

## DRAWING WITH DISTANCE

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**ABSTRACT.** Drawing (a multiset of) coloured balls from an urn is one of the most basic models in discrete probability theory. Three modes of drawing are commonly distinguished: multinomial (draw-replace), hypergeometric (draw-delete), and Pólya (draw-add). These drawing operations are represented as maps from urns to distributions over multisets of draws. The set of urns is a metric space via the Kantorovich distance. The set of distributions over draws is also a metric space, using Kantorovich-over-Kantorovich. It is shown that these three draw operations are all isometries, that is, they exactly preserve the Kantorovich distances. Further, drawing is studied in the limit, both for large urns and for large draws. First it is shown that, as the urn size increases, the Kantorovich distances go to zero between hypergeometric and multinomial draws, and also between Pólya and multinomial draws. Second, it is shown that, as the drawsize increases, the Kantorovich distance goes to zero (in probability) between an urn and (normalised) multinomial draws from the urn. These results are known, but here, they are formulated in a novel metric manner as limits of Kantorovich distances. We call these two limit results the law of large urns and the law of large draws.

### 1. INTRODUCTION

Basic physical models in probability theory are flipping a coin, rolling a dice, or drawing coloured balls from an urn [JK77]. We start with an illustration of these urn models. We consider a situation with a set  $C = \{R, G, B\}$  of three colours: red, green, blue. Assume that we have two urns  $v_1, v_2$  with 10 coloured balls each. We describe these urns as multisets of the form:

$$v_1 = 8|G\rangle + 2|B\rangle \quad \text{and} \quad v_2 = 5|R\rangle + 4|G\rangle + 1|B\rangle.$$

Recall that a multiset is like a set, except that elements may occur multiple times. Here we describe urns as multisets using ‘ket’ notation  $| - \rangle$ . It separates multiplicities of elements (before the ket) from the elements in the multiset (inside the ket). Thus, urn  $v_1$  contains 8 green balls and 2 blue balls (and no red ones). Similarly, urn  $v_2$  contains 5 red, 4 green, and 1 blue ball(s).

Below, we shall describe the Kantorovich distance between multisets (of the same size). How this works does not matter for now; we simply posit that the Kantorovich distance

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$d(v_1, v_2)$  between these two urns is  $\frac{1}{2}$  — where we assume the discrete distance on the set  $C$  of colours.

We turn to draws from these two urns, in this introductory example of size two. These draws are also described as multisets, with elements from the set  $C = \{R, G, B\}$  of colours. There are six multisets (draws) of size 2, namely:

$$2|R\rangle \quad 1|R\rangle + 1|G\rangle \quad 2|G\rangle \quad 1|R\rangle + 1|B\rangle \quad 2|B\rangle \quad 1|G\rangle + 1|B\rangle. \quad (1.1)$$

As we see, there are three draws with 2 balls of the same colour, and three draws with balls of different colours.

We consider the hypergeometric probabilities associated with these draws, from the two urns. Let's illustrate this for the draw  $1|G\rangle + 1|B\rangle$  of one green ball and one blue ball from the urn  $v_1$ . The probability of drawing  $1|G\rangle + 1|B\rangle$  is  $\frac{16}{45}$ ; it is obtained as sum of:

- first drawing-and-deleting a green ball from  $v_1 = 8|G\rangle + 2|B\rangle$ , with probability  $\frac{8}{10}$ . It leaves an urn  $7|G\rangle + 2|B\rangle$ , from which we can draw a blue ball with probability  $\frac{2}{9}$ . Thus drawing “first green then blue” happens with probability  $\frac{8}{10} \cdot \frac{2}{9} = \frac{8}{45}$ .
- Similarly, the probability of drawing “first blue then green” is  $\frac{2}{10} \cdot \frac{8}{9} = \frac{8}{45}$ .

We can similarly compute the probabilities for each of the above six draws (1.1) from urn  $v_1$ . This gives the hypergeometric distribution, which we write using kets-over-kets as:

$$hg[2](v_1) = \frac{28}{45} \left| 2|G\rangle \right\rangle + \frac{16}{45} \left| 1|G\rangle + 1|B\rangle \right\rangle + \frac{1}{45} \left| 2|B\rangle \right\rangle.$$

The fraction written before a big ket is the probability of drawing the multiset (of size 2), written inside that big ket, from the urn  $v_1$ .

Drawing from the second urn  $v_2$  gives a different distribution over these multisets (1.1). Since urn  $v_2$  contains red balls, they additionally appear in the draws.

$$hg[2](v_2) = \frac{2}{9} \left| 2|R\rangle \right\rangle + \frac{4}{9} \left| 1|R\rangle + 1|G\rangle \right\rangle + \frac{2}{15} \left| 2|G\rangle \right\rangle \\ + \frac{1}{9} \left| 1|R\rangle + 1|B\rangle \right\rangle + \frac{4}{45} \left| 1|G\rangle + 1|B\rangle \right\rangle.$$

We can also compute the distance between these two hypergeometric distributions over multisets. It involves a Kantorovich distance over the space of multisets (of size 2) with their own Kantorovich distance. Again, details of the calculation are skipped at this stage. The distance between the above two hypergeometric draw-distributions is:

$$d\left(hg[2](v_1), hg[2](v_2)\right) = \frac{1}{2} = d(v_1, v_2).$$

This coincidence of distances is non-trivial. It holds, in general, for arbitrary urns (of the same size) over arbitrary metric spaces of colours, for draws of arbitrary sizes. Moreover, the same coincidence of distances holds for the multinomial and Pólya modes of drawing. These coincidences form key results of this paper, see Theorems 7.3, 8.2, and 9.3 below.

In order to formulate and obtain these results, we describe multinomial, hypergeometric and Pólya distributions in the form of (Kleisli) maps:

$$\mathcal{D}(X) \xrightarrow{mn[K]} \mathcal{D}(\mathcal{M}[K](X)) \xleftarrow[p[K]]{hg[K]} \mathcal{M}[L](X) \quad (1.2)$$

They all produce distributions (indicated by  $\mathcal{D}$ ), in the middle of this diagram, on multisets (draws) of size  $K$ , indicated by  $\mathcal{M}[K]$ , over a set  $X$  of colours. Details will be provided below. Using the maps in (1.2), the coincidence of distances that we saw above can be described as

a preservation property, in terms of distance preserving maps — called isometries. At this stage we wish to emphasise that the representation of these different drawing operations as maps in (1.2) has a categorical background. It makes it possible to formulate and prove basic properties of drawing from an urn, such as naturality in the set  $X$  of colours. Also, as shown in [Jac21] for the multinomial and hypergeometric case, drawing forms a monoidal transformation (with ‘zipping’ for multisets as coherence map). Below it will be shown that the three draw maps (1.2) are even more well-behaved: they are all isometries, that is, they exactly preserve Kantorovich distances. These remarkable preservation results first appeared in the conference publication [Jac24], which this paper extends. The results are reproduced here, with more details, especially for the Pólya case.

This paper adds two more results about drawing and distance, to which we refer as the law of large urns and the law of large draws. Recall that multinomial and Pólya drawing involves removal and addition of the drawn balls from / to the urn. The effect of such removal / addition is negligible when the urn is very large, in comparison to the drawsize, so that one may expect that there is no difference with multinomial drawing (where the urn remains unchanged). The law of large urns make these intuitions precise in terms of limits of distances going to zero:

$$\lim_{v \rightarrow \infty} d\left(\text{hg}[K](v), \text{mn}[K](\text{Flrn}(v))\right) = 0 = \lim_{v \rightarrow \infty} d\left(\text{pl}[K](v), \text{mn}[K](\text{Flrn}(v))\right).$$

The first equation expresses that the Kantorovich distances between hypergeometric and multinomial distributions goes to zero as the urns become large. The multinomial distribution acts on urns as distributions, so that the normalisation operation  $\text{Flrn}$  must be inserted, see below for details. Similarly, the second equation makes precise that Pólya draws from large urns are close to multinomial draws.

The second law in this paper is what we call the law of large draws. It can be seen as a variation on the law of large numbers, in terms of Kantorovich distances. This law takes the form:

$$\lim_{K \rightarrow \infty} \text{mn}[K](\omega) \models d(\omega, \text{Flrn}(-)) = 0.$$

Informally it says that (normalisations of) large multinomial draws are close to the urn  $\omega$ . This closeness holds “in probability” as expressed by the validity sign  $\models$  in the above formulation. Details can be found in Theorem 11.2 below.

This paper concentrates on the mathematics behind these isometry and large urn/draw results, and not on interpretations or applications. We do like to briefly refer to interpretations in machine learning [RTG00] where the distance that we consider on colours in an urn is called the *ground distance*. Actual distances between colours are used there, based on experiments in psychophysics, using perceived differences [WS82].

The Kantorovich — or Wasserstein-Kantorovich, or Monge-Kantorovich — distance is the standard distance on distributions and on multisets, going back to [KR58]<sup>1</sup>. After some preliminaries on multisets and distributions, and on distances in general, Sections 4 and 6 of this paper recall the Kantorovich distance on distributions and on multisets, together with several basic results. The appendix contains some further background, especially about the dual formulations for these distances. The three subsequent Sections 7 – 9 demonstrate that multinomial, hypergeometric and Pólya drawing are all isometries. Distances occur on

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<sup>1</sup>The history on this topic is not so clear; we refer to the bibliographic notes as the end of Chapter 6 of [Vil09] for details.

multiple levels: on colours, on urns (as multisets or distributions) and on draw-distributions. This may be confusing, but several illustrations are included.

The so-called total variation distance is a special case of the Kantorovich distance. The relation between these two distances is subtle. We elaborate them in Section 5, for convenience of the reader. The large urn / draw results in Theorem 10.3 and 11.2 are proven first for the total variation distance, but can then be transferred to the general Kantorovich distance.

## 2. PRELIMINARIES ON MULTISSETS AND DISTRIBUTIONS

A *multiset* over a set  $X$  is a finite formal sum of the form  $\sum_i n_i |x_i\rangle$ , for elements  $x_i \in X$  and natural numbers  $n_i \in \mathbb{N}$  describing the multiplicities of these elements  $x_i$ . We shall write  $\mathcal{M}(X)$  for the set of such multisets over  $X$ . A multiset  $\varphi \in \mathcal{M}(X)$  may equivalently be described in functional form, as a function  $\varphi: X \rightarrow \mathbb{N}$  with finite support:  $\text{supp}(\varphi) := \{x \in X \mid \varphi(x) \neq 0\}$ . Such a function  $\varphi: X \rightarrow \mathbb{N}$  can be written in ket form as  $\sum_{x \in X} \varphi(x) |x\rangle$ . We switch back-and-forth between the ket and functional form and use the formulation that best suits a particular situation.

For a multiset  $\varphi \in \mathcal{M}(X)$  we write  $\|\varphi\| \in \mathbb{N}$  for the *size* of the multiset. It is the total number of elements, including multiplicities:

$$\|\varphi\| := \sum_{x \in \text{supp}(\varphi)} \varphi(x) = \sum_{x \in X} \varphi(x).$$

For a number  $K \in \mathbb{N}$  we write  $\mathcal{M}[K](X) \subseteq \mathcal{M}(X)$  for the subset of multisets of size  $K$ . When the set  $X$  has  $n \geq 1$  elements, the number of multisets of size  $K$  in the set  $\mathcal{M}[K](X)$  is given by the *multichoose* coefficient:

$$\binom{n}{K} := \binom{n+K-1}{K} = \frac{(n+K-1)!}{K! \cdot (n-1)!}.$$

We refer to [Jac22c, Jac25] for details, but we do recall the analogy that the number of subsets of size  $K$  of an  $n$ -element set is given by the ordinary binomial coefficient  $\binom{n}{K} = \frac{n!}{K! \cdot (n-K)!}$ .

For each set  $X$  and number  $K$  there is an ‘accumulation’ map  $\text{acc}: X^K \rightarrow \mathcal{M}[K](X)$  that turns lists into multisets via  $\text{acc}(x_1, \dots, x_K) := 1|x_1\rangle + \dots + 1|x_K\rangle$ . For instance  $\text{acc}(c, b, a, c, a, c) = 2|a\rangle + 1|b\rangle + 3|c\rangle$ . A standard result (see [Jac25]) is that for a multiset  $\varphi \in \mathcal{M}[K](X)$  there are  $\binom{K!}{\varphi}$  many sequences  $\vec{x} \in X^K$  with  $\text{acc}(\vec{x}) = \varphi$ , where  $\binom{K!}{\varphi} = \prod_x \varphi(x)!$ . This accumulation map is the coequaliser of all transposition maps  $X^K \xrightarrow{\cong} X^K$  induced by permutations of  $K$ , see [Jac22a, Jac25].

Multisets  $\varphi, \psi \in \mathcal{M}(X)$  can be added and compared elementwise, so that  $(\varphi + \psi)(x) = \varphi(x) + \psi(x)$  and  $\varphi \leq \psi$  means  $\varphi(x) \leq \psi(x)$  for all  $x \in X$ . In the latter case, when  $\varphi \leq \psi$ , we can also subtract  $\psi - \varphi$  elementwise.

The mapping  $X \mapsto \mathcal{M}(X)$  is functorial: for a function  $f: X \rightarrow Y$  we have  $\mathcal{M}(f): \mathcal{M}(X) \rightarrow \mathcal{M}(Y)$  given by  $\mathcal{M}(f)(\varphi)(y) = \sum_{x \in f^{-1}(y)} \varphi(x)$ . When we view the function  $f$  as mapping  $X$ -colours to  $Y$ -colours, the associated map  $\mathcal{M}(f)$  is a repainting of balls in urns. This map  $\mathcal{M}(f)$  preserves sums and size. Clearly, repainting of balls in an urn does not change the number of balls in the urn. Preservation of sums by  $\mathcal{M}(f)$  involves: first repainting the balls in two urns separately and then combining their balls, is the same as first combining the urns and then repainting.

For a multiset  $\tau \in \mathcal{M}(X \times Y)$  on a product set we can take its two marginals  $\mathcal{M}(\pi_1)(\tau) \in \mathcal{M}(X)$  and  $\mathcal{M}(\pi_2)(\tau) \in \mathcal{M}(Y)$  via functoriality, using the two projection functions  $\pi_1: X \times Y \rightarrow X$  and  $\pi_2: X \times Y \rightarrow Y$ . Starting from  $\varphi \in \mathcal{M}(X)$  and  $\psi \in \mathcal{M}(Y)$ , we say that  $\tau \in \mathcal{M}(X \times Y)$  is a *coupling* of  $\varphi, \psi$  if  $\varphi$  and  $\psi$  are the two marginals of  $\tau$ . We define the *decoupling* map:

$$\mathcal{M}(X \times Y) \xrightarrow{d\text{cpl} := \langle \mathcal{M}(\pi_1), \mathcal{M}(\pi_2) \rangle} \mathcal{M}(X) \times \mathcal{M}(Y) \quad (2.1)$$

The inverse image  $d\text{cpl}^{-1}(\varphi, \psi) \subseteq \mathcal{M}(X \times Y)$  is thus the subset of couplings of  $\varphi, \psi$ .

For two multisets  $\varphi \in \mathcal{M}(X)$  and  $\psi \in \mathcal{M}(Y)$  we can form a tensor product  $\varphi \otimes \psi \in \mathcal{M}(X \times Y)$  via:

$$(\varphi \otimes \psi)(x, y) := \varphi(x) \cdot \psi(y).$$

Such a tensor  $\varphi \otimes \psi$  is a coupling of  $\varphi, \psi$ .

A *distribution* over a set  $X$  is a finite formal sum of the form  $\sum_i r_i |x_i\rangle$  with elements  $x_i \in X$  and multiplicities / probabilities  $r_i \in [0, 1]$  satisfying  $\sum_i r_i = 1$ . Such a distribution can equivalently be described as a function  $\omega: X \rightarrow [0, 1]$  with finite support, satisfying  $\sum_x \omega(x) = 1$ . We write  $\mathcal{D}(X)$  for the set of distributions on  $X$ . This  $\mathcal{D}$  is functorial, in the same way as  $\mathcal{M}$ . Both  $\mathcal{D}$  and  $\mathcal{M}$  are monads on the category **Sets** of sets and functions, but we only use this for  $\mathcal{D}$ . The unit and multiplication / flatten maps  $\text{unit}: X \rightarrow \mathcal{D}(X)$  and  $\text{flat}: \mathcal{D}^2(X) \rightarrow \mathcal{D}(X)$  are given by:

$$\text{unit}(x) := 1|x\rangle \quad \text{flat}(\Omega) := \sum_{x \in X} \left( \sum_{\omega \in \mathcal{D}(X)} \Omega(\omega) \cdot \omega(x) \right) |x\rangle. \quad (2.2)$$

Kleisli maps  $c: X \rightarrow \mathcal{D}(Y)$  are also called channels and written as  $c: X \rightarrow Y$ . The Kleisli extension  $c_*: \mathcal{D}(X) \rightarrow \mathcal{D}(Y)$  for such a channel, is defined on  $\omega \in \mathcal{D}(X)$  as:

$$c_*(\omega) := \text{flat}(\mathcal{D}(c)(\omega)) = \sum_{y \in Y} \left( \sum_{x \in X} \omega(x) \cdot c(x)(y) \right) |y\rangle.$$

Channels  $c: X \rightarrow Y$  and  $d: Y \rightarrow Z$  can be composed to  $d \circ c: X \rightarrow Z$  via  $(d \circ c)(x) := d_*(c(x))$ . Each function  $f: X \rightarrow Y$  gives rise to a deterministic channel  $\langle f \rangle := \text{unit} \circ f: X \rightarrow Y$ , that is, via  $\langle f \rangle(x) = 1|f(x)\rangle$ .

