formal string diagram notation extending the formal diagram notation for symmetric monoidal categories Selinger (2010). Objects in this diagram refer to stochastic maps, and by interpreting diagrams as symbols we can, in theory, be just as flexible as the purely symbolic approach. However, we avoid complex mixtures of symbols and diagrams elements, and fall back to symbolic representations if it is called for. Finally, we use a matrix-vector product convention that isn’t particularly expressive but can compactly express some common operations.

### 2.1 Standard Symbols

Symbol	Meaning
$[n]$	The natural numbers $\{1, \dots, n\}$
$f : a \mapsto b$	Function definition, equivalent to $f(a) := b$
Dots appearing in function arguments: $f(\cdot, \cdot, z)$	The “curried” function $(x, y) \mapsto f(x, y, z)$
Capital letters: $A, B, X$	sets
Script letters: $\mathcal{A}, \mathcal{B}, \mathcal{X}$	$\sigma$ -algebras on the sets $A, B, X$ respectively
Script $\mathcal{G}$	A directed acyclic graph made up of nodes $V$ and edges
Greek letters $\mu, \xi, \gamma$	Probability measures
$\delta_x$	The Dirac delta measure: $\delta_x(A) = 1$ if $x \in A$ and 0 otherwise
Capital delta: $\Delta(\mathcal{E})$	The set of all probability measures on $\mathcal{E}$
Bold capitals: $\mathbf{A}$	Markov kernel $\mathbf{A} : X \times \mathcal{Y} \rightarrow [0, 1]$ (stochastic maps)
Subscripted bold capitals: $\mathbf{A}_x$	The probability measure given by the curried Markov kernel $\mathbf{A}_x$
$A \rightarrow \Delta(\mathcal{B})$	Markov kernel signature, treated as equivalent to $A \times \mathcal{B}$
$\mathbf{A} : x \mapsto \nu$	Markov kernel definition, equivalent to $\mathbf{A}(x, B) = \nu(B)$ for $B \in \mathcal{B}$
Sans serif capitals: $A, X$	Measurable functions; we will also call them random variables
$\mathbf{F}_X$	The Markov kernel associated with the function $X$ : $\mathbf{F}_X \equiv \mathbf{A}_X$
$\mathbf{N}_{A B}$	The conditional probability (disintegration) of $\mathbf{A}$ given $B$
$\nu \mathbf{F}_X$	The marginal distribution of $X$ under $\nu$

### 2.2 Probability Theory

Given a set  $A$ , a  $\sigma$ -algebra  $\mathcal{A}$  is a collection of subsets of  $A$  where

- $A \in \mathcal{A}$  and  $\emptyset \in \mathcal{A}$
- $B \in \mathcal{A} \implies B^C \in \mathcal{A}$
- $\mathcal{A}$  is closed under countable unions: For any countable collection  $\{B_i | i \in \mathbb{N}\}$  of elements of  $\mathcal{A}$ ,  $\cup_{i \in \mathbb{N}} B_i \in \mathcal{A}$

A measurable space  $(A, \mathcal{A})$  is a set  $A$  along with a  $\sigma$ -algebra  $\mathcal{A}$ . Sometimes the sigma algebra will be left implicit, in which case  $A$  will just be introduced as a measurable space.

**Common  $\sigma$  algebras** For any  $A$ ,  $\{\emptyset, A\}$  is a  $\sigma$ -algebra. In particular, it is the only sigma algebra for any one element set  $\{*\}$ .

For countable  $A$ , the power set  $\mathcal{P}(A)$  is known as the discrete  $\sigma$ -algebra.

Given  $A$  and a collection of subsets of  $B \subset \mathcal{P}(A)$ ,  $\sigma(B)$  is the smallest  $\sigma$ -algebra containing all the elements of  $B$ .

Let  $T$  be all the open subsets of  $\mathbb{R}$ . Then  $\mathcal{B}(\mathbb{R}) := \sigma(T)$  is the *Borel  $\sigma$ -algebra* on the reals. This definition extends to an arbitrary topological space  $A$  with topology  $T$ .

A *standard measurable set* is a measurable set  $A$  that is isomorphic either to a discrete measurable space  $A$  or  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ . For any  $A$  that is a complete separable metric space,  $(A, \mathcal{B}(A))$  is standard measurable.

Given a measurable space  $(E, \mathcal{E})$ , a map  $\mu : \mathcal{E} \rightarrow [0, 1]$  is a *probability measure* if

- $\mu(E) = 1, \mu(\emptyset) = 0$
- Given countable collection  $\{A_i\} \subset \mathcal{E}$ ,  $\mu(\cup_i A_i) = \sum_i \mu(A_i)$

Write by  $\Delta(\mathcal{E})$  the set of all probability measures on  $\mathcal{E}$ .

Given a second measurable space  $(F, \mathcal{F})$ , a *stochastic map* or *Markov kernel* is a map  $\mathbf{M} : E \times \mathcal{F} \rightarrow [0, 1]$  such that

- The map  $\mathbf{M}(\cdot; A) : x \mapsto \mathbf{M}(x; A)$  is  $\mathcal{E}$ -measurable for all  $A \in \mathcal{F}$
- The map  $\mathbf{M}_x : A \mapsto \mathbf{M}(x; A)$  is a probability measure on  $F$  for all  $x \in E$

Extending the subscript notation above, for  $\mathbf{C} : X \times Y \rightarrow \Delta(\mathcal{Z})$  and  $x \in X$  we will write  $\mathbf{C}_x$  for the “curried” map  $y \mapsto \mathbf{C}_{x,y}$ .

The map  $x \mapsto \mathbf{M}_x$  is of type  $E \rightarrow \Delta(\mathcal{F})$ . We will abuse notation somewhat to write  $\mathbf{M} : E \rightarrow \Delta(\mathcal{F})$ , which captures the intuition that a Markov kernel maps from elements of  $E$  to probability measures on  $\mathcal{F}$ . Note that we “reverse” this idea and consider Markov kernels to map from elements of  $\mathcal{F}$  to measurable functions  $E \rightarrow [0, 1]$ , an interpretation found in Clerc et al. (2017), but (at this stage) we don’t make use of this interpretation here.

Given an indiscrete measurable space  $(\{*\}, \{\{*\}, \emptyset\})$ , we identify Markov kernels  $\mathbf{N} : \{*\} \rightarrow \Delta(\mathcal{E})$  with the probability measure  $\mathbf{N}_*$ . In addition, there is a unique Markov kernel  $*$  :  $E \rightarrow \Delta(\{\{*\}, \emptyset\})$  given by  $x \mapsto \delta_*$  for all  $x \in E$  which we will call the “discard” map.