An example of a channel is arrangement  $\text{arr}: \mathcal{M}[K](X) \rightarrow \mathcal{D}(X^K)$ . It maps a multiset  $\varphi \in \mathcal{M}[K](X)$  to the uniform distribution of sequences that accumulate to  $\varphi$ .

$$\text{arr}(\varphi) := \sum_{\vec{x} \in \text{acc}^{-1}(\varphi)} \frac{1}{(\varphi)} |\vec{x}\rangle = \sum_{\vec{x} \in \text{acc}^{-1}(\varphi)} \frac{\varphi_{\circ}^{\parallel}}{K!} |\vec{x}\rangle. \quad (2.3)$$

One can show that  $\langle \text{acc} \rangle \circ \text{arr} = \mathcal{D}(\text{acc}) \circ \text{arr} = \text{unit}: \mathcal{M}[K](X) \rightarrow \mathcal{D}(\mathcal{M}[K](X))$ . The composite in the other direction produces the uniform distribution of all permutations of a sequence:

$$\text{arr} \circ \langle \text{acc} \rangle = \text{arr} \circ \text{acc} = \text{prm} \quad \text{where} \quad \text{prm}(\vec{x}) := \sum_{t: K \xrightarrow{\cong} K} \frac{1}{K!} |t(\vec{x})\rangle, \quad (2.4)$$

in which  $t(x_1, \dots, x_K) := (x_{t(1)}, \dots, x_{t(K)})$ . In writing  $t: K \xrightarrow{\cong} K$  we implicitly identify the number  $K$  with the set  $\{1, \dots, K\}$ .

Each multiset  $\varphi \in \mathcal{M}(X)$  of non-zero size can be turned into a distribution via normalisation. This operation is called frequentist learning, since it involves learning a distribution from a multiset of data, via counting. Explicitly:

$$\text{Flrn}(\varphi) := \sum_{x \in X} \frac{\varphi(x)}{\|\varphi\|} |x\rangle.$$

For instance, if we learn from an urn with three red, two green and five blue balls, we get the probability distribution for drawing a ball of a particular colour from the urn:

$$\text{Flrn}\left(3|R\rangle + 2|G\rangle + 5|B\rangle\right) = \frac{3}{10}|R\rangle + \frac{1}{5}|G\rangle + \frac{1}{2}|B\rangle.$$

This map  $\text{Flrn}$  is a natural transformation (but not a map of monads).

Given two distributions  $\omega \in \mathcal{D}(X)$  and  $\rho \in \mathcal{D}(Y)$ , we can form their parallel product  $\omega \otimes \rho \in \mathcal{D}(X \times Y)$ , given in functional form as:

$$(\omega \otimes \rho)(x, y) := \omega(x) \cdot \rho(y).$$

The tensors of multisets and of distributions are related via frequentist learning:

$$\text{Flrn}(\varphi \otimes \psi) = \text{Flrn}(\varphi) \otimes \text{Flrn}(\psi). \quad (2.5)$$

Like for multisets, we call a joint distribution  $\tau \in \mathcal{D}(X \times Y)$  a *coupling* of  $\omega \in \mathcal{D}(X)$  and  $\rho \in \mathcal{D}(Y)$  when  $\omega, \rho$  are the two marginals of  $\tau$ , that is, when  $\mathcal{D}(\pi_1)(\tau) = \omega$  and  $\mathcal{D}(\pi_2) = \rho$ . We can express this also via a decouple map  $\text{dcpl} = \langle \mathcal{D}(\pi_1), \mathcal{D}(\pi_2) \rangle$  as in (2.1). The tensor  $\omega \otimes \rho$  is an obvious coupling of the distributions  $\omega$  and  $\rho$ .

An *observation* on a set  $X$  is a function of the form  $p: X \rightarrow \mathbb{R}$ . Such a map  $p$ , together with a distribution  $\omega \in \mathcal{D}(X)$ , is called a random variable — but confusingly, the distribution is often left implicit. The map  $p: X \rightarrow \mathbb{R}$  will be called a *factor* if it restricts to non-negative reals  $X \rightarrow \mathbb{R}_{\geq 0}$ . Each element  $x \in X$  gives rise to a point observation  $\mathbf{1}_x: X \rightarrow \mathbb{R}$ , with  $\mathbf{1}_x(x') = 1$  if  $x = x'$  and  $\mathbf{1}_x(x') = 0$  if  $x \neq x'$ .

For a distribution  $\omega \in \mathcal{D}(X)$  and an observation  $p: X \rightarrow \mathbb{R}$  on the same set  $X$  we write  $\omega \models p$  for the validity (expected value) of  $p$  in  $\omega$ , defined as (finite) sum:  $\sum_{x \in X} \omega(x) \cdot p(x)$ . For a function  $f: X \rightarrow Y$ , a distribution  $\omega \in \mathcal{D}(X)$  and an observation  $q: Y \rightarrow \mathbb{R}$  one has the following equality of validities:

$$\mathcal{D}(f)(\omega) \models q = \omega \models (q \circ f). \quad (2.6)$$

This equation is sometimes called ‘the law of the unconscious statistician’, see *e.g.* [CB02, §2.2]. We shall write  $\text{Obs}(X) = \mathbb{R}^X$  and  $\text{Fact}(X) = (\mathbb{R}_{\geq 0})^X$  for the sets of observations and factors on  $X$ .

### 3. PRELIMINARIES ON METRIC SPACES

A metric space will be written as a pair  $(X, d_X)$ , where  $X$  is a set and  $d_X: X \times X \rightarrow \mathbb{R}_{\geq 0}$  is a distance function, also called metric. This metric satisfies:

- separation:  $d_X(x, x') = 0$  iff  $x = x'$ ;
- symmetry:  $d_X(x, x') = d_X(x', x)$ ;
- triangular inequality:  $d_X(x, x'') \leq d_X(x, x') + d_X(x', x'')$ .

Often, we drop the subscript  $X$  in  $d_X$  if it is clear from the context. We use the standard distance  $d(x, y) = |x - y|$  on real and natural numbers.

**Definition 3.1.** Let  $(X, d_X), (Y, d_Y)$  be two metric spaces.

(1) A function  $f: X \rightarrow Y$  is called *short* (or also *non-expansive*) if:

$$d_Y(f(x), f(x')) \leq d_X(x, x'), \quad \text{for all } x, x' \in X.$$

Such a map is called an *isometry* or an *isometric embedding* if the above inequality  $\leq$  is an actual equality  $=$ . This implies that the function  $f$  is injective, and thus an ‘embedding’.

We write  $\mathbf{Met}_S$  for the category of metric spaces with short maps between them.

(2) A function  $f: X \rightarrow Y$  is *Lipschitz* or *M-Lipschitz*, if there is a number  $M \in \mathbb{R}_{>0}$  such that:

$$d_Y(f(x), f(x')) \leq M \cdot d_X(x, x'), \quad \text{for all } x, x' \in X.$$

The number  $M$  is sometimes called the *Lipschitz constant*. Thus, a short function is Lipschitz, with constant 1. We write  $\mathbf{Met}_L$  for the category of metric spaces with Lipschitz maps between them (with arbitrary Lipschitz constants).

It is easy to see that if  $f: X \rightarrow Y$  is  $M$ -Lipschitz and  $g: Y \rightarrow Z$  is  $L$ -Lipschitz, then the composite  $g \circ f: X \rightarrow Z$  is Lipschitz with constant  $M \cdot L$ .

**Lemma 3.2.** For two metric spaces  $(X_1, d_1)$  and  $(X_2, d_2)$  we equip the cartesian product  $X_1 \times X_2$  of sets with the sum of the two metrics:

$$d\left((x_1, x_2), (x'_1, x'_2)\right) := d_{X_1}(x_1, x'_1) + d_{X_2}(x_2, x'_2). \quad (3.1)$$

We shall extend these product distances to  $K$ -ary form  $X_1 \times \cdots \times X_K$  and  $X^K = X \times \cdots \times X$ .

- (1) With the usual projections and tuples this forms a product in the category  $\mathbf{Met}_L$ . The definition yields a monoidal product (tensor) in the category  $\mathbf{Met}_S$  since the diagonal map  $X \rightarrow X \times X$  is 2-Lipschitz and not short.
- (2) If  $f_i: X_i \rightarrow Y_i$  is  $M_i$ -Lipschitz, then  $f_1 \times f_2: X_1 \times X_2 \rightarrow Y_1 \times Y_2$  is  $\max(M_1, M_2)$ -Lipschitz.

Products of metric spaces involve some subtleties, which are not relevant for the main line of the paper, but which we briefly make explicit as background information.

**Remark 3.3.** In the above description (3.1) we have used the sum of the distances in the components. As stated, this formulation yields a categorical product in the category of metric spaces with Lipschitz maps, but not with short maps.

Instead of the sum  $+$  in (3.1) one can use the maximum. This yields a categorical product in the both the categories  $\mathbf{Met}_L$  and  $\mathbf{Met}_S$  of metric spaces with Lipschitz and with short maps. The maximum also works when the metric is 1-bounded, that is, of the form  $d: X \times X \rightarrow [0, 1]$ , restricted to the unit interval  $[0, 1]$ . This restriction is common in program semantics, see *e.g.* [BV96, Bre01]. This 1-bounded case has advantages since it admits infinite products and also coproducts of metric spaces. We do not need such structure and we will work with general  $\mathbb{R}_{\geq 0}$ -valued metrics.

Thus, in the category  $\mathbf{Met}_L$  with Lipschitz maps one can equivalently use the maximum or the sum of distances in (3.1). The resulting products are isomorphic in  $\mathbf{Met}_L$ . This works since for  $r, s \in \mathbb{R}_{\geq 0}$  one has  $\max(r, s) \leq r + s$  and  $r + s \leq 2 \cdot \max(r, s)$ . Here we use the sum of distances in the product, since it is used for certain results, like Lemma 4.3 (9). A

concrete example where the sum of distances is used is for shortness of the addition function  $+: \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ , in:

$$\begin{aligned} d_{\mathbb{R}}(r + s, r' + s') &= |(r + s) - (r' + s')| = |(r - r') + (s - s')| \\ &\leq |r - r'| + |s - s'| \\ &= d_{\mathbb{R}}(r, r') + d_{\mathbb{R}}(s, s') \stackrel{(3.1)}{=} d_{\mathbb{R} \times \mathbb{R}}((r, s), (r', s')). \end{aligned}$$

Below we shall use the familiar zip function. It is in fact an isometry.

**Lemma 3.4.** *For metric spaces  $X, Y$  and for  $K \in \mathbb{N}$  consider the zip function  $\text{zip}: X^K \times Y^K \rightarrow (X \times Y)^K$  given by  $\text{zip}(\vec{x}, \vec{y}) = ((x_1, y_1), \dots, (x_K, y_K))$ . This zip function is a bijective function and an isometry.*

*Similarly, concatenation  $++: X^K \times X^L \rightarrow X^{K+L}$  is a bijection and an isometry.*

*Proof.* We only do the zip case. The zip function is obviously a bijection. For  $\vec{x}, \vec{x}' \in X^K$  and  $\vec{y}, \vec{y}' \in Y^K$  one has via repeated use of (3.1),

$$\begin{aligned} &d_{(X \times Y)^K}(\text{zip}(\vec{x}, \vec{y}), \text{zip}(\vec{x}', \vec{y}')) \\ &= d_{X \times Y}((x_1, y_1), (x'_1, y'_1)) + \dots + d_{X \times Y}((x_K, y_K), (x'_K, y'_K)) \\ &= (d_X(x_1, x'_1) + d_Y(y_1, y'_1)) + \dots + (d_X(x_K, x'_K) + d_Y(y_K, y'_K)) \\ &= (d_X(x_1, x'_1) + \dots + d_X(x_K, x'_K)) + (d_Y(y_1, y'_1) + \dots + d_Y(y_K, y'_K)) \\ &= d_{X^K}(\vec{x}, \vec{x}') + d_{Y^K}(\vec{y}, \vec{y}') = d_{X^K \times Y^K}((\vec{x}, \vec{y}), (\vec{x}', \vec{y}')). \quad \square \end{aligned}$$

#### 4. THE KANTOROVICH DISTANCE BETWEEN DISTRIBUTIONS

This section introduces the Kantorovich distance between probability distributions and recalls some basic results. There are several equivalent formulations for this distance. We express them in terms of validity and couplings, see also *e.g.* [Bre01, Bre18, DD09, FP19, DGJP04].

**Definition 4.1.** Let  $(X, d_X)$  be a metric space. The *Kantorovich* metric  $d = d_{\mathcal{D}(X)}: \mathcal{D}(X) \times \mathcal{D}(X) \rightarrow \mathbb{R}_{\geq 0}$  on distributions over  $X$  is defined by any of the three equivalent formulas:

$$\begin{aligned} d(\omega, \omega') &:= \bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models d_X \\ &= \bigvee_{p, p' \in \text{Obs}(X), p \oplus p' \leq d_X} \omega \models p + \omega' \models p' \\ &= \bigvee_{q \in \text{Facts}(X)} |\omega \models q - \omega' \models q|. \end{aligned} \tag{4.1}$$

This turns  $\mathcal{D}(X)$  into a metric space. The operation  $\oplus$  in the second formulation is defined as  $(p \oplus p')(x, x') = p(x) + p'(x')$ . The set  $\text{Facts}_S(X) \subseteq \text{Fact}(X)$  in the third formulation is the subset of short factors  $X \rightarrow \mathbb{R}_{\geq 0}$ . To be precise, we should write  $\text{Facts}_S(X, d_X)$  since the distance  $d_X$  on  $X$  is a parameter, but we leave it implicit for convenience. The meet  $\bigwedge$  and joins  $\bigvee$  in (4.1) are actually reached, by what are called the *optimal* coupling and the *optimal* observations / factor.



The equivalence of the first and second formulation in (4.1) is an instance of strong duality in linear programming, which can be obtained via Farkas' Lemma, see *e.g.* [MG06]. The second formulation is commonly associated with Monge. The single factor  $q$  in the third formulation can be obtained from the two observations  $p, p'$  in the second formulation, and vice-versa. In [DGJP04] it is shown that instead of using all short factors  $q$  in the third formulation one can restrict to those factors that arise as interpretation of formulas in a logic — since these interpretations are dense. What we call the Kantorovich distance is also called the Wasserstein-Kantorovich, or Monge-Kantorovich distance.

A proof of the equivalence of the three formulations for the Kantorovich distance  $d(\omega, \omega')$  between two distributions  $\omega, \omega'$  in (4.1) is given in the appendix. These three formulations do not immediately suggest how to calculate distances. What helps is that the minimum and maxima are actually reached and can be computed. This is done via linear programming, originally introduced by Kantorovich, see [MG06, Vil09, DD09]. In the sequel, we shall see several examples of distances between distributions. They are obtained via our (adapted) Python implementation of the linear optimisation, which also produces an optimal coupling, observations or factor. This implementation is used only for illustrations.

**Example 4.2.** Consider the set  $X$  containing the first eight natural numbers, so  $X = \{0, 1, \dots, 7\} \subseteq \mathbb{N}$ , with the usual distance, written as  $d_X$ , between natural numbers:  $d_X(n, m) = |n - m|$ . We look at the following two distributions on  $X$ .

$$\omega = \frac{1}{2}|0\rangle + \frac{1}{2}|4\rangle \quad \omega' = \frac{1}{8}|2\rangle + \frac{1}{8}|3\rangle + \frac{1}{8}|6\rangle + \frac{5}{8}|7\rangle.$$

We claim that the Kantorovich distance  $d(\omega, \omega')$  is  $\frac{15}{4}$ . This will be illustrated for each of the three formulations in Definition 4.1.