## 2.3 Product Notation

We can use a notation similar to the standard notation for matrix-vector products to represent operations with Markov kernels. Probability measures  $\mu \in$

$\Delta(\mathcal{X})$  can be read as row vectors, Markov kernels as matrices and measurable functions  $\mathsf{T} : Y \rightarrow T$  as column vectors. Defining  $\mathbf{M} : X \rightarrow \Delta(\mathcal{Y})$  and  $\mathbf{N} : Y \rightarrow \Delta(\mathcal{Z})$ , the measure-kernel product  $\mu\mathbf{A}(G) := \int \mathbf{A}_x(G)d\mu(x)$  yields a probability measure  $\mu\mathbf{A}$  on  $\mathcal{Z}$ , the kernel-kernel product  $\mathbf{MN}(x; H) = \int_Y \mathbf{B}(y; H)d\mathbf{A}_x$  yields a kernel  $\mathbf{MN} : X \rightarrow \Delta(\mathcal{Z})$  and the kernel-function product  $\mathbf{AT}(x) := \int_Y \mathsf{T}(y)d\mathbf{A}_x$  yields a measurable function  $X \rightarrow T$ . Kernel products are associative (Çinlar, 2011).

The tensor product  $(\mathbf{M} \otimes \mathbf{N})(x, y; G, H) := \mathbf{M}(x; G)\mathbf{N}(y; H)$  yields a kernel  $(\mathbf{M} \otimes \mathbf{N}) : X \times Y \rightarrow \Delta(\mathcal{Y} \otimes \mathcal{Z})$ .

## 2.4 String Diagrams

Some constructions are unwieldy in product notation; for example, given  $\mu \in \Delta(\mathcal{E})$  and  $\mathbf{M} : E \rightarrow (\mathcal{F})$ , it is not straightforward to construct a measure  $\nu \in \Delta(\mathcal{E} \otimes \mathcal{F})$  that captures the “joint distribution” given by  $A \times B \mapsto \int_A \mathbf{M}(x; B)d\mu$ .

Such constructions can, however, be straightforwardly captured with string diagrams, a notation developed for category theoretic probability. Cho and Jacobs (2019) also provides an extensive introduction to the notation discussed here.

Some key ideas of string diagrams:

- Basic string diagrams can always be interpreted as a mixture of kernel-kernel products and tensor products of Markov kernels
  - Extended string diagrams can be interpreted as a mixture of kernel-kernel products, kernel-function products, tensor products of kernels and functions and scalar products
- String diagrams are the subject of a coherence theorem: taking a string diagram and applying a planar deformation yields a string diagram that represents the same kernel (Selinger, 2010). This also holds for a number of additional transformations detailed below

A kernel  $\mathbf{M} : X \rightarrow \Delta(\mathcal{Y})$  is written as a box with input and output wires, probability measures  $\mu \in \Delta(\mathcal{X})$  are written as triangles “closed on the left” and measurable functions (which are only elements of the “extended” notation)  $\mathsf{T} : Y \rightarrow T$  as triangles “closed on the right”. For this introduction we will label wires with the names of their corresponding spaces, but in practice we will usually name them with corresponding *random variables*, though additional care is required when using random variables as labels (see paragraph 2.4.2).

For  $\mathbf{M} : X \rightarrow \Delta(\mathcal{Y})$ ,  $\mu \in \Delta(\mathcal{X})$  and  $f : X \rightarrow W$ :

$$X \text{ --- } \boxed{\mathbf{M}} \text{ --- } Y \qquad \triangleleft_{\mu} \text{ --- } X \qquad X \text{ --- } \triangleright_f \qquad (1)$$

**Basic and extended notation** We canonically regard a probability measure  $\mu \in \Delta(\mathcal{E})$  to be a Markov kernel  $\mu : \{*\} \rightarrow \Delta(\mathcal{E})$ . This allows for the definition of “basic” string diagrams for which Markov kernels are the only building blocks. Such a definition isn’t possible for measurable functions. Suppose by analogy with the example probability measures and try to identify a measurable function  $f : E \rightarrow \mathbb{R}$  with a Markov kernel  $f' : E \times \{*\} \rightarrow \mathbb{R}$ . For  $x \in E$  we cannot generally have both  $f'(x, *) = 1$  and  $f'(x, *) = f(x)$ , and so this attempt fails. This lack of normalisation is the reason we require an “extended” string diagram notation if we wish to incorporate functions and expectations which allows for the representation of scalars.

**Elementary operations** We can compose Markov kernels with appropriate spaces - the equivalent operation of the “matrix products” of product notation. Given  $\mathbf{M} : X \rightarrow \Delta(\mathcal{Y})$  and  $\mathbf{N} : Y \rightarrow \Delta(\mathcal{Z})$ , we have

$$\mathbf{MN} := X \text{ --- } \boxed{\mathbf{M}} \text{ --- } \boxed{\mathbf{N}} \text{ --- } Z \quad (2)$$

Probability measures are distinguished in that that they only admit “right composition” while functions only admit “left composition”. For  $\mu \in \Delta(\mathcal{E})$ ,  $h : F \rightarrow X$ :

$$\mu \mathbf{M} := \triangleleft \mu \text{ --- } \boxed{\mathbf{M}} \text{ --- } Z \quad (3)$$

$$\mathbf{M} f := X \text{ --- } \boxed{\mathbf{M}} \text{ --- } \triangleright f \quad (4)$$

We can also combine Markov kernels using tensor products, which we represent with vertical juxtaposition. For  $\mathbf{O} : Z \rightarrow \Delta(\mathcal{W})$ :

$$\mathbf{M} \otimes \mathbf{N} := \begin{array}{c} X \text{ --- } \boxed{\mathbf{M}} \text{ --- } Y \\ Z \text{ --- } \boxed{\mathbf{O}} \text{ --- } W \end{array} \quad (5)$$

Product spaces can be represented either by two parallel wires or a single wire:

$$X \times Y \cong \text{Id}_X \otimes \text{Id}_Y := \begin{array}{c} X \text{ --- } X \\ Y \text{ --- } Y \end{array} \quad (6)$$

$$= X \underline{\otimes} Y \text{ --- } X \underline{\otimes} Y \quad (7)$$

The notation  $X \underline{\otimes} Y$  will be explained in paragraph ?? -  $X \underline{\otimes} Y$  is a meta variable taking values in in the product space  $X \times Y$ .

Because a product space can be represented by parallel wires, a kernel  $\mathbf{L} : X \rightarrow \Delta(\mathcal{Y} \otimes \mathcal{Z})$  can be written using either two parallel output wires or a single output wire:



$$X \text{ --- } \boxed{\mathbf{L}} \text{ --- } \begin{array}{c} Y \\ Z \end{array} \quad (8)$$

$$\equiv \quad (9)$$

$$X \text{ --- } \boxed{\mathbf{L}} \text{ --- } Y \otimes Z \quad (10)$$

**Markov kernels with special notation** A number of Markov kernels are given special notation distinct from the generic “box” representation above. These special representations facilitate intuitive graphical interpretations.