- An optimal coupling  $\tau \in \mathcal{D}(X \times X)$  of  $\omega, \omega'$  is:

$$\tau = \frac{1}{8}|0, 2\rangle + \frac{1}{8}|0, 3\rangle + \frac{1}{8}|0, 6\rangle + \frac{1}{8}|0, 7\rangle + \frac{1}{2}|4, 7\rangle.$$

It is not hard to see that  $\tau$ 's first marginal is  $\omega$ , and its second marginal is  $\omega'$ . We compute the distances as:

$$\begin{aligned} d(\omega, \omega') &= \tau \models d_X \\ &= \frac{1}{8} \cdot d_X(0, 2) + \frac{1}{8} \cdot d_X(0, 3) + \frac{1}{8} \cdot d_X(0, 6) + \frac{1}{8} \cdot d_X(0, 7) + \frac{1}{2} \cdot d_X(4, 7) \\ &= \frac{2}{8} + \frac{3}{8} + \frac{6}{8} + \frac{7}{8} + \frac{3}{2} = \frac{18}{8} + \frac{3}{2} = \frac{9}{4} + \frac{6}{4} = \frac{15}{4}. \end{aligned}$$

- There are the following two optimal observations  $p, p': X \rightarrow \mathbb{R}$ , described as sums of weighted point predicates:

$$\begin{aligned} p &= -1 \cdot \mathbf{1}_1 - 2 \cdot \mathbf{1}_2 - 3 \cdot \mathbf{1}_3 - 4 \cdot \mathbf{1}_4 - 5 \cdot \mathbf{1}_5 - 6 \cdot \mathbf{1}_6 - 7 \cdot \mathbf{1}_7 \\ p' &= 1 \cdot \mathbf{1}_1 + 2 \cdot \mathbf{1}_2 + 3 \cdot \mathbf{1}_3 + 4 \cdot \mathbf{1}_4 + 5 \cdot \mathbf{1}_5 + 6 \cdot \mathbf{1}_6 + 7 \cdot \mathbf{1}_7. \end{aligned}$$

It is not hard to see that  $(p \oplus p')(i, j) := p(i) + p'(j) \leq d_X(i, j)$  holds for all  $i, j \in X$ . Using the second formulation in (4.1) we get:

$$\begin{aligned} (\omega \models p) + (\omega' \models p') &= \frac{1}{2} \cdot p(0) + \frac{1}{2} \cdot p(4) + \frac{1}{8} \cdot p'(2) + \frac{1}{8} \cdot p'(3) + \frac{1}{8} \cdot p'(6) + \frac{5}{8} \cdot p'(7) \\ &= \frac{-4}{2} + \frac{2}{8} + \frac{3}{8} + \frac{6}{8} + \frac{35}{8} = -2 + \frac{46}{8} = \frac{30}{8} = \frac{15}{4}. \end{aligned}$$

- Finally, there is a (single) short factor  $q: X \rightarrow \mathbb{R}_{\geq 0}$  given by:

$$q = 7 \cdot \mathbf{1}_0 + 6 \cdot \mathbf{1}_1 + 5 \cdot \mathbf{1}_2 + 4 \cdot \mathbf{1}_3 + 3 \cdot \mathbf{1}_4 + 2 \cdot \mathbf{1}_5 + 1 \cdot \mathbf{1}_6.$$

Then:

$$\begin{aligned} (\omega \models q) - (\omega' \models q) &= \frac{1}{2} \cdot q(0) + \frac{1}{2} \cdot q(4) - \left( \frac{1}{8} \cdot q(2) + \frac{1}{8} \cdot q(3) + \frac{1}{8} \cdot q(6) + \frac{5}{8} \cdot q(7) \right) \\ &= \frac{7}{2} + \frac{3}{2} - \left( \frac{5}{8} + \frac{4}{8} + \frac{1}{8} \right) = \frac{10}{2} - \frac{10}{8} = \frac{20}{4} - \frac{5}{4} = \frac{15}{4}. \end{aligned}$$

From the fact that the coupling  $\tau$ , the two observations  $p, p'$ , and the single factor  $q$  produce the same distance one can deduce that they are optimal, using the formula (4.1).

We proceed with several standard properties of the Kantorovich distance on distributions.

**Lemma 4.3.** *In the context of Definition 4.1, the following properties hold.*

- (1) *For an  $M$ -Lipschitz function  $f: X \rightarrow Y$ , the pushforward map  $\mathcal{D}(f): \mathcal{D}(X) \rightarrow \mathcal{D}(Y)$  is also  $M$ -Lipschitz; as a result,  $\mathcal{D}$  lifts to a functor  $\mathcal{D}: \mathbf{Met}_L \rightarrow \mathbf{Met}_L$ , and also to  $\mathcal{D}: \mathbf{Met}_S \rightarrow \mathbf{Met}_S$ .*
- (2) *If  $f: X \rightarrow Y$  is an isometry, then so is  $\mathcal{D}(f): \mathcal{D}(X) \rightarrow \mathcal{D}(Y)$ .*
- (3) *For an  $M$ -Lipschitz factor  $q: X \rightarrow \mathbb{R}_{\geq 0}$ , the validity-of- $q$  factor  $(-) \models q: \mathcal{D}(X) \rightarrow \mathbb{R}_{\geq 0}$  is also  $M$ -Lipschitz.*
- (4) *For each element  $x \in X$  and distribution  $\omega \in \mathcal{D}(X)$  one has:  $d(1|x\rangle, \omega) = \omega \models d_X(x, -)$ ; especially,  $d(1|x\rangle, 1|x'\rangle) = d_X(x, x')$ , making the map  $\text{unit}: X \rightarrow \mathcal{D}(X)$  an isometry.*
- (5) *The monad multiplication  $\text{flat}: \mathcal{D}^2(X) \rightarrow \mathcal{D}(X)$  is short, so that  $\mathcal{D}$  lifts from a monad on  $\mathbf{Sets}$  to a monad on  $\mathbf{Met}_S$  and on  $\mathbf{Met}_L$ .*
- (6) *If a channel  $c: X \rightarrow \mathcal{D}(Y)$  is  $M$ -Lipschitz, then so is its Kleisli extension  $c_* := \text{flat} \circ \mathcal{D}(c): \mathcal{D}(X) \rightarrow \mathcal{D}(Y)$ .*
- (7) *If channel  $c: X \rightarrow Y$  is  $M$ -Lipschitz and channel  $d: Y \rightarrow Z$  is  $L$ -Lipschitz, then their (channel) composite  $d \circ c: X \rightarrow Z$  is  $(M \cdot L)$ -Lipschitz.*
- (8) *For distributions  $\omega_i, \omega'_i \in \mathcal{D}(X)$  and numbers  $r_i \in [0, 1]$  with  $\sum_i r_i = 1$  one has:*

$$d\left(\sum_i r_i \cdot \omega_i, \sum_i r_i \cdot \omega'_i\right) \leq \sum_i r_i \cdot d(\omega_i, \omega'_i).$$

- (9) *The permutation channel  $\text{prm}: X^K \rightarrow \mathcal{D}(X^K)$  from (2.4) is short.*

*Proof.*

- (1) Let  $f: X \rightarrow Y$  be  $M$ -Lipschitz. If  $\tau \in \mathcal{D}(X \times X)$  is a coupling of  $\omega, \omega' \in \mathcal{D}(X)$ , then  $\mathcal{D}(f \times f)(\tau) \in \mathcal{D}(Y \times Y)$  is a coupling of  $\mathcal{D}(f)(\omega), \mathcal{D}(f)(\omega') \in \mathcal{D}(Y)$ . Thus:

$$\begin{aligned} d_{\mathcal{D}(Y)}\left(\mathcal{D}(f)(\omega), \mathcal{D}(f)(\omega')\right) &\stackrel{(4.1)}{=} \bigwedge_{\sigma \in \text{dcpl}^{-1}(\mathcal{D}(f)(\omega), \mathcal{D}(f)(\omega'))} \sigma \models d_Y \\ &\leq \bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \mathcal{D}(f \times f)(\tau) \models d_Y \\ &\stackrel{(2.6)}{=} \bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models d_Y \circ (f \times f) \\ &\leq \bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models M \cdot d_X \\ &= M \cdot \left( \bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models d_X \right) \stackrel{(4.1)}{=} M \cdot d_{\mathcal{D}(X)}(\omega, \omega'). \end{aligned}$$

- (2) Let  $f: X \rightarrow Y$  be an isometry. Then it is 1-Lipschitz, so  $\mathcal{D}(f)$  is as well, by the previous item. It thus suffices to prove:  $d(\omega, \omega') \leq d(\mathcal{D}(f)(\omega), \mathcal{D}(f)(\omega'))$ , for  $\omega, \omega' \in \mathcal{D}(X)$ . Let  $p: X \rightarrow \mathbb{R}_{\geq 0}$  be short. We turn it into a short factor  $q: Y \rightarrow \mathbb{R}_{\geq 0}$  via the definition:

$$q(y) := \bigwedge_{x \in X} p(x) + d_Y(f(x), y) \quad \text{satisfying, by construction,} \quad q \circ f = p.$$

This map  $q$  is short, since for arbitrary  $y, y' \in Y$  we have:

$$\begin{aligned} |q(y) - q(y')| &= \bigwedge_{x, x' \in X} |(p(x) + d_Y(f(x), y)) - (p(x') + d_Y(f(x'), y'))| \\ &\leq \bigwedge_{x \in X} |p(x) + d_Y(f(x), y) - p(x) - d_Y(f(x), y')| \\ &= \bigwedge_{x \in X} |d_Y(f(x), y) - d_Y(f(x), y')| \leq d_Y(y, y'). \end{aligned}$$

The latter inequality — sometimes called the reverse triangle inequality — follows easily from the triangular inequality.

Using  $q \circ f = p$  we get:

$$\begin{aligned} |\omega \models p - \omega' \models p| &= |\omega \models (q \circ f) - \omega' \models (q \circ f)| \\ &\stackrel{(2.6)}{=} |\mathcal{D}(f)(\omega) \models q - \mathcal{D}(f)(\omega') \models q| \leq d(\mathcal{D}(f)(\omega), \mathcal{D}(f)(\omega')). \end{aligned}$$

Since this holds for all short factors  $p$  we obtain, as required:

$$d(\omega, \omega') = \bigvee_{p \in \text{Fact}_S(X)} |\omega \models p - \omega' \models p| \leq d(\mathcal{D}(f)(\omega), \mathcal{D}(f)(\omega')).$$

- (3) Let  $q: X \rightarrow \mathbb{R}_{\geq 0}$  be  $M$ -Lipschitz, then  $\frac{1}{M} \cdot q: X \rightarrow \mathbb{R}_{\geq 0}$  is short. The function  $(-) \models q: \mathcal{D}(X) \rightarrow \mathbb{R}_{\geq 0}$  is then also  $M$ -Lipschitz, since for  $\omega, \omega' \in \mathcal{D}(X)$ ,

$$\begin{aligned} |\omega \models q - \omega' \models q| &= M \cdot |\omega \models \frac{1}{M} \cdot q - \omega' \models \frac{1}{M} \cdot q| \\ &\leq M \cdot \bigvee_{p \in \text{Fact}_S(X)} |\omega \models p - \omega' \models p| = M \cdot d(\omega, \omega'). \end{aligned}$$

- (4) The only coupling of  $1|x\rangle, \omega \in \mathcal{D}(X)$  is  $1|x\rangle \otimes \omega \in \mathcal{D}(X \times X)$ . Hence:

$$d(1|x\rangle, \omega) = 1|x\rangle \otimes \omega \models d_X = \sum_{x' \in X} \omega(x') \cdot d_X(x, x') = \omega \models d_X(x, -).$$

- (5) We first note that for a distribution of distributions  $\Omega \in \mathcal{D}^2(X)$  and a short factor  $p: X \rightarrow \mathbb{R}_{\geq 0}$  the validity in  $\Omega$  of the short validity factor  $(-) \models p: \mathcal{D}(X) \rightarrow \mathbb{R}_{\geq 0}$  from item (3) satisfies:

$$\begin{aligned} \Omega \models ((-) \models p) &= \sum_{\omega \in \mathcal{D}(X)} \Omega(\omega) \cdot (\omega \models p) = \sum_{\omega \in \mathcal{D}(X)} \sum_{x \in X} \Omega(\omega) \cdot \omega(x) \cdot p(x) \\ &\stackrel{(2.2)}{=} \sum_{x \in X} \text{flat}(\Omega)(x) \cdot p(x) = \text{flat}(\Omega) \models p. \end{aligned}$$

Thus for  $\Omega, \Omega' \in \mathcal{D}^2(X)$ ,

$$\begin{aligned}
& d_{\mathcal{D}(X)}(\text{flat}(\Omega), \text{flat}(\Omega')) \\
&= \bigvee_{p \in \text{Fact}_S(X)} |\text{flat}(\Omega) \models p - \text{flat}(\Omega') \models p| \\
&= \bigvee_{p \in \text{Fact}_S(X)} |\Omega \models ((-) \models p) - \Omega' \models ((-) \models p)| \quad \text{as just shown} \\
&\leq \bigvee_{Q \in \text{Fact}_S(\mathcal{D}(X))} |\Omega \models Q - \Omega' \models Q| \quad \text{by item (3)} \\
&= d_{\mathcal{D}^2(X)}(\Omega, \Omega').
\end{aligned}$$

(6) Directly by points (1) and (5).

(7) The channel composite  $d \circ c = \text{flat} \circ \mathcal{D}(d) \circ c$  consists of a functional composite of  $M$ -Lipschitz,  $L$ -Lipschitz, and 1-Lipschitz maps, and is thus  $(M \cdot L \cdot 1)$ -Lipschitz. This uses items (1) and (5).

(8) If we have couplings  $\tau_i$  for  $\omega_i, \omega'_i$ , then  $\sum_i r_i \cdot \tau_i$  is a coupling of  $\sum_i r_i \cdot \omega_i$  and  $\sum_i r_i \cdot \omega'_i$ . Moreover:

$$d\left(\sum_i r_i \cdot \omega_i, \sum_i r_i \cdot \omega'_i\right) \leq \left(\sum_i r_i \cdot \tau_i\right) \models d_X = \sum_i r_i \cdot (\tau_i \models d_X).$$

Since this holds for all  $\tau_i$ , we get:  $d(\sum_i r_i \cdot \omega_i, \sum_i r_i \cdot \omega'_i) \leq \sum_i r_i \cdot d(\omega_i, \omega'_i)$ .

(9) We unfold the definition of the *prm* map from (2.4) and use the previous item in the first step below. We also use that the distance between two sequences is invariant under permutation (of both).

$$\begin{aligned}
d_{\mathcal{D}(X^K)}(\text{prm}(\vec{x}), \text{prm}(\vec{y})) &\leq \sum_{t: K \cong K} \frac{1}{K!} \cdot d_{\mathcal{D}(X^K)}(1|\underline{t}(\vec{x})\rangle, 1|\underline{t}(\vec{y})\rangle) \\
&= \sum_{t: K \cong K} \frac{1}{K!} \cdot d_{X^K}(\underline{t}(\vec{x}), \underline{t}(\vec{y})) \quad \text{by item (4)} \\
&= \sum_{t: K \cong K} \frac{1}{K!} \cdot d_{X^K}(\vec{x}, \vec{y}) = d_{X^K}(\vec{x}, \vec{y}). \quad \square
\end{aligned}$$

Later on we need the following facts about tensors of distributions.

**Proposition 4.4.** *Let  $X, Y$  be metric spaces, and  $K$  be a positive natural number.*

- (1) *The tensor map  $\otimes: \mathcal{D}(X) \times \mathcal{D}(Y) \rightarrow \mathcal{D}(X \times Y)$  is an isometry.*
- (2) *The  $K$ -fold tensor map  $\text{iid}[K]: \mathcal{D}(X) \rightarrow \mathcal{D}(X^K)$ , given by  $\text{iid}[K](\omega) := \omega^K = \omega \otimes \dots \otimes \omega$ , is  $K$ -Lipschitz. Actually, there is an equality:  $d(\text{iid}[K](\omega), \text{iid}[K](\rho)) = K \cdot d(\omega, \rho)$ .*

*Proof.* (1) Let distributions  $\omega, \omega' \in \mathcal{D}(X)$  and  $\rho, \rho' \in \mathcal{D}(Y)$  be given. For the inequality  $d_{\mathcal{D}(X) \times \mathcal{D}(Y)}((\omega, \rho), (\omega', \rho')) \leq d_{\mathcal{D}(X \times Y)}(\omega \otimes \rho, \omega' \otimes \rho')$  one uses that a coupling  $\tau \in \mathcal{D}((X \times Y) \times (X \times Y))$  of  $\omega \otimes \rho, \omega' \otimes \rho' \in \mathcal{D}(X \times Y)$  can be turned into two couplings  $\tau_1, \tau_2$  of  $\omega, \omega'$  and of  $\rho, \rho'$ , namely as  $\tau_i := \mathcal{D}(\pi_i \times \pi_i)(\tau)$ . For the reverse inequality one turns two couplings  $\tau_1, \tau_2$  of  $\omega, \omega'$  and  $\rho, \rho'$  into a coupling  $\tau$  of  $\omega \otimes \rho, \omega' \otimes \rho'$  via  $\tau := \mathcal{D}(\langle \pi_1 \times \pi_1, \pi_2 \times \pi_2 \rangle)(\tau_1 \otimes \tau_2)$ .

(2) For  $\omega, \rho \in \mathcal{D}(X)$  and  $K \in \mathbb{N}$ , using the previous item, we get:

$$d_{\mathcal{D}(X^K)}(\omega^K, \rho^K) \stackrel{(1)}{=} d_{\mathcal{D}(X) \times \dots \times \mathcal{D}(X)}((\omega, \dots, \omega), (\rho, \dots, \rho)) \stackrel{(3.1)}{=} K \cdot d_{\mathcal{D}(X)}(\omega, \rho). \quad \square$$

For the next result we use for an arbitrary set  $Y$  and natural number  $K > 0$  the set  $\mathcal{D}[K](Y)$  of ‘fractional distributions’ obtained from multisets of size  $K$ :

$$\mathcal{D}[K](Y) := \{Flrn(\varphi) \mid \varphi \in \mathcal{M}[K](Y)\}.$$

**Fact 4.5.** For fractional distributions  $\omega, \omega' \in \mathcal{D}[K](X)$  over a metric space  $X$  there is an optimal coupling  $\tau \in \mathcal{D}[K](X \times X)$  with  $d(\omega, \omega') = \tau \models d_X$ .

The fact that this coupling  $\tau$  is also fractional, for the same number  $K$ , can be seen by inspecting the simplex algorithm that is standardly used in linear programming, see *e.g.* [MG06]. The details of this go beyond the scope of this paper. Since this fact is given without proof we shall make explicit which results depend on it.

We illustrate that these matters are subtle.

**Example 4.6.** Consider the set  $X = \{1, 2, 3\}$  with the following two distributions  $\omega, \omega' \in \mathcal{D}[4](X)$ , namely:  $\omega = \frac{3}{4}|1\rangle + \frac{1}{4}|2\rangle$  and  $\omega' = \frac{1}{2}|1\rangle + \frac{1}{4}|2\rangle + \frac{1}{4}|3\rangle$ . We consider the following two couplings of  $\omega, \omega'$

$$\begin{aligned} \tau &= \frac{1}{2}|1, 1\rangle + \frac{1}{4}|1, 2\rangle + \frac{1}{4}|2, 3\rangle \\ \sigma &= \frac{1}{2}|1, 1\rangle + \frac{1}{8}|1, 2\rangle + \frac{1}{8}|1, 3\rangle + \frac{1}{8}|2, 2\rangle + \frac{1}{8}|2, 3\rangle \end{aligned}$$

The first coupling  $\tau$  is in  $\mathcal{D}[4](X \times X)$  and forms an optimal coupling, giving rise to  $d(\omega, \omega') = \frac{1}{2}$ . Interestingly,  $\sigma$  is also an optimal coupling of  $\omega, \omega'$  giving rise to the same distance, but inhabits the set  $\mathcal{D}[8](X \times X)$ . Explicitly:

$$\begin{aligned} \tau \models d_X &= \frac{1}{4} \cdot d_X(1, 2) + \frac{1}{4} \cdot d_X(2, 3) = \frac{1}{4} \cdot 1 + \frac{1}{4} \cdot 1 = \frac{1}{2}. \\ \sigma \models d_X &= \frac{1}{8} \cdot d_X(1, 2) + \frac{1}{8} \cdot d_X(1, 3) + \frac{1}{8} \cdot d_X(2, 3) = \frac{1}{8} \cdot 1 + \frac{1}{8} \cdot 2 + \frac{1}{8} \cdot 1 = \frac{1}{2}. \end{aligned}$$

The conclusion is that, in general, if  $\tau \in \mathcal{D}(X \times X)$  is an optimal coupling of  $\omega, \omega' \in \mathcal{D}[K](X)$ , then  $K \cdot \tau$  need not be a multiset of (size  $K$ ). Fact 4.5 says that there is at least one optimal coupling  $\tau$  such that  $K \cdot \tau$  does form a multiset.

## 5. KANTOROVICH DISTANCE AND TOTAL VARIATION DISTANCE

In this section we relate the so-called total variation distance between distributions to the Kantorovich distance, in two different ways.

- The total variation distance is an instance of the Kantorovich distance, for discrete metric spaces, see Proposition 5.2.
- The total variation distance forms a (scaled) upperbound for the Kantorovich distance, see Proposition 5.3.

Both facts are familiar from the literature, but proofs are scattered around or left implicit for the discrete case. We include the details for the record and for convenience of the reader. The second point will be useful to prove further (limit) properties of the Kantorovich distance, via the total variation distance. The latter distance is easier to calculate and reason about.

We first recall the *total variation distance*  $tvd$  for distributions  $\omega, \omega' \in \mathcal{D}(X)$ , on a set  $X$ .

$$tvd(\omega, \omega') := \frac{1}{2} \sum_{x \in X} |\omega(x) - \omega'(x)|. \quad (5.1)$$

Since  $|\omega(x) - \omega'(x)| \leq |\omega(x)| + |\omega'(x)| = \omega(x) + \omega'(x)$  this distance is 1-bounded, with values in the unit interval  $[0, 1]$ . This total variation distance is quite common, see *e.g.* [JW20] and the references given there.

We first introduce a reformulation that is convenient to reason about the total variation distance.

**Lemma 5.1.** *Fix two distributions  $\omega, \omega' \in \mathcal{D}(X)$  and write:*

$$\begin{cases} X_{>} := \{x \in X \mid \omega(x) > \omega'(x)\} \\ X_{=} := \{x \in X \mid \omega(x) = \omega'(x)\} \\ X_{<} := \{x \in X \mid \omega(x) < \omega'(x)\} \end{cases} \quad \begin{cases} X\uparrow := \sum_{x \in X_{>}} \omega(x) - \omega'(x) \geq 0 \\ X\downarrow := \sum_{x \in X_{<}} \omega'(x) - \omega(x) \geq 0. \end{cases}$$

*Then:*  $X\uparrow = X\downarrow = \text{tvd}(\omega, \omega')$ .

The sets  $X_{>}, X_{=}, X_{<}$  and the numbers  $X\uparrow, X\downarrow$  depend on the distributions  $\omega, \omega'$  but this is left implicit for simplicity.

*Proof.* We have both:

$$\begin{aligned} 1 &= \sum_{x \in X} \omega(x) = \sum_{x \in X_{>}} \omega(x) + \sum_{x \in X_{=}} \omega(x) + \sum_{x \in X_{<}} \omega(x) \\ 1 &= \sum_{x \in X} \omega'(x) = \sum_{x \in X_{>}} \omega'(x) + \sum_{x \in X_{=}} \omega'(x) + \sum_{x \in X_{<}} \omega'(x). \end{aligned}$$

Subtraction yields  $0 = X\uparrow - X\downarrow$ , so that  $X\uparrow = X\downarrow$ . Further:

$$\begin{aligned} \text{tvd}(\omega, \omega') &= \frac{1}{2} \sum_{x \in X} |\omega(x) - \omega'(x)| = \frac{1}{2} \left( \sum_{x \in X_{>}} \omega(x) - \omega'(x) + \sum_{x \in X_{<}} \omega'(x) - \omega(x) \right) \\ &= \frac{1}{2} (X\uparrow + X\downarrow) = \frac{1}{2} (X\uparrow + X\uparrow) = X\uparrow = X\downarrow. \quad \square \end{aligned}$$

Each set  $X$  forms a ‘discrete’ metric with distance  $d_{=} : X \times X \rightarrow [0, 1] \subseteq \mathbb{R}_{\geq 0}$  given by:

$$d_{=}(x, x') := \begin{cases} 0 & \text{if } x = x' \\ 1 & \text{if } x \neq x'. \end{cases} \quad (5.2)$$

**Proposition 5.2.** *For each set  $X$  with distributions  $\omega, \omega' \in \mathcal{D}(X)$  one has:*

$$\text{tvd}(\omega, \omega') = \bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models d_{=} = d(\omega, \omega'). \quad (5.3)$$

*The latter distance  $d$  is the Kantorovich distance for distributions on the discrete metric space  $(X, d_{=})$ .*

*Proof.* Let  $\tau$  be an arbitrary coupling of  $\omega, \omega'$ . Then:

$$\begin{aligned} \omega(x) &= \sum_{y \in X} \tau(x, y) = \tau(x, x) + \sum_{y \neq x} \tau(x, y) \\ &\leq \sum_{z \in X} \tau(z, x) + \sum_{y \neq x} \tau(x, y) = \omega'(x) + \sum_{y \neq x} \tau(x, y). \end{aligned}$$

Thus, using Lemma 5.1 we have:

$$\begin{aligned} \text{tvd}(\omega, \omega') = X\uparrow &= \sum_{x \in X_{>}} \omega(x) - \omega'(x) \leq \sum_{x \in X_{>}} \sum_{y \neq x} \tau(x, y) \\ &\leq \sum_{x \in X} \sum_{y \in X} \tau(x, y) \cdot d_{=} (x, y) = \tau \models d_{=} . \end{aligned}$$

Since this holds for all couplings  $\tau$  we get the inequality ( $\leq$ ) in (5.3).

For the inequality ( $\geq$ ) we may assume  $\omega \neq \omega'$  and so  $\text{tvd}(\omega, \omega') \neq 0$ . One uses the function  $\rho: X \times X \rightarrow \mathbb{R}_{\geq 0}$  defined as:

$$\rho(x, y) := \begin{cases} \min(\omega(x), \omega'(x)) & \text{if } x = y \\ \frac{(\omega(x) \dot{-} \omega'(x)) \cdot (\omega'(y) \dot{-} \omega(y))}{\text{tvd}(\omega, \omega')} & \text{otherwise,} \end{cases} \quad (5.4)$$

where  $a \dot{-} b := \max(a - b, 0)$ , for  $a, b \in \mathbb{R}$ . This formula occurs for instance in [Vil09, proof of Thm. 6.15] (for the continuous case).

We first check that this  $\rho$  is a coupling of  $\omega, \omega'$ . Let  $x \in X_{>}$  so that  $\omega(x) > \omega'(x)$ ; then:

$$\begin{aligned} \sum_{y \in X} \rho(x, y) &= \min(\omega(x), \omega'(x)) + (\omega(x) \dot{-} \omega'(x)) \cdot \sum_{y \neq x} \frac{\omega'(y) \dot{-} \omega(y)}{\text{tvd}(\omega, \omega')} \\ &= \omega'(x) + (\omega(x) - \omega'(x)) \cdot \frac{\sum_{y \in X_{<}} \omega'(y) - \omega(y)}{\text{tvd}(\omega, \omega')} \\ &= \omega'(x) + (\omega(x) - \omega'(x)) \cdot \frac{X\downarrow}{\text{tvd}(\omega, \omega')} \\ &= \omega'(x) + (\omega(x) - \omega'(x)) \cdot 1 \quad \text{see Lemma 5.1} \\ &= \omega(x). \end{aligned}$$

If  $x \notin X_{>}$ , so that  $\omega(x) \leq \omega'(x)$ , then it is obvious that  $\sum_y \rho(x, y) = \min(\omega(x), \omega'(x)) + 0 = \omega(x)$ . This shows that the first marginal  $\mathcal{D}(\pi_1)(\rho)$  is  $\omega$ . In a similar way one obtains  $\mathcal{D}(\pi_2)(\rho) = \omega'$ . In particular, we can conclude that  $\rho$  is a distribution.

Finally,

$$\begin{aligned} 1 - (\rho \models d_{=}) &= \sum_{x, y} \rho(x, y) - \sum_{x \neq y} \rho(x, y) = \sum_{x \in X} \rho(x, x) \\ &= \sum_{x \in X} \min(\omega(x), \omega'(x)) \\ &= \sum_{x \in X_{>}} \omega'(x) + \sum_{x \notin X_{>}} \omega(x) \\ &= \sum_{x \in X_{>}} \omega'(x) + 1 - \sum_{x \in X_{>}} \omega(x) \\ &= 1 - \sum_{x \in X_{>}} \omega(x) - \omega'(x) \\ &= 1 - X\uparrow = 1 - \text{tvd}(\omega, \omega'). \end{aligned}$$

Hence  $\text{tvd}(\omega, \omega') = \rho \models d_{=} \geq \bigwedge_{\tau \in \text{dcp1}^{-1}(\omega, \omega')} \tau \models d_{=} = 1 - \text{tvd}(\omega, \omega')$ . In particular  $\rho$  in (5.4) is an optimal coupling.  $\square$

For the next result we need the following notion. The diameter  $\text{diam}(U)$  of a subset  $U \subseteq X$  of a metric space  $X$ , if it exists, is the supremum:

$$\text{diam}(U) := \bigvee_{x, x' \in U} d_X(x, x'). \quad (5.5)$$

The subset  $U$  is called bounded if this join exists. This is the case when  $U$  is finite, as in the proposition below. This diameter is used to show that the total variation distance forms a scaled upperbound for the Kantorovich distance. The continuous version of this result occurs in [Vil09, 6.16].

**Proposition 5.3.** *Let  $X$  be a metric space, with distributions  $\omega, \omega' \in \mathcal{D}(X)$ . The Kantorovich distance  $d$  and the total variation distance  $\text{tvd}$  are related via the following inequality.*

$$d(\omega, \omega') \leq D \cdot \text{tvd}(\omega, \omega'), \quad (5.6)$$

where:

$$D := \max\{d_X(x, x') \mid x \in \text{supp}(\omega), x' \in \text{supp}(\omega')\} \\ \stackrel{(5.5)}{=} \text{diam}(\text{supp}(\omega) \cup \text{supp}(\omega')).$$

*Proof.* We use the coupling  $\rho \in \mathcal{D}(X \times X)$  from (5.4). It satisfies, as we have seen:

$$\begin{aligned} d(\omega, \omega') \leq \rho \models d_X &= \sum_{x, x' \in X} \rho(x, x') \cdot d_X(x, x') \\ &\leq \sum_{x \neq x'} \rho(x, x') \cdot D = (\rho \models d_{\neq}) \cdot D = D \cdot \text{tvd}(\omega, \omega'). \quad \square \end{aligned}$$

## 6. THE KANTOROVICH DISTANCE BETWEEN MULTISSETS

There is also a Kantorovich distance between multisets of the same size. This section recalls the definition and the main results.

**Definition 6.1.** Let  $(X, d_X)$  be a metric space and  $K \in \mathbb{N}_{>0}$  a positive natural number. We can turn the metric  $d_X: X \times X \rightarrow \mathbb{R}_{\geq 0}$  into the *Kantorovich* metric  $d: \mathcal{M}[K](X) \times \mathcal{M}[K](X) \rightarrow \mathbb{R}_{\geq 0}$  on multisets (of the same size  $K$ ), via:

$$\begin{aligned} d(\varphi, \varphi') &:= \bigwedge_{\tau \in \text{dcpl}^{-1}(\varphi, \varphi')} \text{Flrn}(\tau) \models d_X \\ &= \bigwedge_{\vec{x} \in \text{acc}^{-1}(\varphi), \vec{y} \in \text{acc}^{-1}(\varphi')} \frac{1}{K} \cdot d_{X^K}(\vec{x}, \vec{y}) \\ &\stackrel{(3.1)}{=} \bigwedge_{\vec{x} \in \text{acc}^{-1}(\varphi), \vec{y} \in \text{acc}^{-1}(\varphi')} \sum_{1 \leq i \leq K} \frac{1}{K} \cdot d_X(x_i, y_i). \end{aligned} \quad (6.1)$$

This distance is defined for  $K > 0$ . We can extend it trivially to  $K = 0$  since there is only one multiset of size  $K = 0$ , namely the empty multiset, so  $\mathcal{M}[0](X) = \{\mathbf{0}\}$ . We set  $d(\mathbf{0}, \mathbf{0}) = 0$ .

All meets in (6.1) are finite and can be computed via enumeration. Alternatively, one can use linear optimisation. We give an illustration below. The equality of the first two formulations is standard; a proof is included in Appendix B. In the above formulation (6.1) the decouple map has type  $\text{dcpl}: \mathcal{M}[K](X \times X) \rightarrow \mathcal{M}[X] \times \mathcal{M}[X]$ . Thus it is required that



the couplings  $\tau$  in (6.1) are inhabitants of the set  $\mathcal{M}[K](X \times X)$  and are thus multisets, with natural numbers as multiplicities. The latter requirement is not so explicit in formulations in the literature. It is justified by Lemma B.1 in the appendix. The requirement is relevant and relates to Fact 4.5, see the proof of Lemma 6.3 (1) below.