The identity kernel  $\mathbf{Id} : X \rightarrow \Delta(X)$  maps a point  $x$  to the measure  $\delta_x$  that places all mass on the same point:

$$\mathbf{Id}_x : x \mapsto \delta_x \equiv X \text{ --- } X \quad (11)$$

The copy map  $\Upsilon : X \rightarrow \Delta(\mathcal{X} \times \mathcal{X})$  maps a point  $x$  to two identical copies of  $x$ :

$$\Upsilon : x \mapsto \delta_{(x,x)} \equiv X \text{ --- } \begin{array}{c} X \\ X \end{array} \quad (12)$$

The swap map  $\sigma : X \times Y \rightarrow \Delta(\mathcal{Y} \otimes \mathcal{X})$  swaps its inputs:

$$\sigma := (x, y) \mapsto \delta_{(y,x)} \equiv \begin{array}{c} Y \\ X \end{array} \text{ --- } \begin{array}{c} X \\ Y \end{array} \quad (13)$$

Apart from identity, copy and swap maps, we assign different names to the input and output wires of Markov kernels.

The discard map  $*$  :  $X \rightarrow \Delta(\{*\})$  maps every input to  $\delta_*$ . Note that the only non-empty event in  $\{\emptyset, \{*\}\}$  must have probability 1.

$$* : x \mapsto \delta_* \equiv X \text{ --- } * \quad (14)$$

We can associate a Markov kernel  $F \rightarrow \Delta(\mathcal{X})$  with any measurable function  $F \rightarrow X$ . A useful property of functional kernels is that products with functional kernels induce push-forward measures.

**Definition 2.1** (Function induced kernel). Given a measurable function  $g : F \rightarrow X$ , define the function induced kernel  $\mathbf{F}_g : F \rightarrow \Delta(\mathcal{X})$  to be the Markov kernel  $a \mapsto \delta_{g(a)}$  for all  $a \in X$ .

**Definition 2.2** (Pushforward kernel). Given a kernel  $\mathbf{M} : E \rightarrow \Delta(\mathcal{F})$  and a measurable function  $g : F \rightarrow X$ , the *pushforward kernel*  $g_\# \mathbf{M} : E \rightarrow \Delta(\mathcal{X})$  is the kernel such that  $g_\# \mathbf{M}(a; B) = \mathbf{M}(a; g^{-1}(B))$ .

If  $E$  is the indiscrete space  $\{*\}$ , then  $\mathbf{M}$  can be identified with the probability measure  $\mu := \mathbf{M}_*$  and the pushforward kernel  $g_\# \mathbf{M}$  identified with the pushforward measure  $g_\# \mu$ , so pushforward kernels reduce to pushforward measures.

**Lemma 2.3** (Pushforward kernels are functional kernel products). *Given a kernel  $\mathbf{M} : E \rightarrow \Delta(\mathcal{F})$  and a measurable function  $g : F \rightarrow X$ , the pushforward  $g\#\mathbf{M} = \mathbf{M}\mathbf{F}_g$ .*

*Proof.*

$$\mathbf{M}\mathbf{F}_g(a; B) = \int_F \delta_{g(y)}(B) d\mathbf{M}_a(y) \quad (15)$$

$$= \int_F \delta_y(g^{-1}(B)) d\mathbf{M}_a(y) \quad (16)$$

$$= \int_{g^{-1}(B)} d\mathbf{M}_a(y) \quad (17)$$

$$= g\#\mathbf{M}(a; B) \quad (18)$$

□

#### 2.4.1 Comparison of notations

We are in a position to compare the three introduced notations using a few examples. Given  $\mu \in \Delta(X)$ ,  $\mathbf{A} : X \rightarrow \Delta(Y)$  and  $A \in \mathcal{X}$ ,  $B \in \mathcal{Y}$ , the following correspondences hold, where we express the same object in elementary notation, product notation and string notation respectively:

$$\nu := A \times B \mapsto \int_A A(x; B) d\mu(x) \equiv \mu \curlyvee (\mathbf{Id}_X \otimes \mathbf{A}) \equiv \begin{array}{c} \text{Diagram: A triangle with } \mu \text{ at the top vertex, a horizontal line to the left, and a curved line to the right. The right side splits into two branches: the top branch is labeled } X \text{ and the bottom branch is labeled } \boxed{\mathbf{A}} - Y. \end{array} \quad (19)$$

Where the resulting object is a probability measure  $\nu \in \Delta(\mathcal{X} \otimes \mathcal{Y})$ . Note that the elementary notation requires a function definition here, while the product and string notations can represent the measure without explicitly addressing its action on various inputs and outputs. Cho and Jacobs (2019) calls this construction “integrating  $\mathbf{A}$  with respect to  $\mu$ ”.

Define the marginal  $\nu_Y \in \Delta(\mathcal{Y}) : B \mapsto \nu(X \times B)$  for  $B \in \mathcal{Y}$  and similarly for  $\nu_X$ . We can then express the result of marginalising 19 over  $X$  in our three separate notations as follows:

$$\nu_Y(B) = \nu(X \times B) = \int_X A(x; B) d\mu(x) \quad (20)$$

$$\nu_Y = \mu \mathbf{A} = \mu \curlyvee (\mathbf{Id}_X \otimes \mathbf{A})(\ast \otimes \mathbf{Id}_Y) \quad (21)$$

$$\nu_Y = \begin{array}{c} \text{Diagram: A triangle with } \mu \text{ at the top vertex, a horizontal line to the left, and a curved line to the right. The right side splits into two branches: the top branch is labeled } \ast \text{ and the bottom branch is labeled } \boxed{\mathbf{A}} - Y. \end{array} = \begin{array}{c} \text{Diagram: A triangle with } \mu \text{ at the top vertex, a horizontal line to the left, and a curved line to the right. The right side splits into two branches: the top branch is labeled } X \text{ and the bottom branch is labeled } \boxed{\mathbf{A}} - Y. \end{array} \quad (22)$$

The elementary notation 20 makes the relationship between  $\nu_Y$  and  $\nu$  explicit and, again, requires the action on each event to be defined. The product

notation 21 is, in my view, the least transparent but also the most compact in the form  $\mu\mathbf{A}$ , and does not demand the explicit definition of how  $\nu_Y$  treats every event. The graphical notation is the least compact in terms of space taken up on the page, but unlike the product notation it shows a clear relationship to the graphical construction in 19, and displays a clear graphical logic whereby marginalisation corresponds to “cutting off branches”. Like product notation, it also allows for the definition of derived measures such as  $\nu_Y$  without explicit definition of the handling of all events. It also features a much smaller collection of symbols than does elementary notation.

String diagrams often achieve a good balance between interpretational transparency, expressive power and symbol economy. Downsides of string diagrams are that they can be time consuming to typeset, and formal reasoning with them takes some practice.

### 2.4.2 Random Variables

The summary of this section is:

- We label wires with the names of random variables
- Diagrams with random variable labeled wires correspond to conditional/marginal distributions of those random variables in the obvious way
- We work with *conditional probability spaces* which are like probability spaces except some random variables don’t have marginal distributions

Probability theory is primarily concerned with the behaviour of *random variables*. This behaviour can be analysed via a collection of probability measures and Markov kernels representing joint, marginal and conditional distributions of random variables of interest. In the framework developed by Kolmogorov, this collection of joint, marginal and conditional distributions is modeled by a single underlying *probability space*, and random variables by measurable functions on the probability space.

We use the same approach here, with a couple of additions.