**Example 6.2.** Consider the following two multisets of size 4 on the set  $X = \{1, 2, 3\} \subseteq \mathbb{N}$ , with standard distance between natural numbers.

$$\varphi = 3|1\rangle + 1|2\rangle \qquad \varphi' = 2|1\rangle + 1|2\rangle + 1|3\rangle.$$

An optimal coupling  $\tau \in \mathcal{M}[4](X \times X)$  is:

$$\tau = 2|1, 1\rangle + 1|1, 2\rangle + 1|2, 3\rangle.$$

The resulting Kantorovich distance  $d(\varphi, \varphi')$  is:

$$\text{Flrn}(\tau) \models d_X = \frac{1}{2} \cdot d_X(1, 1) + \frac{1}{4} \cdot d_X(1, 2) + \frac{1}{4} \cdot d_X(2, 3) = \frac{1}{4} \cdot 1 + \frac{1}{4} \cdot 1 = \frac{1}{2}.$$

Alternatively, we may proceed as follows. There are  $\binom{4!}{3! \cdot 1!} = 4$  lists that accumulate to  $\varphi$ , and  $\binom{4!}{2! \cdot 1! \cdot 1!} = 12$  lists that accumulate to  $\varphi'$ . We can align them all and compute the minimal distance. It is achieved for instance at:

$$\frac{1}{4} \cdot d_{X^4} \left( (1, 1, 1, 2), (1, 1, 2, 3) \right) \stackrel{(3.1)}{=} \frac{1}{4} \cdot (0 + 0 + 1 + 1) = \frac{2}{4} = \frac{1}{2}.$$

As an aside: if we zip these two lists and then accumulate we recover the coupling multiset  $\tau$ , in:

$$\begin{aligned} \text{acc} \left( \text{zip} \left( (1, 1, 1, 2), (1, 1, 2, 3) \right) \right) &= \text{acc} \left( (1, 1), (1, 1), (1, 2), (2, 3) \right) \\ &= 2|1, 1\rangle + 1|1, 2\rangle + 1|2, 3\rangle = \tau. \end{aligned}$$

This is a more general phenomenon, see Lemma B.1.

**Lemma 6.3.** *We consider the situation in Definition 6.1.*

- (1) *Frequentist learning  $\text{Flrn}: \mathcal{M}[K](X) \rightarrow \mathcal{D}(X)$  is short, for  $K > 0$ . It is even an isometry by Fact 4.5.*
- (2) *For numbers  $K, n \geq 1$  the scalar multiplication function  $n \cdot (-): \mathcal{M}[K](X) \rightarrow \mathcal{M}[n \cdot K](X)$  is also short, and an isometry by Fact 4.5.*
- (3) *The sum of distributions  $+: \mathcal{M}[K](X) \times \mathcal{M}[L](X) \rightarrow \mathcal{M}[K + L](X)$  is short.*
- (4) *If  $f: X \rightarrow Y$  is  $M$ -Lipschitz, then  $\mathcal{M}[K](f): \mathcal{M}[K](X) \rightarrow \mathcal{M}[K](Y)$  is  $M$ -Lipschitz too. Thus, the fixed size multiset functor  $\mathcal{M}[K]$  lifts to categories of metric spaces  $\mathbf{Met}_S$  and  $\mathbf{Met}_L$ .*
- (5) *For  $K > 0$  the accumulation map  $\text{acc}: X^K \rightarrow \mathcal{M}[K](X)$  is  $\frac{1}{K}$ -Lipschitz, and thus short.*
- (6) *The arrangement channel  $\text{arr}: \mathcal{M}[K](X) \rightarrow X^K$  is  $K$ -Lipschitz; in fact there is an equality  $d(\text{arr}(\varphi), \text{arr}(\varphi')) = K \cdot d(\varphi, \varphi')$ .*

We have already seen an illustration of item (1): multisets  $\varphi, \varphi'$  in Example 6.2 have the same distance  $\frac{1}{2}$  as the distributions  $\omega = \text{Flrn}(\varphi)$ ,  $\omega' = \text{Flrn}(\varphi')$  in Example 4.6.

*Proof.* (1) Via naturality of frequentist learning  $\text{Flrn}: \mathcal{M}[K] \Rightarrow \mathcal{D}$  we obtain that if the multiset  $\tau \in \mathcal{M}[K](X \times X)$  is a coupling of  $\varphi, \varphi' \in \mathcal{M}[K](X)$ , then the distribution  $\text{Flrn}(\tau) \in \mathcal{D}(X \times X)$  is a coupling of  $\text{Flrn}(\varphi), \text{Flrn}(\varphi') \in \mathcal{D}(X)$ . This gives:

$$d(\text{Flrn}(\varphi), \text{Flrn}(\varphi')) = \bigwedge_{\sigma \in \text{dcpl}^{-1}(\text{Flrn}(\varphi), \text{Flrn}(\varphi'))} \sigma \models d_X \leq \text{Flrn}(\tau) \models d_X.$$

Since this holds for all  $\tau$  we get shortness of  $\text{Flrn}$  in:

$$d(\text{Flrn}(\varphi), \text{Flrn}(\varphi')) \leq \bigwedge_{\tau \in \text{dcpl}^{-1}(\varphi, \varphi')} \text{Flrn}(\tau) \models d_X = d(\varphi, \varphi').$$

For the reverse inequality ( $\geq$ ), let  $\sigma \in \mathcal{D}(X \times X)$  be an optimal coupling of  $\text{Flrn}(\varphi), \text{Flrn}(\varphi') \in \mathcal{D}[K](X)$ . By Fact 4.5 we may assume  $\sigma \in \mathcal{D}[K](X \times X)$ , so that  $K \cdot \sigma \in \mathcal{M}[K](X \times X)$ . This is then a coupling of  $\varphi, \varphi' \in \mathcal{M}[K](X)$ . We thus get:

$$\begin{aligned} d(\text{Flrn}(\varphi), \text{Flrn}(\varphi')) &= \sigma \models d_X = \text{Flrn}(K \cdot \sigma) \models d_X \\ &\geq \bigwedge_{\tau \in \text{dcpl}^{-1}(\varphi, \varphi')} \text{Flrn}(\tau) \models d_X = d(\varphi, \varphi'). \end{aligned}$$

- (2) If  $\tau \in \mathcal{M}[K](X \times X)$  is a coupling of  $\varphi, \varphi' \in \mathcal{M}[K](X)$ , then  $n \cdot \tau \in \mathcal{M}[n \cdot K](X \times X)$  is obviously a coupling of  $n \cdot \varphi, n \cdot \varphi' \in \mathcal{M}[n \cdot K](X)$ . This gives:

$$d(n \cdot \varphi, n \cdot \varphi') = \bigwedge_{\sigma \in \text{dcpl}^{-1}(n \cdot \varphi, n \cdot \varphi')} \text{Flrn}(\sigma) \models d_X \leq \text{Flrn}(n \cdot \tau) \models d_X = \text{Flrn}(\tau) \models d_X.$$

Since this holds for all  $\tau$  we get  $d(n \cdot \varphi, n \cdot \varphi') \leq d(\varphi, \varphi')$ .

For the reverse inequality ( $\geq$ ), let multisets  $\varphi, \varphi' \in \mathcal{M}[K](X)$  be given. Using that  $\text{Flrn}$  is an isometry, via Fact 4.5, we get:

$$\begin{aligned} d_{\mathcal{M}[K](X)}(\varphi, \varphi') &= d_{\mathcal{D}(X)}(\text{Flrn}(\varphi), \text{Flrn}(\varphi')) \\ &= d_{\mathcal{D}(X)}(\text{Flrn}(n \cdot \varphi), \text{Flrn}(n \cdot \varphi')) = d_{\mathcal{M}[n \cdot K](X)}(n \cdot \varphi, n \cdot \varphi'). \end{aligned}$$

- (3) Let  $\sigma \in \mathcal{M}[K](X \times X)$  and  $\tau \in \mathcal{M}[L](X \times X)$  be couplings of multisets  $\varphi, \varphi' \in \mathcal{M}[K](X)$  and  $\psi, \psi' \in \mathcal{M}[L](X)$ . The multiset sum  $\sigma + \tau \in \mathcal{M}[K + L](X \times X)$  is then a coupling of  $\varphi + \varphi'$  and  $\psi + \psi'$ . Hence:

$$\begin{aligned} d(\varphi + \psi, \varphi' + \psi') &\leq \text{Flrn}(\sigma + \tau) \models d_X \\ &= \left( \frac{K}{K+L} \cdot \text{Flrn}(\sigma) + \frac{L}{K+L} \cdot \text{Flrn}(\tau) \right) \models d_X \\ &= \frac{K}{K+L} \cdot (\text{Flrn}(\sigma) \models d_X) + \frac{L}{K+L} \cdot (\text{Flrn}(\tau) \models d_X) \\ &\leq \text{Flrn}(\sigma) \models d_X + \text{Flrn}(\tau) \models d_X. \end{aligned}$$

Since this holds for each coupling  $\sigma$  and  $\tau$  we get:

$$\begin{aligned} d(\varphi + \psi, \varphi' + \psi') &\leq \bigwedge_{\sigma \in \text{dcpl}^{-1}(\varphi, \varphi')} \text{Flrn}(\sigma) \models d_X + \bigwedge_{\tau \in \text{dcpl}^{-1}(\psi, \psi')} \text{Flrn}(\tau) \models d_X \\ &= d(\varphi, \varphi') + d(\psi, \psi') \\ &\stackrel{(3.1)}{=} d((\varphi, \psi), (\varphi', \psi')). \end{aligned}$$

- (4) Let  $f: X \rightarrow Y$  be  $M$ -Lipschitz. For sequences  $\vec{x} \in \text{acc}^{-1}(\varphi)$ ,  $\vec{x}' \in \text{acc}^{-1}(\varphi')$  we have, by naturality of accumulation,

$$\text{acc}(f^K(\vec{x})) = \mathcal{M}(f)(\text{acc}(\vec{x})) = \mathcal{M}(f)(\varphi).$$

This means that  $f^K(\vec{x}) \in \text{acc}^{-1}(\mathcal{M}(f)(\varphi))$ . Thus:

$$\begin{aligned} d(\mathcal{M}(f)(\varphi), \mathcal{M}(f)(\varphi')) &= \frac{1}{K} \cdot \bigwedge_{\vec{y} \in \text{acc}^{-1}(\mathcal{M}(f)(\varphi)), \vec{y}' \in \text{acc}^{-1}(\mathcal{M}(f)(\varphi'))} d_{Y^K}(\vec{y}, \vec{y}') \\ &\leq \frac{1}{K} \cdot \bigwedge_{\vec{x} \in \text{acc}^{-1}(\varphi), \vec{x}' \in \text{acc}^{-1}(\varphi')} d_{Y^K}(f^K(\vec{x}), f^K(\vec{x}')) \\ &\leq \frac{1}{K} \cdot \bigwedge_{\vec{x} \in \text{acc}^{-1}(\varphi), \vec{x}' \in \text{acc}^{-1}(\varphi')} M \cdot d_{X^K}(\vec{x}, \vec{x}') \\ &= M \cdot d(\varphi, \varphi'). \end{aligned}$$

(5) The map  $\text{acc}: X^K \rightarrow \mathcal{M}[K](X)$  is  $\frac{1}{K}$ -Lipschitz since for  $\vec{y}, \vec{y}' \in X^K$ ,

$$\begin{aligned} d(\text{acc}(\vec{y}), \text{acc}(\vec{y}')) &= \frac{1}{K} \cdot \bigwedge_{\vec{x} \in \text{acc}^{-1}(\text{acc}(\vec{y})), \vec{x}' \in \text{acc}^{-1}(\text{acc}(\vec{y}'))} d_{X^K}(\vec{x}, \vec{x}') \\ &\leq \frac{1}{K} \cdot d_{X^K}(\vec{y}, \vec{y}'). \end{aligned}$$

(6) For fixed  $\varphi, \varphi' \in \mathcal{M}[K](X)$ , take arbitrary  $\vec{x} \in \text{acc}^{-1}(\varphi)$  and  $\vec{x}' \in \text{acc}^{-1}(\varphi')$ . Then:

$$\begin{aligned} d_{\mathcal{D}(X^K)}(\text{arr}(\varphi), \text{arr}(\varphi')) &= d_{\mathcal{D}(X^K)}(\text{arr}(\text{acc}(\vec{x})), \text{arr}(\text{acc}(\vec{x}'))) \\ &\stackrel{(2.4)}{=} d_{\mathcal{D}(X^K)}(\text{prm}(\vec{x}), \text{prm}(\vec{x}')) \\ &\leq d_{X^K}(\vec{x}, \vec{x}') \quad \text{by Lemma 4.3 (9)}. \end{aligned}$$

Since this holds for all sequences  $\vec{x} \in \text{acc}^{-1}(\varphi)$ ,  $\vec{x}' \in \text{acc}^{-1}(\varphi')$  we get an inequality  $d_{\mathcal{D}(X^K)}(\text{arr}(\varphi), \text{arr}(\varphi')) \leq K \cdot d_{\mathcal{M}[K](X)}(\varphi, \varphi')$ , see Definition 6.1. This inequality is an actual equality since  $\text{acc}$ , and thus  $\mathcal{D}(\text{acc})$ , is  $\frac{1}{K}$ -Lipschitz:

$$\begin{aligned} d_{\mathcal{M}[K](X)}(\varphi, \varphi') &= d_{\mathcal{D}(\mathcal{M}[K](X))}(1|\varphi, 1|\varphi') \\ &= d_{\mathcal{D}(\mathcal{M}[K](X))}(\mathcal{D}(\text{acc})(\text{arr}(\varphi)), \mathcal{D}(\text{acc})(\text{arr}(\varphi'))) \\ &\leq \frac{1}{K} \cdot d_{\mathcal{D}(X^K)}(\text{arr}(\varphi), \text{arr}(\varphi')) \quad \square \end{aligned}$$

We recall the multiset-zip operation  $mzip: \mathcal{M}[K](X) \times \mathcal{M}[K](Y) \rightarrow \mathcal{D}(\mathcal{M}[K](X \times Y))$  from [Jac21]. It turns two multisets into a distribution over couplings of these multisets, via the composite:

$$\begin{aligned} \mathcal{M}[K](X) \times \mathcal{M}[K](Y) &\xrightarrow{\text{arr} \times \text{arr}} \mathcal{D}(X^K) \times \mathcal{D}(Y^K) \xrightarrow{\otimes} \mathcal{D}(X^K \times Y^K) \\ &\quad \mathcal{D}(\text{zip}) \downarrow \cong \\ &\quad \mathcal{D}((X \times Y)^K) \xrightarrow{\mathcal{D}(\text{acc})} \mathcal{D}(\mathcal{M}[K](X \times Y)) \end{aligned} \quad (6.2)$$

An example of how  $mzip$  works can be found in Example 6.5 below, and also in [Jac21, Ex. 16].

**Proposition 6.4.** *Consider the  $mzip$  operation (6.2) for metric spaces  $X, Y$ .*

- (1) *This  $mzip$  function is short.*
- (2) *It is even an isometry, via Fact 4.5 (in an indirect way, through Lemma 6.3 (1)).*

*Proof.* (1) As we can see in Diagram (6.2), the composite  $mzip = \mathcal{D}(\text{acc}) \circ \mathcal{D}(\text{zip}) \circ \otimes \circ (\text{arr} \times \text{arr})$  is a composite of:

- a  $K$ -Lipschitz function  $arr \times arr$ , by Lemma 6.3 (6) and Lemma 3.2;
- a 1-Lipschitz function  $\otimes$ , by Proposition 4.4 (1);
- a 1-Lipschitz function  $\mathcal{D}(zip)$ , by Lemma 3.4 and Lemma 4.3 (1);
- a  $\frac{1}{K}$ -Lipschitz function  $\mathcal{D}(acc)$ , by Lemma 6.3 (5) and Lemma 4.3 (1).

The composite  $mzip$  is thus Lipschitz with constant  $K \cdot 1 \cdot 1 \cdot \frac{1}{K} = 1$ , making it short.

- (2) We use the equation  $Flrn_*(mzip(\varphi, \psi)) = Flrn(\varphi \otimes \psi)$ , from [Jac21, Thm. 18]. Then, for multisets  $\varphi, \varphi' \in \mathcal{M}[K](X)$  and  $\psi, \psi' \in \mathcal{M}[K](Y)$  one has:

$$\begin{aligned}
& d\left(mzip(\varphi, \psi), mzip(\varphi', \psi')\right) \\
& \geq d\left(Flrn_*(mzip(\varphi, \psi)), Flrn_*(mzip(\varphi', \psi'))\right) \quad \text{by Lemma 4.3 (6)} \\
& = d\left(Flrn(\varphi \otimes \psi), Flrn(\varphi' \otimes \psi')\right) \\
& = d\left(Flrn(\varphi) \otimes Flrn(\psi), Flrn(\varphi') \otimes Flrn(\psi')\right) \quad \text{by (2.5)} \\
& = d(Flrn(\varphi), Flrn(\varphi')) + d(Flrn(\psi), Flrn(\psi')) \quad \text{by Proposition 4.4 (1)} \\
& = d(\varphi, \varphi') + d(\psi, \psi') \quad \text{by Lemma 6.3 (1)} \\
& = d\left((\varphi, \psi), (\varphi', \psi')\right) \quad \text{by (3.1)}. \quad \square
\end{aligned}$$

A central operation from [Jac21] is the distributive law  $pml: \mathcal{M}[K](\mathcal{D}(X)) \rightarrow \mathcal{D}(\mathcal{M}[K](X))$ , called parallel multinomial law. One way to describe it is as composite  $pml = \mathcal{D}(acc) \circ \otimes \circ arr: \mathcal{M}[K](\mathcal{D}(X)) \rightarrow \mathcal{D}(X)^K \rightarrow \mathcal{D}(X^K) \rightarrow \mathcal{D}(\mathcal{M}[K](X))$ . The map in the middle is the  $K$ -ary tensor  $\otimes: \mathcal{D}(X)^K \rightarrow \mathcal{D}(X^K)$  of distributions — which is short, generalising Proposition 4.4 (1). Via an argument as for  $mzip$  — in the proof of Proposition 6.4 (1) — one shows that  $pml$  is short.

There is one more point we like to make about the multiset-zip operation  $mzip$ .

**Example 6.5.** We shall now use the multiset-zip function (6.2) with  $Y = X$  and check if the Kantorovich distance between multisets can be described via this  $mzip$  operation (channel) — assuming that  $X$  is a metric space.

The obvious way to do this would be via the following composite.

$$\mathcal{M}[K](X) \times \mathcal{M}[K](X) \xrightarrow{mzip} \mathcal{D}(\mathcal{M}[K](X \times X)) \xrightarrow{\mathcal{D}(\dashv=d_X)} \mathcal{D}(\mathbb{R}_{\geq 0}) \xrightarrow{sum} \mathbb{R}_{\geq 0} \quad (6.3)$$

The sum operation  $sum: \mathcal{D}(\mathbb{R}_{\geq 0}) \rightarrow \mathbb{R}_{\geq 0}$  is defined in the obvious way as  $sum(\sum_i r_i |s_i\rangle) = \sum_i r_i \cdot s_i$ , exploiting that  $\mathbb{R}_{\geq 0}$  is a convex set.

We demonstrate that the approach via (6.3) does not produce the Kantorovich distance, for  $X = \{1, 2, 3\} \subseteq \mathbb{N}$  with usual distance and with multisets  $\varphi = 3|1\rangle + 2|3\rangle$  and  $\varphi' = 1|1\rangle + 3|2\rangle + 1|3\rangle$  of size 5. The Kantorovich distance  $d(\varphi, \varphi')$  is 3. The multiset-zip gives the following distribution over couplings of  $\varphi, \varphi'$ .

$$\begin{aligned}
mzip(\varphi, \varphi') &= \frac{3}{10} \left| 2|1, 2\rangle + 1|1, 3\rangle + 1|3, 1\rangle + 1|3, 2\rangle \right\rangle \\
&+ \frac{3}{10} \left| 1|1, 1\rangle + 1|1, 2\rangle + 1|1, 3\rangle + 2|3, 2\rangle \right\rangle \\
&+ \frac{1}{10} \left| 3|1, 2\rangle + 1|3, 1\rangle + 1|3, 3\rangle \right\rangle + \frac{3}{10} \left| 1|1, 1\rangle + 2|1, 2\rangle + 1|3, 2\rangle + 1|3, 3\rangle \right\rangle.
\end{aligned}$$

By applying the function  $(-) \models d_X$  to the couplings inside the big ket's, as in (6.3), one gets:

$$\mathcal{D}(\text{sum})\left(\frac{3}{10}|7\rangle + \frac{3}{10}|5\rangle + \frac{1}{10}|5\rangle + \frac{3}{10}|3\rangle\right) = \frac{50}{10} = 5.$$

This outcome according to (6.3) differs from Kantorovich distance  $d(\varphi, \varphi') = 3$ .

## 7. MULTINOMIAL DRAWING IS ISOMETRIC

At this stage we have prepared the ground so that we are able to show that the three draw channels — multinomial  $mn[K]$ , hypergeometric  $hg[K]$  and Pólya  $pl[K]$ , for a fixed drawsize  $K$  — are all isometric. The equality of metrics involved in an isometry will be split in two inequalities, where one is for shortness. The other inequality, for each of the drawing modes, will be proven in basically the same manner. Each of the drawing channels interacts well with frequentist learning, in the following manner:

$$\begin{aligned} \text{Flrn}_*(mn[K](\omega)) = \omega & \quad \text{Flrn}_*(hg[K](v)) = \text{Flrn}(v) & \quad \text{Flrn}_*(pl[K](v)) = \text{Flrn}(v). \end{aligned} \tag{7.1}$$

With these equations we can already prove, without having seen the details of  $mn[K]$ ,  $hg[K]$  or  $pl[K]$ , via Lemma 6.3 (1), including Fact 4.5, and Lemma 4.3 (6):

$$\begin{aligned} d(\omega, \omega') & \stackrel{(7.1)}{=} d(\text{Flrn}_*(mn[K](\omega)), \text{Flrn}_*(mn[K](\omega'))) \\ & \leq d(mn[K](\omega), mn[K](\omega')) \\ d(v, v') & = d(\text{Flrn}(v), \text{Flrn}(v')) \\ & \stackrel{(7.1)}{=} d(\text{Flrn}_*(hg[K](v)), \text{Flrn}_*(hg[K](v'))) \\ & \leq d(hg[K](v), hg[K](v')) \\ d(v, v') & = d(\text{Flrn}(v), \text{Flrn}(v')) \\ & \stackrel{(7.1)}{=} d(\text{Flrn}_*(pl[K](v)), \text{Flrn}_*(pl[K](v'))) \\ & \leq d(pl[K](v), pl[K](v')). \end{aligned} \tag{7.2}$$

Hence in the next three sections, we shall prove for the multinomial, hypergeometric, and Pólya draw channel the corresponding equation in (7.1). This means that we only have to prove shortness in order to get isometry, since the reverse inequality is already handled in (7.2).

We start with the multinomial case. Multinomial draws are of the draw-and-replace kind. This means that a drawn ball is returned to the urn, so that the urn remains unchanged. Thus we may use a distribution  $\omega \in \mathcal{D}(X)$  as urn, giving for each colour  $x \in X$  the probability  $\omega(x)$  of drawing a ball of that colour. For a drawsize number  $K \in \mathbb{N}$ , the multinomial distribution  $mn[K](\omega) \in \mathcal{D}(\mathcal{M}[K](X))$  on multisets / draws of size  $K$  can be defined via

accumulated sequences of draws:

$$\begin{aligned}
mn[K](\omega) &:= \mathcal{D}(\text{acc})(\text{iid}[K](\omega)) = \mathcal{D}(\text{acc})(\omega^K) \\
&= \sum_{\vec{x} \in X^K} \omega^K(\vec{x}) | \text{acc}(\vec{x}) \rangle \\
&= \sum_{\varphi \in \mathcal{M}[K](X)} \sum_{\vec{x} \in \text{acc}^{-1}(\varphi)} \prod_{1 \leq i \leq K} \omega(x_i) | \varphi \rangle \quad (7.3) \\
&= \sum_{\varphi \in \mathcal{M}[K](X)} (\varphi) \cdot \prod_{x \in X} \omega(x)^{\varphi(x)} | \varphi \rangle.
\end{aligned}$$

We recall that  $(\varphi) = \frac{K!}{\prod_x \varphi(x)!}$  is the number of sequences that accumulate to a multiset / draw  $\varphi \in \mathcal{M}[K](X)$ .

**Example 7.1.** Consider the following two distributions  $\omega, \omega' \in \mathcal{D}(\mathbb{N})$ .

$$\omega = \frac{1}{3}|0\rangle + \frac{2}{3}|2\rangle \quad \text{and} \quad \omega' = \frac{1}{2}|1\rangle + \frac{1}{2}|2\rangle \quad \text{with} \quad d(\omega, \omega') = \frac{1}{2}.$$

This distance  $d(\omega, \omega')$  involves the standard distance on  $\mathbb{N}$ , using as an optimal coupling  $\frac{1}{3}|0, 1\rangle + \frac{1}{6}|2, 1\rangle + \frac{1}{2}|2, 2\rangle \in \mathcal{D}(\mathbb{N} \times \mathbb{N})$ .

We take draws of size  $K = 3$ . There are 10 multisets of size 3 over  $\{0, 1, 2\}$ :

$$\begin{aligned}
\varphi_1 &= 3|0\rangle & \varphi_2 &= 2|0\rangle + 1|1\rangle & \varphi_3 &= 1|0\rangle + 2|1\rangle & \varphi_4 &= 3|1\rangle \\
\varphi_5 &= 2|0\rangle + 1|2\rangle & \varphi_6 &= 1|0\rangle + 1|1\rangle + 1|2\rangle & \varphi_7 &= 2|1\rangle + 1|2\rangle \\
\varphi_8 &= 1|0\rangle + 2|2\rangle & \varphi_9 &= 1|1\rangle + 2|2\rangle & \varphi_{10} &= 3|2\rangle.
\end{aligned}$$

These multisets occur in the following multinomial distributions of draws of size 3.

$$\begin{aligned}
mn[3](\omega) &= \frac{1}{27}|\varphi_1\rangle + \frac{2}{9}|\varphi_5\rangle + \frac{4}{9}|\varphi_8\rangle + \frac{8}{27}|\varphi_{10}\rangle \\
mn[3](\omega') &= \frac{1}{8}|\varphi_4\rangle + \frac{3}{8}|\varphi_7\rangle + \frac{3}{8}|\varphi_9\rangle + \frac{1}{8}|\varphi_{10}\rangle.
\end{aligned} \quad (7.4)$$

An optimal coupling  $\tau \in \mathcal{D}(\mathcal{M}[3](\mathbb{N}) \times \mathcal{M}[3](\mathbb{N}))$  between these two multinomial distributions is:

$$\begin{aligned}
\tau &= \frac{1}{27}|\varphi_1, \varphi_4\rangle + \frac{19}{216}|\varphi_5, \varphi_4\rangle + \frac{1}{8}|\varphi_{10}, \varphi_{10}\rangle + \frac{29}{216}|\varphi_5, \varphi_7\rangle \\
&\quad + \frac{5}{72}|\varphi_8, \varphi_7\rangle + \frac{3}{8}|\varphi_8, \varphi_9\rangle + \frac{37}{216}|\varphi_{10}, \varphi_7\rangle.
\end{aligned}$$

We compute the distance between the multinomial distributions, using  $d_{\mathcal{M}} = d_{\mathcal{M}[3](\mathbb{N})}$ .

$$\begin{aligned}
d(mn[3](\omega), mn[3](\omega')) &= \tau \models d_{\mathcal{M}} \\
&= \frac{1}{27} \cdot d_{\mathcal{M}}(\varphi_1, \varphi_4) + \frac{19}{216} \cdot d_{\mathcal{M}}(\varphi_5, \varphi_4) + \frac{1}{8} \cdot d_{\mathcal{M}}(\varphi_{10}, \varphi_{10}) + \frac{29}{216} \cdot d_{\mathcal{M}}(\varphi_5, \varphi_7) \\
&\quad + \frac{5}{72} \cdot d_{\mathcal{M}}(\varphi_8, \varphi_7) + \frac{3}{8} \cdot d_{\mathcal{M}}(\varphi_8, \varphi_9) + \frac{37}{216} \cdot d_{\mathcal{M}}(\varphi_{10}, \varphi_7) \\
&= \frac{1}{27} \cdot 1 + \frac{19}{216} \cdot 1 + \frac{1}{8} \cdot 0 + \frac{29}{216} \cdot \frac{2}{3} + \frac{5}{72} \cdot \frac{2}{3} + \frac{3}{8} \cdot \frac{1}{3} + \frac{37}{216} \cdot \frac{2}{3} = \frac{1}{2}.
\end{aligned}$$

This distance between multinomial distributions coincides with the distance  $d(\omega, \omega') = \frac{1}{2}$  between the original urn distributions. This is a general phenomenon, see Theorem 7.3 below. One sees here that the computation of the distance between the multinomial distributions is more complex, involving ‘Kantorovich-over-Kantorovich’.

As shown in the beginning of this section, for one part of the isometry of multinomial drawing we use the equation  $\text{Flrn}_*(mn[K](\omega)) = \omega$  in (7.1) (originally from [Jac21, Prop. 3]). It implies, for instance, that if we apply  $\text{Flrn}$  to the multisets  $\varphi_i$  inside the kets in (7.4) and then apply flattening, the original distributions  $\omega$  and  $\omega'$  appear.

The proposition below contains a few more similar results, for future use.

**Proposition 7.2.** *Let  $\omega \in \mathcal{D}(X)$  be a distribution with a drawsize number  $K \in \mathbb{N}$ .*

(1) *For each element  $y \in X$ ,*

$$\sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot \varphi(y) = K \cdot \omega(y).$$

*As a result, the validity  $mn[K](\omega) \models Flrn(-)(y)$  equals  $\omega(y)$ .*

(2)  *$Flrn_*(mn[K](\omega)) = \omega$ .*

(3) *For two elements  $y \neq z$  in  $X$ ,*

$$\sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot \varphi(y) \cdot \varphi(z) = K \cdot (K - 1) \cdot \omega(y) \cdot \omega(z).$$

(4) *For a single element  $y \in X$ ,*

$$\sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot \varphi(y) \cdot (\varphi(y) - 1) = K \cdot (K - 1) \cdot \omega(y)^2.$$

(5)  $mn[K](\omega) \models Flrn(-)(y)^2 = \frac{(K - 1) \cdot \omega(y)^2 + \omega(y)}{K}$ .

*Proof.* (1) The equation holds for  $K = 0$ , since then  $\varphi(y) = 0$ . Hence we may assume  $K > 0$ .

Then:

$$\begin{aligned} & \sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot \varphi(y) \\ & \stackrel{(7.3)}{=} \sum_{\varphi \in \mathcal{M}[K](X), \varphi(y) \neq 0} \varphi(y) \cdot \frac{K!}{\prod_x \varphi(x)!} \cdot \prod_x \omega(x)^{\varphi(x)} \\ & = \sum_{\varphi \in \mathcal{M}[K](X), \varphi(y) \neq 0} K \cdot \frac{(K - 1)!}{\prod_x (\varphi - 1|y)(x)!} \cdot \omega(y) \cdot \prod_x \omega(x)^{(\varphi - 1|y)(x)} \\ & = K \cdot \omega(y) \cdot \sum_{\varphi \in \mathcal{M}[K-1](X)} (\varphi) \cdot \prod_x \omega(x)^{\varphi(x)} \\ & = K \cdot \omega(y) \cdot \sum_{\varphi \in \mathcal{M}[K-1](X)} mn[K-1](\omega)(\varphi) \\ & = K \cdot \omega(y). \end{aligned}$$

(2) By the previous point:

$$\begin{aligned} Flrn_*(mn[K](\omega))(y) & = \sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot Flrn(\varphi)(y) \\ & = \sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot \frac{\varphi(y)}{K} = K \cdot \omega(y) \cdot \frac{1}{K} = \omega(y). \end{aligned}$$

(3) + (4) Essentially as for item (1)

(5) We use the equation  $a^2 = a \cdot (a - 1) + a$  in a combination of the previous items (4) and (1):

$$\begin{aligned} mn[K](\omega) \models Flrn(-)(y)^2 & = \frac{1}{K^2} \sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot \left( \varphi(y) \cdot (\varphi(y) - 1) + \varphi(y) \right) \\ & = \frac{K \cdot (K - 1) \cdot \omega(y)^2 + K \cdot \omega(y)}{K^2} = \frac{(K - 1) \cdot \omega(y)^2 + \omega(y)}{K}. \quad \square \end{aligned}$$

We can now formulate and prove our first isometry result.

**Theorem 7.3.** *Let  $X$  be an arbitrary metric space (of colours), and  $K > 0$  be a positive natural (drawsize) number. The multinomial channel*

$$\mathcal{D}(X) \xrightarrow{mn[K]} \mathcal{D}(\mathcal{M}[K](X))$$

is an isometry. This involves the Kantorovich metric (4.1) for distributions over  $X$  on the domain  $\mathcal{D}(X)$ , and the Kantorovich metric for distributions over multisets of size  $K$ , with their Kantorovich metric (6.1), on the codomain  $\mathcal{D}(\mathcal{M}[K](X))$ .

*Proof.* Let distributions  $\omega, \omega' \in \mathcal{D}(X)$  be given. The map  $mn[K]$  is short since:

$$\begin{aligned} & d_{\mathcal{D}(\mathcal{M}[K](X))} \left( mn[K](\omega), mn[K](\omega') \right) \\ & \stackrel{(7.3)}{=} d_{\mathcal{D}(\mathcal{M}[K](X))} \left( \mathcal{D}(\text{acc})(iid[K](\omega)), \mathcal{D}(\text{acc})(iid[K](\omega')) \right) \\ & \leq \frac{1}{K} \cdot d_{\mathcal{D}(X^K)} \left( iid[K](\omega), iid[K](\omega') \right) && \text{by Lemma 6.3 (5)} \\ & = \frac{1}{K} \cdot K \cdot d_{\mathcal{D}(X)}(\omega, \omega') && \text{by Proposition 4.4 (2)} \\ & = d_{\mathcal{D}(X)}(\omega, \omega'). \end{aligned}$$

The reverse inequality ( $\geq$ ) follows by combining Proposition 7.2 (2) with the argument in (7.2).  $\square$

## 8. HYPERGEOMETRIC DRAWING IS ISOMETRIC

We start with some preparatory observations on probabilistic projection and drawing of single balls.