1. First, we are interested in variables whose outcomes depend both on random processes and decisions. These variables are better modelled by a Markov kernels than probability measure - *given* a particular decision, they inherit a particular probability distribution. Thus, variables in our work are modeled by an underlying Markov kernel rather than a probability measure; we call this a *conditional probability space*
2. Secondly, we show how Markov kernel diagrams representing joint, marginal and conditional distributions within a conditional probability space can be identified by labels on the wires, analogously to the argument labels in  $\mathbb{P}(X, Y)$  identifying the joint distribution of  $X$  and  $Y$

With regard to the first point, Hájek (2003) notes that there are many Markov kernels that cannot be uniquely specified by conditionals of probability

measures. Thus, in general, conditional probability spaces cannot be identified with probability spaces. However, rather than dealing with the issues raised by this possibility, we limit ourselves to conditional probability spaces that can be identified with probability spaces.

As a general motivation, suppose the following identity holding for some  $\mu$ ,  $\mathbf{K}$ :

$$\triangleleft \mathbb{P} = \triangleleft \mathbb{P} * \boxed{\mathbf{K}} \quad (23)$$

This implies, roughly, that  $\mathbf{K}$  is the probability of the lower wire of  $\mu$  conditional on the upper (it is a *disintegration* of  $\mu$ , defined later). We will want to deal with conditional probabilities such as  $\mathbf{K}$  regularly; it would be nice to be able to define it as such without having to explicitly write out an equation like 23. Instead, we will adopt a system whereby the wires of a distinguished probability measure (or general Markov kernel) have names:

$$\triangleleft \mathbb{P} \begin{array}{c} \mathbf{X} \\ \mathbf{Y} \end{array} \quad (24)$$

And then we adopt the convention that any kernel labelled as

$$\mathbf{X} \boxed{\mathbb{P}_{\mathbf{Y}|\mathbf{X}}} \mathbf{Y} \quad (25)$$

satisfies Equation 23 when substituted for  $\mathbf{K}$ . These names stand for random variables on an appropriately defined *conditional probability space*.

**Definition 2.4** (Probability space, conditional probability space). A *probability space*  $(\mathbb{P}, \Omega, \mathcal{F})$  is a probability measure  $\mathbb{P}$ , which we call the *ambient measure*, along with the *sample space*  $\Omega$  and the *events*  $\mathcal{F}$ .

A *conditional probability space*  $(\mathcal{K}, \Omega, \mathcal{F}, D, \mathcal{D})$  is a Markov kernel  $\mathcal{K}$ , called the *ambient kernel*, along with the sample space  $\Omega$  and the *global conditioning space*  $D$ .

Note that we use the blackboard and script fonts to distinguish ambient measures and kernels. They are formally the same thing as ordinary probability measures and kernels, but it is useful to distinguish them.

**Definition 2.5** (Random variable). Given a sample space  $\Omega$  and an input space  $D$ , a random variable  $\mathbf{X}$  is a measurable function  $\Omega \times D \rightarrow E$  for arbitrary measurable  $E$ . If the input space is trivial, it is simply a measurable function  $\Omega \rightarrow X$ .

We call the random variable  $\mathbf{D} : \Omega \times D \rightarrow D$  given by  $(w, d) \mapsto d$  to be the *global conditioning variable*.  $\mathbf{D}$  does not have a marginal distribution on a nontrivial conditional probability space (i.e. we don't have  $D$  isomorphic to the indiscrete set  $\{*\}$ ).

**Definition 2.6** (Coupled tensor product  $\otimes$ ). Given two Markov kernels  $\mathbf{M}$  and  $\mathbf{N}$  or functions  $f$  and  $g$  with shared domain  $E$ , let  $\mathbf{M} \otimes \mathbf{N} := \Upsilon(\mathbf{M} \otimes \mathbf{N})$  and  $f \otimes g := \Upsilon(f \otimes g)$  where these expressions are interpreted using standard product notation. Graphically:

$$\mathbf{M} \otimes \mathbf{N} := \begin{array}{c} \begin{array}{c} \boxed{\mathbf{M}} - \mathbf{X} \\ \boxed{\mathbf{N}} - \mathbf{Y} \end{array} \\ E \text{ --- } \end{array} \quad (26)$$

$$f \otimes g := \begin{array}{c} \begin{array}{c} \triangle f \\ \triangle g \end{array} \\ E \text{ --- } \end{array} \quad (27)$$

The operation denoted by  $\otimes$  is associative (Lemma 2.7), so we can without ambiguity write  $f \otimes g \otimes \dots \otimes h$  for finite groups of functions or Markov kernels sharing a domain.

**Lemma 2.7** ( $\otimes$  is associative). For Markov kernels  $\mathbf{L}$ ,  $\mathbf{M}$  and  $\mathbf{N}$  sharing a domain  $E$ ,  $(\mathbf{L} \otimes \mathbf{M}) \otimes \mathbf{N} = \mathbf{L} \otimes (\mathbf{M} \otimes \mathbf{N})$ .

**Definition 2.8** (Marginal distribution, marginal kernel). Given  $\mathbb{P} \in \Delta(\mathcal{F})$ , random variable  $\mathbf{X} : \Omega \rightarrow G$  the *marginal distribution* of  $\mathbf{X}$   $\mathbb{P}_{\mathbf{X}} \in \Delta(\mathcal{G})$  of  $\mathbf{X}$  is the product measure  $\mathbb{P}\mathbf{F}_{\mathbf{X}}$ .

See Lemma 2.3 for the proof that this matches the usual definition of marginal distribution.

Following this, given  $\mathcal{K} : D \rightarrow \Delta(\mathcal{F})$  and random variable  $\mathbf{X} : \Omega \rightarrow G$ , the *marginal kernel* is  $\mathcal{K}_{\mathbf{X}|D} := \mathcal{K}\mathbf{F}_{\mathbf{X}}$ . Note that we include the global conditioning variable  $D$  in this notation.

**Definition 2.9** (Joint distribution, joint kernel). Given  $\mathbb{P} \in \Delta(\mathcal{F})$ ,  $\mathbf{X} : \Omega \rightarrow G$  and  $\mathbf{Y} : \Omega \rightarrow H$ , the *joint distribution*  $\mathbb{P}_{\mathbf{X}\mathbf{Y}} \in \Delta(\mathcal{G} \otimes \mathcal{H})$  of  $\mathbf{X}$  and  $\mathbf{Y}$  is the marginal distribution of  $\mathbf{X} \otimes \mathbf{Y}$ .

This is identical to the definition in, for example, Çinlar (2011) if we note that the random variable  $(\mathbf{X}, \mathbf{Y}) : \omega \mapsto (\mathbf{X}(\omega), \mathbf{Y}(\omega))$  (Çinlar's definition) is the same thing as  $\mathbf{X} \otimes \mathbf{Y}$ .

Analogously, the joint kernel  $\mathcal{K}_{\mathbf{X}\mathbf{Y}|D}$  is the product  $\mathcal{K}\mathbf{F}_{\mathbf{X} \otimes \mathbf{Y}}$ .

This is just an aside

Joint distributions and kernels have a nice visual representation, as a result of Lemma 2.10 which follows.

**Lemma 2.10** (Joint distributions and coupled products). Given  $\mathbf{X} : \Omega \rightarrow G$  and  $\mathbf{Y} : \Omega \rightarrow H$ ,  $\mathbf{F}_{\mathbf{X} \otimes \mathbf{Y}} = \mathbf{F}_{\mathbf{X}} \otimes \mathbf{F}_{\mathbf{Y}}$

*Proof.* For  $a \in \Omega$ ,  $B \in \mathcal{G}$ ,  $C \in \mathcal{H}$ ,

$$\mathbf{F}_{\mathbf{X} \otimes \mathbf{Y}}(a; B \times C) = \delta_{\mathbf{X}(a), \mathbf{Y}(a)}(B \times C) \quad (28)$$

$$= \delta_{\mathbf{X}(a)}(B) \delta_{\mathbf{Y}(a)}(C) \quad (29)$$

$$= (\delta_{\mathbf{X}(a)} \otimes \delta_{\mathbf{Y}(a)})(B \times C) \quad (30)$$

$$= \mathbf{F}_{\mathbf{X}} \otimes \mathbf{F}_{\mathbf{Y}} \quad (31)$$

Equality follows from the monotone class theorem.  $\square$

Therefore the following holds:

$$\boxed{\mathcal{K}_{\mathbf{X}\mathbf{Y}}} = \boxed{\mathcal{K}} \begin{array}{c} \boxed{\mathbf{F}_{\mathbf{X}}} \\ \boxed{\mathbf{F}_{\mathbf{Y}}} \end{array} \quad (32)$$

We are now in a position to define wire labels for “output” wires.

**Definition 2.11** (Wire labels - joint probabilities). Given a conditional probability space with ambient kernel  $\mathcal{K} : D \rightarrow \Delta(\mathcal{F})$  (or a probability space with measure  $\mathbb{P}$ ) and some collection of random variables  $\mathbf{X}, \mathbf{Y}, \dots$  on  $\Omega \times D$ , any diagram representing a kernel  $\mathbf{L} : D \rightarrow \Delta(\mathcal{E})$  with *output* wires labeled  $\mathbf{X}, \mathbf{Y}, \dots$  represents the corresponding marginal of  $\mathcal{K}$  (we assume that the space  $E$  factorises appropriately). For example

$$\boxed{\mathbf{L}} \begin{array}{c} \mathbf{X} \\ \mathbf{Y} \end{array} \quad (33)$$

asserts that  $\mathbf{L} = \mathbf{K}_{\mathbf{X}\mathbf{Y}|D}$ , the joint kernel of  $\mathbf{X}$  and  $\mathbf{Y}$ .

If we have an ambient measure  $\mathbb{P}$ , then  $D = \{*\}$  and the diagram

$$\triangleleft \mu \begin{array}{c} \mathbf{X} \\ \mathbf{Y} \end{array} \quad (34)$$

asserts that  $\mu = \mathbb{P}_{\mathbf{X}\mathbf{Y}}$ .

**Definition 2.12** (Disintegration). Given a probability space  $(\mathbb{P}, \Omega, \mathcal{F})$ , random variables  $\mathbf{X}$  and  $\mathbf{Y}$  and joint probability measure  $\mu := \mathbb{P}_{\mathbf{X}\mathbf{Y}} \in \Delta(\mathcal{E} \otimes \mathcal{F})$ , we say that  $\mathbf{M} : E \rightarrow \Delta(\mathcal{F})$  is a disintegration of  $\mu$  if

$$\triangleleft \mu \begin{array}{c} \mathbf{X} \\ \mathbf{Y} \end{array} = \triangleleft \mu \begin{array}{c} \mathbf{X} \\ \mathbf{Y} \end{array} \begin{array}{c} \mathbf{M} \end{array} \quad (35)$$

Notationally,  $\mathbf{N}$  is a version of  $\mathbb{P}_{\mathbf{Y}|\mathbf{X}}$ , “the probability of  $\mathbf{Y}$  given  $\mathbf{X}$ ”, or  $\mathbf{M} \in \mathbb{P}_{\mathbf{Y}|\mathbf{X}}$ .

Given a conditional probability space  $(\mathcal{K}, \Omega, D)$ , define  $\mathcal{K}^*$  to be the kernel

$$\begin{array}{c} \boxed{\mathcal{K}} \\ \curvearrowright \end{array} \quad (36)$$

Given random variables  $X, Y$  on  $\Omega \times D$  and kernel  $\mathbf{L} := \mathcal{K}_{X,Y}^* : D \rightarrow \Delta(\mathcal{E} \otimes \mathcal{F})$ , we say that  $\mathbf{M} : D \times E \rightarrow \Delta(\mathcal{F})$  is a disintegration of  $\mathbf{L}$  if

$$\text{---} \boxed{\mathbf{L}} \text{---} \begin{matrix} X \\ Y \end{matrix} = \text{---} \boxed{\mathbf{L}} \text{---} * \boxed{\mathbf{M}} \text{---} \begin{matrix} X \\ Y \end{matrix} \quad (37)$$

Similarly, recalling that  $D$  is the global conditioning variable, we can say  $\mathbf{M} \in \mathcal{K}_{Y|XD}$ . We require disintegrations of kernel spaces to be conditional on the global conditioning variable, as this along with certain other conditions guarantees the existence of a disintegration.

Note that Eq. 38 also implies

$$\text{---} \boxed{\mathbf{L}} \text{---} \begin{matrix} X \\ Y \\ D \end{matrix} = \text{---} \boxed{\mathbf{L}} \text{---} * \boxed{\mathbf{M}} \text{---} \begin{matrix} X \\ Y \\ D \end{matrix} \quad (38)$$

**Definition 2.13** (Wire labels - disintegrations). Given a conditional probability space with ambient kernel  $\mathcal{K} : D \rightarrow \Delta(\mathcal{F})$  (or a probability space with measure  $\mathbb{P}$ ),

Note that  $\mathbb{P}^*$  is simply  $\mathbb{P}$  for a probability space

Recall that  $D$  is the global conditioning variable. Given two collections of random variables  $c_1 = [X_1, X_2, \dots]$  and  $c_2 = [Y_1, Y_2]$ , we adopt the convention that any diagram with the input wires labeled with  $c_1$  and the output wires labeled with  $c_2$  is an element of  $\mathcal{K}_{Y_1 Y_2 \dots | X_1 X_2 \dots}^*$ .

That is, by this convention, the diagram

$$\begin{matrix} X \\ D \end{matrix} \text{---} \boxed{\mathbf{M}} \text{---} Y \quad (39)$$

implies that  $\mathbf{M} \in \mathcal{K}_{Y|XD}$ . Note further that by Theorem 2.15, we can rely on the existence of disintegrations such as  $\mathbf{M}$  that are conditional on the global conditioning variable  $D$  provided we have countable  $D$  and standard measurable  $(Y, \mathcal{Y})$ .