**Lemma 8.1.** *For a metric space  $X$  and a number  $K$ , consider the probabilistic projection-delete PD and probabilistic draw-delete DD channels.*

$$X^{K+1} \xrightarrow{PD} \mathcal{D}(X^K) \qquad \mathcal{M}[K+1](X) \xrightarrow{DD} \mathcal{D}(\mathcal{M}[K](X))$$

They are defined via deletion of elements from sequences and from multisets:

$$\begin{aligned} PD(x_1, \dots, x_{K+1}) & := \sum_{1 \leq i \leq K+1} \frac{1}{K+1} |x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{K+1}\rangle \\ DD(\psi) & := \sum_{x \in \text{supp}(\psi)} \frac{\psi(x)}{K+1} |\psi - 1|x\rangle \\ & = \sum_{x \in \text{supp}(\psi)} \text{Flrn}(\psi)(x) |\psi - 1|x\rangle. \end{aligned}$$

We write  $\psi - 1|x\rangle$  for the multiset  $\psi$  with one of its elements  $x \in \text{supp}(\psi)$  removed. Then:

- (1)  $\langle \text{acc} \rangle \circ PD = DD \circ \langle \text{acc} \rangle$ ;
- (2)  $\text{Flrn}_*(DD(\psi)) = \text{Flrn}(\psi)$ ;
- (3)  $PD$  is  $\frac{K}{K+1}$ -Lipschitz, and thus short;
- (4)  $DD$  is short, and even an isometry using Fact 4.5.

*Proof.* The first point is easy and the second one is [Jac21, Lem. 5 (ii)].



(3) For  $\vec{x}, \vec{y} \in X^{K+1}$ , via Lemma 4.3 (8) and (4),

$$\begin{aligned}
d\left(PD(\vec{x}), PD(\vec{y})\right) &= d\left(\sum_{1 \leq i \leq K+1} \frac{1}{K+1} |x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{K+1}\rangle, \right. \\
&\quad \left. \sum_{1 \leq i \leq K+1} \frac{1}{K+1} |y_1, \dots, y_{i-1}, y_{i+1}, \dots, y_{K+1}\rangle\right) \\
&\leq \sum_{1 \leq i \leq K+1} \frac{1}{K+1} \cdot d\left(1 |x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{K+1}\rangle, \right. \\
&\quad \left. 1 |y_1, \dots, y_{i-1}, y_{i+1}, \dots, y_{K+1}\rangle\right) \\
&= \sum_{1 \leq i \leq K+1} \frac{1}{K+1} \cdot d_{X^K}\left((x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{K+1}), \right. \\
&\quad \left. (y_1, \dots, y_{i-1}, y_{i+1}, \dots, y_{K+1})\right) \\
&= \sum_{1 \leq i \leq K+1} \frac{1}{K+1} \cdot K \cdot d_X(x_i, y_i) \\
&\stackrel{(3.1)}{=} \frac{K}{K+1} \cdot d_{X^{K+1}}(\vec{x}, \vec{y}).
\end{aligned}$$

(4) Via item 1 we get:

$$\langle acc \rangle \circ PD \circ arr = DD \circ \langle acc \rangle \circ arr = DD \circ unit = DD. \quad (*)$$

Now we can show that  $DD$  is short: for  $\psi, \psi' \in \mathcal{M}[K+1](X)$

$$\begin{aligned}
&d_{\mathcal{D}(\mathcal{M}[K](X))}(DD(\psi), DD(\psi')) \\
&= d_{\mathcal{D}(\mathcal{M}[K](X))}\left(\mathcal{D}(acc)(PD_*(arr(\psi))), \mathcal{D}(acc)(PD_*(arr(\psi')))\right) \quad \text{by } (*) \\
&\leq \frac{1}{K} \cdot d_{\mathcal{D}(X^K)}\left(PD_*(arr(\psi)), PD_*(arr(\psi'))\right) \quad \text{by Lemma 6.3 (5)} \\
&\leq \frac{1}{K} \cdot \frac{K}{K+1} \cdot d_{\mathcal{D}(X^{K+1})}(arr(\psi), arr(\psi')) \quad \text{by item (3)} \\
&= \frac{1}{K+1} \cdot (K+1) \cdot d_{\mathcal{M}[K+1](X)}(\psi, \psi') \quad \text{by Lemma 6.3 (6)} \\
&= d_{\mathcal{M}[K+1](X)}(\psi, \psi').
\end{aligned}$$

For the reverse inequality we use that  $Flrn$  is an isometry, via Fact 4.5, and (thus) that  $Flrn_*$  is short.

$$\begin{aligned}
d_{\mathcal{D}(\mathcal{M}[K](X))}(DD(\psi), DD(\psi')) &\geq d_{\mathcal{D}(X)}\left(Flrn_*(DD(\psi)), Flrn_*(DD(\psi'))\right) \\
&= d_{\mathcal{D}(X)}(Flrn(\psi), Flrn(\psi')) \quad \text{by item 2} \\
&= d_{\mathcal{M}[K+1](X)}(\psi, \psi'). \quad \square
\end{aligned}$$

Hypergeometric drawing uses the draw-delete mode, where a drawn ball is removed from the urn. The urn thus changes with every draw. It will be presented as a multiset, say initially of size  $L$ . The size  $K$  of draws (multisets) must thus be restricted as  $K \leq L$ , since one cannot draw more balls than the urn contains — unless one uses negative probabilities, see [JS23]. In addition, we must require that drawn multisets  $\varphi$  are sub-multisets of the urn, that is  $\varphi \leq v$ , if  $v$  is the urn. This requirement ensures that the number of drawn balls for each color is below the number of balls of that colour in the urn.

The hypergeometric channel thus takes the form  $hg[K]: \mathcal{M}[L](X) \rightarrow \mathcal{D}(\mathcal{M}[K](X))$ , for  $L \geq K$ . It can be described as an iteration of draw-delete's, see [Jac21, Thm. 6]:

$$hg[K](v) := \left( \underbrace{DD \circ \dots \circ DD}_{L-K \text{ times}} \right)(v) = \sum_{\varphi \in \mathcal{M}[K](X), \varphi \leq v} \frac{\binom{v}{\varphi}}{\binom{L}{K}} |\varphi\rangle, \quad (8.1)$$

where  $\binom{v}{\varphi} := \prod_{x \in X} \binom{v(x)}{\varphi(x)}$ .

**Theorem 8.2.** *The hypergeometric channel  $hg[K]: \mathcal{M}[L](X) \rightarrow \mathcal{D}(\mathcal{M}[K](X))$  defined in (8.1), for  $L \geq K$ , is short and an isometry, via Fact 4.5.*

*Proof.* We see in (8.1) that  $hg[K]$  is a (channel) iteration of short channels  $DD$ , and thus short itself. Via iterated use of Lemma 8.1 (2) we get  $Flrn_*(hg[K](\psi)) = Flrn(\psi)$ . The proof is then completed via the argumentation in (7.2).  $\square$

The introduction of this paper contains an illustration of this hypergeometric isometry result, for urns over the set of colours  $C = \{R, G, B\}$ , considered as a discrete metric space.

## 9. PÓLYA DRAWING IS ISOMETRIC

Hypergeometric distributions use the draw-delete mode: a drawn ball is removed from the urn. The less well-known Pólya draws [Hop84] use the draw-add mode. This means that a drawn ball is returned to the urn, together with another ball of the same colour (as the drawn ball). Thus, with hypergeometric draws the urn decreases in size, so that only finitely many draws are possible, whereas with Pólya draws the urn grows in size, and the drawing may be repeated arbitrarily many times. As a result, for Pólya distributions we do not need to impose restrictions on the size  $K$  of draws. We do have to restrict draws from urn  $v$  to multisets  $\varphi \in \mathcal{M}[K](X)$  with  $\text{supp}(\varphi) \subseteq \text{supp}(v)$  since we can only draw balls of colours that are in the urn. Following [Jac22c], Pólya distributions are formulated in terms of multichoose binomials  $\binom{n}{m} := \binom{n+m-1}{m} = \frac{(n+m-1)!}{m!(n-1)!}$ , for  $n > 0$ .

$$pl[K](v) := \sum_{\varphi \in \mathcal{M}[K](X), \text{supp}(\varphi) \subseteq \text{supp}(v)} \frac{\binom{v}{\varphi}}{\binom{L}{K}} |\varphi\rangle, \quad (9.1)$$

where  $\binom{v}{\varphi} := \prod_{x \in \text{supp}(v)} \binom{v(x)}{\varphi(x)}$ .

The following result was already announced in the beginning of Section 7 and is used for part of the isometry proof.

**Proposition 9.1.** *For a non-empty urn  $v$  and drawsize  $K > 0$  one has  $Flrn_*(pl[K](v)) = Flrn(v)$ .*

*Proof.* We use:

$$\begin{aligned}
& \sum_{\varphi \in \mathcal{M}[K](\text{supp}(v))} pl[K](v)(\varphi) \cdot Flrn(\varphi)(y) \\
& \stackrel{(9.1)}{=} \sum_{\varphi \in \mathcal{M}[K](\text{supp}(v))} \frac{\binom{v}{\varphi} \cdot \varphi(y)}{\binom{L}{K} \cdot K} \\
& \stackrel{(*)}{=} \sum_{\varphi \in \mathcal{M}[K](\text{supp}(v))} \frac{v(y) \cdot \binom{v+1|y}{\varphi-1|y}}{L \cdot \binom{L+1}{K-1}} \\
& = \frac{v(y)}{L} \cdot \sum_{\varphi \in \mathcal{M}[K-1](\text{supp}(v+1|y))} \frac{\binom{v+1|y}{\varphi}}{\binom{L+1}{K-1}} \\
& = Flrn(v)(y) \cdot \sum_{\varphi \in \mathcal{M}[K-1](\text{supp}(v+1|y))} pl[K-1](v+1|y)(\varphi) \\
& = Flrn(v)(y).
\end{aligned}$$

The marked equation  $\stackrel{(*)}{=}$  uses the following property:

$$\binom{L}{K} \cdot K = \frac{(L+K-1)!}{(L-1)! \cdot K!} \cdot K = L \cdot \frac{(L+K-1)!}{L! \cdot (K-1)!} = L \cdot \binom{L+1}{K-1}. \quad \square$$

In Equation (8.1) we have seen that the hypergeometric channel can be expressed as an iteration of single-draw-delete's. It is not the case that the Pólya channel is an iteration of analogous single-draw-add channels. But we do have the following result.

**Lemma 9.2.** *Consider channel PSA, for ‘projection-store-add’, of the form:*

$$X^L \times X^N \xrightarrow{\text{PSA}} \mathcal{D}(X^L \times X^{N+1})$$

defined as:

$$\text{PSA}(\vec{x}, \vec{y}) := \sum_{1 \leq i \leq L+N} \sum_{1 \leq j \leq N+1} \frac{1}{(L+N)(N+1)} |\vec{x}, y_1, \dots, y_{j-1}, z_i, y_j, \dots, y_N \rangle \quad (9.2)$$

where  $z_i$  is the  $i$ -th element of the concatenation  $\vec{x} ++ \vec{y}$

Then:

- (1) PSA has Lipschitz constant  $\frac{L+N+1}{L+N}$ ;
- (2) The  $K$ -fold Kleisli iteration  $\text{PSA}^K = \text{PSA} \circ \dots \circ \text{PSA}: X^L \times X^N \rightarrow \mathcal{D}(X^L \times X^{N+K})$  has Lipschitz constant  $\frac{L+N+K}{L+N}$ ;
- (3) Using the empty sequence  $\langle \rangle \in X^0$  as fixed second argument in the  $K$ -fold iteration gives a function  $\text{PSA}^K(-, \langle \rangle): X^L \rightarrow \mathcal{D}(X^L \times X^K)$  with Lipschitz constant  $\frac{L+K}{L}$ . This function is of the form:

$$\text{PSA}^K(\vec{x}, \langle \rangle) = 1|\vec{x} \rangle \otimes \text{spol}[K](\vec{x}),$$

where  $\text{spol}[K] := \mathcal{D}(\pi_2) \circ \text{PSA}^K(-, \langle \rangle): X^L \rightarrow \mathcal{D}(X^K)$  is ‘sequence Pólya’. We claim that has Lipschitz constant  $\frac{K}{L}$ .

- (4)  $K$ -fold Pólya drawing (in terms of multisets) can be described in terms of sequence Pólya, namely as:

$$pl[K] = \langle \text{acc} \rangle \circ \text{spol}[K] \circ \text{arr} : \mathcal{M}[L](X) \rightarrow \mathcal{D}(\mathcal{M}[K](X)).$$

*Proof.* (1) For arbitrary sequences  $\vec{x}, \vec{x}' \in X^L$  and  $\vec{y}, \vec{y}' \in X^N$  we have, by immediately using Lemma 4.3 (8):

$$\begin{aligned}
& d\left(\text{PSA}(\vec{x}, \vec{y}), \text{PSA}(\vec{x}', \vec{y}')\right) \\
& \leq \sum_{1 \leq i \leq L+N} \sum_{1 \leq j \leq N+1} \frac{1}{(L+N)(N+1)} \cdot d_{X^L \times X^{N+1}}\left(\begin{array}{c} (\vec{x}, y_1, \dots, y_{j-1}, z_i, y_j, \dots, y_N), \\ (\vec{x}', y'_1, \dots, y'_{j-1}, z'_i, y'_j, \dots, y'_N) \end{array}\right) \\
& \stackrel{(3.1)}{=} \sum_{1 \leq i \leq L+N} \frac{1}{L+N} \cdot \left(d_{X^L}(\vec{x}, \vec{x}') + d_X(z_i, z'_i) + d_{X^N}(\vec{y}, \vec{y}')\right) \\
& = d_{X^L}(\vec{x}, \vec{x}') + \frac{1}{L+N} \cdot d_{X^L \times X^N}((\vec{x}, \vec{y}), (\vec{x}', \vec{y}')) + d_{X^N}(\vec{y}, \vec{y}') \\
& = \frac{L+N+1}{L+N} \cdot d_{X^L \times X^N}((\vec{x}, \vec{y}), (\vec{x}', \vec{y}')).
\end{aligned}$$

(2) By a simple iteration, using that function composition involves multiplication of Lipschitz constants:

$$\frac{L+N+1}{L+N} \cdot \frac{L+N+2}{L+N+1} \cdot \dots \cdot \frac{L+N+K}{L+N+K-1} = \frac{L+N+K}{L+N}.$$

(3) The distribution  $\text{DSA}(\vec{x}, \vec{y})$  in (9.2) is defined as a sum of ket's that all have  $\vec{x}$  as first component. This first component can be extracted via a tensor, as  $|\vec{x}, -\rangle = 1|\vec{x}\rangle \otimes -$ . Subsequently, this  $1|\vec{x}\rangle$  can be pulled outside the two sums in (9.2). This allows us in the calculations below to use that the tensor  $\otimes$  is an isometry, see Proposition 4.4 (1).

The previous point gives, for  $N = 0$ , that the function  $\text{PSA}^K(-, \vec{\cdot})$  has Lipschitz constant  $\frac{L+K}{L}$ , since:

$$d\left(\text{PSA}^K(\vec{x}, \langle \rangle), \text{PSA}^K(\vec{x}', \langle \rangle)\right) \leq \frac{L+0+K}{L+0} \cdot \left(d(\vec{x}, \vec{x}') + d(\langle \rangle, \langle \rangle)\right) = \frac{L+K}{L} \cdot d(\vec{x}, \vec{x}').$$

At the same time, using Proposition 4.4 (1) and Lemma 4.3 (4),

$$\begin{aligned}
d\left(\text{PSA}^K(\vec{x}, \langle \rangle), \text{PSA}^K(\vec{x}', \langle \rangle)\right) & = d\left(1|\vec{x}\rangle \otimes \text{spol}[K](\vec{x}), 1|\vec{x}'\rangle \otimes \text{spol}[K](\vec{x}')\right) \\
& = d(1|\vec{x}\rangle, 1|\vec{x}'\rangle) + d(\text{spol}[K](\vec{x}), \text{spol}[K](\vec{x}')) \\
& = d(\vec{x}, \vec{x}') + d(\text{spol}[K](\vec{x}), \text{spol}[K](\vec{x}')).
\end{aligned}$$

Combining these two facts gives Lipschitz constant  $\frac{K}{L}$  for sequence Pólya:

$$d(\text{spol}[K](\vec{x}), \text{spol}[K](\vec{x}')) \leq \frac{L+K}{L} \cdot d(\vec{x}, \vec{x}') - d(\vec{x}, \vec{x}') = \frac{K}{L} \cdot d(\vec{x}, \vec{x}').$$

(4) We prove  $\langle \text{acc} \rangle \circ \text{spol}[K] \circ \text{arr} = \text{pl}[K]$  by induction on  $K \geq 0$ , where  $\text{spol}[K] = \mathcal{D}(\pi_2) \circ \text{PSA}^K(-, \langle \rangle)$ . The case  $K = 0$  is easy since  $\text{PSA}^0(\vec{x}, \langle \rangle) = 1|\vec{x}, \langle \rangle\rangle$ , so that:

$$\begin{aligned}
(\langle \text{acc} \rangle \circ \text{spol}[0] \circ \text{arr})(v) & = \mathcal{D}(\text{acc})\left(\mathcal{D}(\pi_2)(1|\vec{x}, \langle \rangle\rangle)\right) \\
& = \mathcal{D}(\text{acc})(1|\langle \rangle\rangle) = 1|\text{acc}(\langle \rangle)\rangle = 1|\mathbf{0}\rangle = \text{pl}[0](v).
\end{aligned}$$

The latter equation holds because the only possible draw of size 0 is the empty multiset  $\mathbf{0}$ .