If we have some version  $\mathbf{M}$  of  $\mathcal{K}_{Y|XD}$  that does not depend on the value of  $D$  - i.e.  $\mathbf{M}_{(x,d)} = \mathbf{M}_{(x,d')}$  for all  $x \in X$ ,  $d, d' \in D$ , then there exists some  $\mathbf{M}'$  such that:

$$\begin{matrix} X \\ D \end{matrix} \text{---} \boxed{\mathbf{M}} \text{---} Y = \begin{matrix} X \\ D \end{matrix} \text{---} \boxed{\mathbf{M}'} \text{---} Y \quad (40)$$

Under these circumstances, we will abuse notation to say  $\mathbf{M}' = \mathcal{K}_{Y|X}$ .

We can't expect Equation 40 to hold in an arbitrary conditional probability spaces. For a very simple example, take  $\mathcal{K} : \{0, 1\} \rightarrow \Delta(\{0, 1\})$  where  $\mathcal{K}_0 =$

$\mathcal{K}_1 = \text{Bernoulli}(0.5)$ , and let  $\mathbf{X} : (x, d) \mapsto x$  - i.e. the random variable projecting the output of  $\mathcal{K}$ . Then there is no disintegration  $\mathcal{K}_{D|\mathbf{X}}$  - we can't recover the input  $D$  from  $\mathbf{X}$ .

Under some (strong) regularity conditions, disintegrations of conditional probability spaces do exist.

**Theorem 2.14** (Disintegration existence - probability space). *Given a probability measure  $\mu \in \Delta(\mathcal{E} \otimes \mathcal{F})$ , if  $(F, \mathcal{F})$  is standard then a disintegration  $\mathbf{K} : E \rightarrow \Delta(\mathcal{F})$  exists (Çinlar, 2011).*

**Theorem 2.15** (Disintegration existence - conditional probability space). *Given a kernel  $\mathbf{L} : D \rightarrow \Delta(\mathcal{E} \otimes \mathcal{F})$ , define  $\mathbf{L}^*$ :*

$$\text{---} \boxed{\mathbf{L}} \text{---} \quad (41)$$

*If  $D$  is countable and  $(F, \mathcal{F})$  is standard, then there is a disintegration  $\mathbf{M} : D \times E \rightarrow \Delta(\mathcal{F})$  of  $\mathbf{L}^*$ .*

*Proof.* By Theorem 2.14, for each  $d \in D$  we have a disintegration  $\mathbf{K}^{(d)} : E \rightarrow \Delta(\mathcal{F})$  of  $\mathbf{L}_d$ . Define  $\mathbf{M} : D \times E \rightarrow \Delta(\mathcal{F})$  by  $\mathbf{M}(d, e; A) = \mathbf{K}^{(d)}(e; A)$  for  $d \in D$ ,  $e \in E$ ,  $A \in \mathcal{F}$ . Clearly  $\mathbf{M}_{(d,e)}$  is a probability measure. Furthermore, for  $B \in \mathcal{B}(\mathbb{R})$ ,  $\mathbf{M}^{-1}(\cdot; A)(B) = \cup_{d \in D} \{d\} \times \mathbf{K}^{(d)-1}(\cdot; A)(B)$ , which is a countable union of measurable sets and therefore measurable.  $\square$

From here on out, we will assume whether explicitly stated or not that any global conditioning space is countable and any other measurable space is standard, guaranteeing the existence of disintegrations.

In general, we don't want to spent time explicitly setting up conditional probability spaces. Rather, we will specify key marginals and disintegrations from which a conditional probability space can be constructed - call these marginals and conditional "components". Clearly we cannot build a conditional probability space from two kernels that represent the same component but disagree with each other on a non-negligible set. Also, in general, for an arbitrary collection of components there may be many ambient kernels from which we can extract these components. There is no particular problem if we have multiple ambient kernels over undefined random variable; if we are only interested in  $\mathbf{X}$  then the possibility of many joint kernels over  $\mathbf{X}$  and  $\mathbf{Y}$  is no cause for concern. We do, however, want to avoid ambient kernels supporting non-negligibly distinct marginals or disintegrations over the random variables that have been defined.

**Example 2.16** (Implicit conditional probability space). Suppose we have labeled Markov kernels

$$D \text{---} \boxed{\mathbf{L}} \text{---} \mathbf{X} \quad \mathbf{X} \text{---} \boxed{\mathbf{M}} \text{---} \mathbf{Y} \quad (42)$$

We want to define a conditional probability space  $(\mathcal{K}, \Omega, D)$  supporting random variables  $D$ ,  $\mathbf{X}$  and  $\mathbf{Y}$  yielding the above kernels as the relevant marginals and disintegrations. Strictly:



- Take  $\Omega = W \times X \times Y \times Z$  and define  $\mathcal{K}$  such that

Where  $\mathcal{K}^*$  is the copy map composed with  $\mathcal{K}$  as in previous definitions.  $\mathcal{K}$  is the unique Markov kernel  $D \rightarrow \Delta(\mathcal{X} \otimes \mathcal{Y})$  supporting the two criteria above, assuming finite  $D$  and standard measurable  $X, Y$ .

$$= \begin{array}{c} D - \boxed{\text{L}} - \boxed{\text{M}} - Y \\ \quad \quad \quad \quad \quad X \\ \quad \quad \quad \quad \quad D \end{array} \quad (46)$$

This example was chosen to illustrate a peculiarity of our notation of conditional probability spaces. Consider a problem that appears similar: find an ambient measure  $\mathbb{P}$  decomposing into the following marginal and conditionals:

Here there are many choices of  $\mathbb{P}$  that satisfy our conditions arising from different choices of  $\mathbb{P}_{Y|X,D}$ . This is not possible in the conditional probability space because  $\mathcal{K}_{Y|X}$  only exists if  $\mathcal{K}_{Y|X,D}$  is independent of  $D$ . That is, in a conditional probability space every disintegration is conditional on  $D$ , but we may not explicitly write this if it does not actually depend on  $D$ .

A sufficient condition for the construction of a unique ambient kernel from a collection of components  $\{C_1, \dots, C_n\}$  is if there is some ordering of components  $\{i_1, i_2, \dots, i_n\}$  such that the input labels of  $C_{i_{k+1}}$  is the union of the inputs and outputs of  $C_{i_1}, \dots, C_{i_j}$ . This can be shown by repeated application of Theorem 2.15.

In general, diagram labels are “well behaved” with regard to the application of any of the special Markov kernels: identities 11, swaps 13, discards 14 and copies 12 as well as with respect to the coherence theorem of the CD category. They are not “well behaved” with respect to composition.

**Lemma 2.17** (Diagrammatic consequences of labels). *Fix some conditional probability space  $(\mathcal{K}, \Omega, D)$  and random variables  $X, Y, Z$  taking values in arbitrary spaces.  $\text{Sat} :$  indicates that a labeled diagram satisfies definitions 2.11 and 2.13 with respect to  $(\mathcal{K}, \Omega, D)$  and  $X, Y, Z$ . The following always holds:*

$$\text{Sat} : X - X \quad (48)$$

and the following implications hold:

$$\text{Sat} : Z - \boxed{K} - \begin{array}{c} X \\ \diagdown \\ Y \end{array} \implies \text{Sat} : Z - \boxed{K} - * \quad (49)$$

$$\text{Sat} : Z - \boxed{K} - \begin{array}{c} X \\ \diagdown \\ Y \end{array} \implies \text{Sat} : Z - \boxed{K} - \begin{array}{c} Y \\ \diagup \\ X \end{array} \quad (50)$$

$$\text{Sat} : Z - \boxed{L} - X \implies \text{Sat} : Z - \boxed{L} - \begin{array}{c} X \\ \diagup \\ X \end{array} \quad (51)$$

$$\text{Sat} : Z - \boxed{K} - Y \implies \text{Sat} : \begin{array}{c} Z \\ \diagup \\ \boxed{K} - Y \end{array} \quad (52)$$

*Proof.* •  $\text{Id}_X$  is a version of  $\mathbb{P}_{X|X}$  for all  $\mathbb{P}$ ;  $\mathbb{P}_X \text{Id}_X = \mathbb{P}_X$

$$\bullet \mathbf{K} \text{Id} \otimes * (w; A) = \int_{X \times Y} \delta_x(A) \mathbb{1}_Y(y) d\mathbf{K}_w(x, y) = \mathbf{K}_w(A \times Y) = \mathbb{P}_{X|Z}(w; A)$$

$$\bullet \int_{X \times Y} \delta_{\text{swap}(x, y)}(A \times B) d\mathbf{K}_w(x, y) = \mathbb{P}_{YX|Z}(w; A \times B)$$

$$\bullet \mathbf{K} \vee (w; A \times B) = \int_X \delta_{x, x}(A \times B) d\mathbf{K}_w(x) = \mathbb{P}_{XX|Z}(w; A \times B)$$

52: Suppose  $\mathbf{K}$  is a version of  $\mathbb{P}_{Y|Z}$ . Then

$$\mathbb{P}_{ZY} = \begin{array}{c} \triangleleft \mathbb{P}_Z \\ \text{---} \boxed{K} \text{---} \begin{array}{c} Z \\ \diagdown \\ Y \end{array} \end{array} \quad (53)$$

$$\mathbb{P}_{ZZY} = \begin{array}{c} \triangleleft \mathbb{P}_Z \\ \text{---} \boxed{K} \text{---} \begin{array}{c} Z \\ \diagup \\ Z \\ \diagdown \\ Y \end{array} \end{array} \quad (54)$$

$$= \begin{array}{c} \triangleleft \mathbb{P}_Z \\ \text{---} \boxed{K} \text{---} \begin{array}{c} Z \\ \diagup \\ Z \\ \diagdown \\ Y \end{array} \end{array} \quad (55)$$

Therefore  $\vee(\text{Id}_X \otimes \mathbf{K})$  is a version of  $\mathbb{P}_{Z|Y}$  by ?? □

The following property, on the other hand, does *not* generally hold:

$$\text{Sat} : Z - \boxed{\mathbf{K}} - Y, Y - \boxed{\mathbf{L}} - X \implies \text{Sat} : Z - \boxed{\mathbf{K}} - \boxed{\mathbf{L}} - X \quad (56)$$

Consider some ambient measure  $\mathbb{P}$  with  $Z = X$  and  $\mathbb{P}_{Y|X} = x \mapsto \text{Bernouli}(0.5)$  for all  $z \in Z$ . Then  $\mathbb{P}_{Z|Y} = y \mapsto \mathbb{P}_Z$ ,  $\forall y \in Y$  and therefore  $\mathbb{P}_{Y|Z}\mathbb{P}_{Z|Y} = x \mapsto \mathbb{P}_Z$  but  $\mathbb{P}_{Z|X} = x \mapsto \delta_x \neq \mathbb{P}_{Y|Z}\mathbb{P}_{Z|Y}$ .

### 2.4.3 Working With String Diagrams

todo:

- Functional generalisation
- Conditioning
- Infinite copy map
- De Finetti's representation theorem

There are a relatively small number of manipulation rules that are useful for string diagrams. In addition, we will define graphically analogues of the standard notions of *conditional probability*, *conditioning*, and infinite sequences of exchangeable random variables.

**Axioms of Symmetric Monoidal Categories** For the following, we either omit labels or label diagrams with their domain and codomain spaces, as we are discussing identities of kernels rather than identities of components of a conditional probability space. Recalling the unique Markov kernels defined above, the following equivalences, known as the *commutative comonoid axioms*, hold among string diagrams:

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} = \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} := \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \quad (57)$$

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array}^* = \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array}^* = \text{---} \quad (58)$$

$$\begin{array}{c} \text{X} \text{---} \text{---} \text{X} \\ \text{X} \text{---} \text{---} \text{X} \end{array} = \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \quad (59)$$

The discard map  $*$  can “fall through” any Markov kernel:

$$\boxed{\mathbf{A}} * = * \quad (60)$$

Combining 58 and 60 we can derive the following: integrating  $\mathbf{A} : X \rightarrow \Delta(\mathcal{Y})$  with respect to  $\mu \in \Delta(\mathcal{X})$  and then discarding the output of  $\mathbf{A}$  leaves us with  $\mu$ :

$$\begin{array}{c} \triangleleft \mu \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \boxed{\mathbf{A}} * = \begin{array}{c} \triangleleft \mu \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} * = \begin{array}{c} \triangleleft \mu \\ \text{---} \end{array} \quad (61)$$

In elementary notation, this is equivalent to the fact that, for all  $B \in \mathcal{X}$ ,  $\int_B \mathbf{A}(x; B) d\mu(x) = \mu(B)$ .

The following additional properties hold for  $*$  and  $\curlyvee$ :

$$X \times Y \longrightarrow * = \begin{array}{c} X \\ Y \end{array} \begin{array}{c} \longrightarrow * \\ \longrightarrow * \end{array} \quad (62)$$

$$X \times Y \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} X \times Y \\ X \times Y \end{array} = \begin{array}{c} X \\ Y \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} X \\ Y \end{array} \quad (63)$$

A key fact that *does not* hold in general is

$$\boxed{\mathbf{A}} \begin{array}{c} \text{---} \\ \text{---} \end{array} = \begin{array}{c} \boxed{\mathbf{A}} \\ \boxed{\mathbf{A}} \end{array} \quad (64)$$

In fact, it holds only when  $\mathbf{A}$  is a *deterministic* kernel.

**Definition 2.18** (Deterministic Markov kernel). A *deterministic* Markov kernel  $\mathbf{A} : E \rightarrow \Delta(\mathcal{F})$  is a kernel such that  $\mathbf{A}_x(B) \in \{0, 1\}$  for all  $x \in E$ ,  $B \in \mathcal{F}$ .

**Theorem 2.19** (Copy map commutes for deterministic kernels (Fong, 2013)). Equation 64 holds iff  $\mathbf{A}$  is deterministic.

### 3 Statistical Decision Problems to Causal Statistical Decision Problems

Statistical decision theory (SDT) is a theory of data-driven decision making that was set out in detail by Wald (1950). Many core concepts of machine

learning have precursors in SDT including statistical experiments, losses and risk functionals. SDT also sets out foundational theorems such as the complete class theorem, which establishes the completeness of Bayes decision rules, and the Blackwell-Sherman-Stein theorem characterising the comparison of statistical experiments. SDT, however, does not feature any notion of *consequences* and as a result is not suited to causal problems. CSDT is an extension of SDT that features consequences.