The induction step is more work.

$$\begin{aligned}
& (\langle \text{acc} \rangle \circ \text{spol}[K+1] \circ \text{arr})(v) \\
&= \sum_{\vec{x} \in \text{acc}^{-1}(v)} \frac{1}{\binom{v}{\vec{x}}} \cdot \sum_{\vec{z} \in \text{supp}(v)^{K+1}} (\text{PSA} \circ \text{PSA}^K)(\vec{x}, \langle \rangle)(\vec{x}, \vec{z} \mid \text{acc}(\vec{z})) \\
&= \sum_{\vec{x} \in \text{acc}^{-1}(v)} \frac{1}{\binom{v}{\vec{x}}} \cdot \sum_{\vec{y} \in \text{supp}(v)^K} \sum_{z \in \vec{x} + \vec{y}} \frac{1}{L+K} \cdot \text{PSA}^K(\vec{x}, \langle \rangle)(\vec{x}, \vec{y} \mid \text{acc}(\vec{y}) + 1|z\rangle) \\
&= \sum_{\vec{x} \in \text{acc}^{-1}(v)} \frac{1}{\binom{v}{\vec{x}}} \cdot \sum_{\varphi \in \mathcal{M}[K](\text{supp}(v))} \sum_{z \in \text{supp}(v)} \frac{v(z) + \varphi(z)}{L+K} \cdot \mathcal{D}(\text{acc})(\text{spol}[K](\vec{x}))(\varphi \mid \varphi + 1|z\rangle) \\
&\stackrel{\text{(IH)}}{=} \sum_{\varphi \in \mathcal{M}[K](\text{supp}(v))} \sum_{z \in \text{supp}(v)} \frac{v(z) + \varphi(z)}{L+K} \cdot \text{pl}[K](v)(\varphi \mid \varphi + 1|z\rangle) \\
&\stackrel{\text{(9.1)}}{=} \sum_{\varphi \in \mathcal{M}[K](\text{supp}(v))} \sum_{z \in \text{supp}(v)} \frac{v(z) + \varphi(z)}{L+K} \cdot \frac{\binom{v}{\varphi}}{\binom{L}{K}} \mid \varphi + 1|z\rangle) \\
&\stackrel{(*)}{=} \sum_{\varphi \in \mathcal{M}[K](\text{supp}(v))} \sum_{z \in \text{supp}(v)} \frac{\varphi(z) + 1}{K+1} \cdot \frac{\binom{v}{\varphi+1|z\rangle}}{\binom{L}{K+1}} \mid \varphi + 1|z\rangle) \\
&= \sum_{\psi \in \mathcal{M}[K+1](\text{supp}(v))} \left( \sum_{z \in \text{supp}(v)} \frac{\psi(z)}{K+1} \right) \cdot \frac{\binom{v}{\psi}}{\binom{L}{K+1}} \mid \psi) \\
&\stackrel{\text{(9.1)}}{=} \text{pl}[K+1](v).
\end{aligned}$$

The marked equation  $\stackrel{(*)}{=}$  follows from an easy calculation. For instance:

$$\begin{aligned}
(L+K) \cdot \binom{L}{K} &= (L+K) \cdot \frac{(L+K-1)!}{(L-1)! \cdot K!} \\
&= (K+1) \cdot \frac{(L+K)!}{(L-1)! \cdot (K+1)!} = (K+1) \cdot \binom{L}{K+1}. \quad \square
\end{aligned}$$

We now obtain isometry for Pólya.

**Theorem 9.3.** *Each Pólya channel  $\text{pl}[K]: \mathcal{M}[L](X) \rightarrow \mathcal{D}(\mathcal{M}[K](X))$ , for urn size  $L > 0$ ,  $K > 0$ , is short and, indirectly via Fact 4.5, also an isometry.*

*Proof.* The hard work has already been done in Lemma 9.2. Shortness of Pólya drawing is obtained from its description  $\text{pl}[K] = \langle \text{acc} \rangle \circ \text{spol}[K] \circ \text{arr}: \mathcal{M}[L](X) \rightarrow \mathcal{D}(\mathcal{M}[K](X))$  in Lemma 9.2 (4). This allows us to use the Lipschitz constants for accumulation and arrangement from Lemma 6.3 (5), (6), and for sequence Pólya from Lemma 9.2 (3). Thus, for urns  $v, v' \in \mathcal{M}[L](X)$ ,

$$\begin{aligned}
d(\text{pl}[K](v), \text{pl}[K](v')) &= d(\mathcal{D}(\text{acc})(\text{spol}[K]_*(\text{arr}(v))), \mathcal{D}(\text{acc})(\text{spol}[K]_*(\text{arr}(v')))) \\
&\leq \frac{1}{K} \cdot d(\text{spol}[K]_*(\text{arr}(v)), \text{spol}[K]_*(\text{arr}(v'))) \\
&\leq \frac{1}{K} \cdot \frac{K}{L} \cdot d(\text{arr}(v), \text{arr}(v')) \\
&\leq \frac{1}{L} \cdot L \cdot d(v, v') \\
&= d(v, v').
\end{aligned}$$

The reverse inequality ( $\geq$ ) follows from Proposition 9.1 and the argument in (7.2).  $\square$

We illustrate that the Pólya channel is an isometry.

**Example 9.4.** We take as space of colours  $X = \{0, 10, 50\} \subseteq \mathbb{N}$  with two urns of size 4

$$v_1 = 3|0\rangle + 1|10\rangle \quad v_2 = 1|0\rangle + 2|10\rangle + 1|50\rangle.$$

The Kantorovich distance between these urns is 15, via an optimal coupling  $1|0, 0\rangle + 2|0, 10\rangle + 1|10, 50\rangle$ , yielding the distance  $\frac{1}{4} \cdot (0 - 0) + \frac{1}{2} \cdot (10 - 0) + \frac{1}{4} \cdot (50 - 10) = 5 + 10 = 15$ .

We look at Pólya draws of size  $K = 2$ . This gives distributions:

$$\begin{aligned} pl[2](v_1) &= \frac{3}{5} \left| 2|0\rangle \right\rangle + \frac{3}{10} \left| 1|0\rangle + 1|10\rangle \right\rangle + \frac{1}{10} \left| 2|10\rangle \right\rangle \\ pl[2](v_2) &= \frac{1}{10} \left| 2|0\rangle \right\rangle + \frac{1}{5} \left| 1|0\rangle + 1|10\rangle \right\rangle + \frac{3}{10} \left| 2|10\rangle \right\rangle + \frac{1}{10} \left| 1|0\rangle + 1|50\rangle \right\rangle \\ &\quad + \frac{1}{5} \left| 1|10\rangle + 1|50\rangle \right\rangle + \frac{1}{10} \left| 2|50\rangle \right\rangle \end{aligned}$$

We compute the distance between these two distributions via the last formulation in (4.1), using an optimal short factor  $p: \mathcal{M}[2](X) \rightarrow \mathbb{R}_{\geq 0}$  given by  $p(\varphi) = \sum_x \varphi(x) \cdot \frac{x}{2}$ , that is:

$$\begin{aligned} p(2|0\rangle) &= 0 & p(1|0\rangle + 1|10\rangle) &= 5 & p(2|10\rangle) &= 10 \\ p(1|0\rangle + 1|50\rangle) &= 25 & p(1|10\rangle + 1|50\rangle) &= 30 & p(2|50\rangle) &= 50. \end{aligned}$$

Then:

$$\begin{aligned} pl[2](v_1) \models p &= \frac{3}{5} \cdot 0 + \frac{3}{10} \cdot 5 + \frac{1}{10} \cdot 10 = \frac{5}{2} \\ pl[2](v_2) \models p &= \frac{1}{10} \cdot 0 + \frac{1}{5} \cdot 5 + \frac{3}{10} \cdot 10 + \frac{1}{10} \cdot 25 + \frac{1}{5} \cdot 30 + \frac{1}{10} \cdot 50 = \frac{35}{2}. \end{aligned}$$

As predicted by Theorem 9.3, the distance between the Pólya distributions then coincides with the distance between the urns:

$$\begin{aligned} d(pl[2](v_1), pl[2](v_2)) &= \left| pl[2](v_1) \models p - pl[2](v_2) \models p \right| \\ &= \frac{35}{2} - \frac{5}{2} = 15 = d(v_1, v_2). \end{aligned}$$

## 10. THE LAW OF LARGE URNS

Hypergeometric and Pólya draws involve removals from, and additions to, the urn. When the urn  $v$  is very large, in comparison to the drawsize, the effects of such removals and additions are relatively small. Thus, hypergeometric and Pólya draws from large urns look very much like multinomial draws — which do not change the urn. For the corresponding multinomial draws one uses the distribution  $Flrn(v)$  as urn, the normalised version of the original urn  $v$ . This statement that hypergeometric and Pólya draws from large urns are like multinomial draws is intuitively clear and well-known. We make it mathematically precise in terms of limits of Kantorovich-over-Kantorovich distances going to zero.

The starting point is the following observation about binomial and multichoose coefficients.

**Lemma 10.1.** *Fix a number  $m \in \mathbb{N}$ . Then:*

$$\lim_{n \rightarrow \infty} \frac{\binom{n}{m}}{n^m} = \frac{1}{m!} = \lim_{n \rightarrow \infty} \frac{\left(\!\!\binom{n}{m}\!\!\right)}{n^m}.$$

*We shall use these equations in the following alternative form.*

$$\lim_{n \rightarrow \infty} \frac{n!}{(n-m)! \cdot n^m} = 1 = \lim_{n \rightarrow \infty} \frac{(n+m-1)!}{(n-1)! \cdot n^m}. \quad (10.1)$$

*Proof.* We may assume  $n \geq m$ . Then:

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{\binom{n}{m}}{n^m} &= \frac{1}{m!} \cdot \lim_{n \rightarrow \infty} \frac{n!}{(n-m)! \cdot n^m} \\ &= \frac{1}{m!} \cdot \lim_{n \rightarrow \infty} \frac{n}{n} \cdot \frac{n-1}{n} \cdot \dots \cdot \frac{n-m+1}{n} \\ &= \frac{1}{m!} \cdot \left( \lim_{n \rightarrow \infty} \frac{n}{n} \right) \cdot \left( \lim_{n \rightarrow \infty} \frac{n-1}{n} \right) \cdot \dots \cdot \left( \lim_{n \rightarrow \infty} \frac{n-m+1}{n} \right) = \frac{1}{m!}. \end{aligned}$$

Similarly, for the multichoose coefficient:

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{\binom{n}{m}}{n^m} &= \lim_{n \rightarrow \infty} \frac{(n+m-1)!}{m! \cdot (n-1)! \cdot n^m} \\ &= \frac{1}{m!} \cdot \lim_{n \rightarrow \infty} \frac{n}{n} \cdot \frac{n+1}{n} \cdot \dots \cdot \frac{n+m-1}{n} = \frac{1}{m!}. \quad \square \end{aligned}$$

**Proposition 10.2.** *Let  $X = \{x_1, \dots, x_N\}$  be a finite set with  $N \geq 2$  elements and let  $\varphi \in \mathcal{M}[K](X)$  be a draw of size  $K \in \mathbb{N}_{>0}$ .*

- (1) *The hypergeometric probability of drawing  $\varphi$  from an urn becomes equal to the multinomial probability of drawing  $\varphi$  from the frequentist learning of the urn, when the number of balls in the urn for each color  $x_i$  goes to infinity:*

$$\lim_{n_1, \dots, n_N \rightarrow \infty} \frac{mn[K](\text{Flrn}(\sum_i n_i | x_i))(\varphi)}{hg[K](\sum_i n_i | x_i)(\varphi)} = 1.$$

- (2) *Similarly, Pólya draw probabilities from a large urn are like multinomial probabilities:*

$$\lim_{n_1, \dots, n_N \rightarrow \infty} \frac{mn[K](\text{Flrn}(\sum_i n_i | x_i))(\varphi)}{pl[K](\sum_i n_i | x_i)(\varphi)} = 1.$$

*Proof.* (1) By unpacking the relevant definitions:

$$\begin{aligned} &\lim_{n_1, \dots, n_N \rightarrow \infty} \frac{mn[K](\text{Flrn}(\sum_i n_i | x_i))(\varphi)}{hg[K](\sum_i n_i | x_i)(\varphi)} \\ &= \lim_{n_1, \dots, n_N \rightarrow \infty} \frac{K!}{\prod_i \varphi(x_i)!} \cdot \prod_i \left( \frac{n_i}{\sum_j n_j} \right)^{\varphi(x_i)} \cdot \frac{\binom{\sum_j n_j}{K}}{\prod_i \binom{n_i}{\varphi(x_i)}} \\ &= \lim_{n_1, \dots, n_N \rightarrow \infty} \frac{(\sum_j n_j)!}{((\sum_j n_j) - K)! \cdot (\sum_j n_j)^K} \cdot \prod_i \frac{(n_i - \varphi(x_i))! \cdot n_i^{\varphi(x_i)}}{n_i!} \\ &= \left( \lim_{n \rightarrow \infty} \frac{n!}{(n-K)! \cdot n^K} \right) \cdot \left( \prod_i \lim_{n_i \rightarrow \infty} \frac{(n_i - \varphi(x_i))! \cdot n_i^{\varphi(x_i)}}{n_i!} \right) \\ &\stackrel{(10.1)}{=} 1. \end{aligned}$$

(2) Similarly:

$$\begin{aligned}
& \lim_{n_1, \dots, n_N \rightarrow \infty} \frac{mn[K](\text{Flrn}(\sum_i n_i | x_i))(\varphi)}{pl[K](\sum_i n_i | x_i)(\varphi)} \\
&= \lim_{n_1, \dots, n_N \rightarrow \infty} \frac{K!}{\prod_i \varphi(x_i)!} \cdot \prod_i \left( \frac{n_i}{\sum_j n_j} \right)^{\varphi(x_i)} \cdot \frac{\binom{\sum_j n_j}{K}}{\prod_i \binom{n_i}{\varphi(x_i)}} \\
&= \lim_{n_1, \dots, n_N \rightarrow \infty} \frac{((\sum_j n_j) + K - 1)!}{((\sum_j n_j) - 1)! \cdot (\sum_j n_j)^K} \cdot \prod_i \frac{(n_i - 1)! \cdot n_i^{\varphi(x_i)}}{(n_i + \varphi(x_i) - 1)!} \\
&= \left( \lim_{n \rightarrow \infty} \frac{(n + K - 1)!}{(n - 1)! \cdot n^K} \right) \cdot \left( \prod_i \lim_{n_i \rightarrow \infty} \frac{(n_i - 1)! \cdot n_i^{\varphi(x_i)}}{(n_i + \varphi(x_i) - 1)!} \right) \\
&\stackrel{(10.1)}{=} 1. \quad \square
\end{aligned}$$

We translate these results into limits of Kantorovich distances going to zero.

**Theorem 10.3.** *Let  $X = \{x_1, \dots, x_N\} \subseteq X$  be a finite set of colors, in a metric space  $X$ , of size  $N \geq 2$ , and let  $K \in \mathbb{N}$  be a fixed drawsize.*

(1) *When the urn size increases, the Kantorovich distance between hypergeometric and multinomial distributions goes to zero, as in:*

$$\lim_{n_1, \dots, n_N \rightarrow \infty} d\left(\text{hg}[K](\sum_i n_i | x_i), mn[K](\text{Flrn}(\sum_i n_i | x_i))\right) = 0.$$

(2) *Similarly, for Pólya distributions:*

$$\lim_{n_1, \dots, n_N \rightarrow \infty} d\left(pl[K](\sum_i n_i | x_i), mn[K](\text{Flrn}(\sum_i n_i | x_i))\right) = 0.$$

*Proof.* By Proposition 5.3 it suffices to prove the result for the total variation distance, where we take as constant  $D = \text{diam}(\{x_1, \dots, x_N\})$ . We prove the first point only, since the proof of the second one works similarly. We use Proposition 10.2 (1) in:

$$\begin{aligned}
& \lim_{n_1, \dots, n_N \rightarrow \infty} \text{tvd}\left(\text{hg}[K](\sum_i n_i | x_i), mn[K](\text{Flrn}(\sum_i n_i | x_i))\right) \\
&\stackrel{(5.1)}{=} \lim_{n_1, \dots, n_N \rightarrow \infty} \frac{1}{2} \sum_{\varphi \in \mathcal{M}[K](X)} \left| \text{hg}[K](\sum_i n_i | x_i)(\varphi) - mn[K](\text{Flrn}(\sum_i n_i | x_