A statistical decision problem (SDP) poses the following scenario: suppose we have a set of “states of nature”  $\Theta$ , a set of decisions  $D$  and a loss function  $l : \Theta \times D \rightarrow \mathbb{R}$ . For each state of nature  $\theta \in \Theta$  there is an associated probability measure  $\mu_\theta \in \Delta(\mathcal{E})$  where  $(E, \mathcal{E})$  is some measurable space. Call the stochastic map  $\mathbf{H} : \theta \mapsto \mu_\theta$  a *statistical experiment*. Given a *decision strategy*  $\mathbf{J} : E \rightarrow \Delta(\mathcal{D})$ , define the *risk* of  $\mathbf{J}$  given state  $\theta$  to be the expected loss of  $\mathbf{J}$  in state  $\theta$ . Specifically, the risk  $R : \Delta(\mathcal{D})^E \times \Theta \rightarrow \mathbb{R}$  is given by  $R : (\mathbf{J}, \theta) \mapsto \mathbf{H}_\theta \mathbf{J} l_\theta$ , where we make use of kernel product notation for brevity.

We would ideally find a strategy  $\mathbf{J}$  that minimises the risk in the “true state”  $\theta^*$ . Unfortunately, we don’t know the true state. If there were a decision strategy that minimised the loss in every state, such a strategy would clearly minimise the loss in the true state, but most statistical decision problems don’t admit such a strategy. Two alternative decision rules are available:

Given a measure  $\xi \in \Delta(\Theta)$  called a prior,  $\xi$ -*Bayes decision rule* is a decision rule  $\mathbf{J}_{\text{Ba}}^*$  such that the *Bayes risk*  $R_\xi : \mathbf{J} \mapsto \int_\Theta H_\theta \mathbf{J} l_\theta d\xi$  is minimised. A *minimax* decision rule  $\mathbf{J}_{\text{MM}}^*$  minimises the worst-case risk:  $\mathbf{J}_{\text{MM}}^* \in \arg \min_{\mathbf{J}} \max_{\theta \in \Theta} R(\mathbf{J}, \theta)$ . Unlike a Bayes rule, a minimax rule does not invoke a prior. In general, a decision rule is some rule that selects a decision on the basis of the risk functional  $R(\mathbf{J}, \cdot)$ .

Our representation of statistical experiment is slightly different to, for example, Le Cam (1996), who introduces statistical experiments as an ordered collection of probability measures. Both representations do the same job, and the representation as a map makes for a clearer connection with causal statistical decision problems.

Formally, we define an SDP as the tuple  $\langle \Theta, E, D, \mathbf{H}, l \rangle$  where  $\Theta, E$  and  $D$  are measurable sets,  $\mathbf{H}$  is a stochastic map  $\Theta \rightarrow \Delta(\mathcal{E})$  and  $l$  a measurable function  $E \rightarrow \mathbb{R}$ . We leave implicit the set of decision strategies  $E \rightarrow \Delta(\mathcal{D})$ . This is a very bare bones exposition of the theory of SDPs, and for more details we refer readers to Ferguson (1967).

Observe that a statistical decision problem supplies a loss  $l$  that tells us immediately how desirable a pair  $(\theta, d) \in \Theta \times D$  is. It is more typical to talk about how desirable the *consequences* of a decision are than how desirable a (state, decision) pair is. If the set of possible consequences of a decision is denoted by a set  $F$ , let the desirability of an element  $f \in F$  be given by a utility function  $u : F \rightarrow \mathbb{R}$ . Given such a  $u$ , the tuple  $\langle \Theta, E, D, \mathbf{H}, u \rangle$  is an ill-posed problem: we want to evaluate the desirability of decision strategies  $\mathbf{J}$ , but we have no means of connecting decisions with consequences  $F$ . We introduce for each state of nature  $\theta$  a *consequence map*  $\mathbf{C}_\theta : D \rightarrow \Delta(\mathcal{F})$ ; let  $\mathbf{C}$  be the Markov kernel  $\theta \mapsto \kappa_\theta$ . We can then define the *causal risk*  $S : \Delta(\mathcal{D})^E \times \Theta \rightarrow \mathbb{R}$  by

$S : (\mathbf{J}, \theta) \mapsto -H_\theta \mathbf{F} C_\theta u$ , and Bayes and minimax risks are defined analogously. For each state  $\theta \in \Theta$ , the Markov kernel

$$\mathbf{T}_\theta := \begin{array}{c} \triangle \delta_\theta \\ \text{---} \end{array} \begin{array}{c} \boxed{H} \text{---} E \\ \boxed{C} \text{---} F \end{array} \quad (65)$$

Is sufficient to compute the causal risk. Thus we can replace  $\mathbf{H}$  and  $\mathbf{C}$  with the *causal theory*  $\mathbf{T} : \Theta \times D \rightarrow \Delta(\mathcal{E} \otimes \mathcal{F})$  given by  $(\theta, d) \mapsto \mathbf{T}_\theta(d; \cdot)$ . A causal statistical decision problem (CSDP) is therefore a tuple  $\langle \Theta, E, F, D, \mathbf{T}, u \rangle$ .

Given a CSDP  $\alpha = \langle \Theta, E, F, D, T, u \rangle$  where  $\mathbf{T}$  is a theory arising from some  $\mathbf{H}$  and  $\mathbf{C}$  as in Equation 65, we can recover the original kernels by marginalisation:  $\mathbf{H} = T(\text{Id} \otimes *)$  and  $\mathbf{C} = \mathbf{T}(* \otimes \text{Id})$ . Given  $\alpha$  and letting  $l := \mathbf{C}u$  we induce the canonical SDP  $\beta = \langle \Theta, E, D, \mathbf{H}', l \rangle$  such that for any  $\theta \in \Theta$ ,  $\mathbf{J}$ ,  $R^{(\beta)}(\mathbf{J}, \theta) = S^{(\alpha)}(\mathbf{J}, \theta)$ , and thus  $\alpha$  and  $\beta$  will always produce identical recommendations.

It is also possible to induce a CSDP from an arbitrary SDP  $\beta := \langle \Theta, E, D, \mathbf{H}, l \rangle$ . First, define  $F := \Theta \times D$  and then let  $u := -l$ . Define  $\mathbf{C} : \Theta \rightarrow (D \rightarrow \Delta(\mathcal{F}))$  by  $\mathbf{C} : \theta \mapsto (d \mapsto (\theta, d))$ , and then construct  $\mathbf{T}$  from  $\Theta, \mathbf{H}$  and  $\mathbf{C}$  as in 65. Then the CSDP  $\alpha := \langle \Theta, E, F, D, \mathbf{T}, u \rangle$  has the property  $S^{(\alpha)}(\mathbf{J}, \theta) = R^{(\beta)}(\mathbf{J}, \theta)$ .

Causal theories are the central object of study here. They provide a bridge between the experiment  $\mathbf{H}$  and the consequences  $\mathbf{C}$  and allow us to use the former to make inferences about the latter.

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## Appendix: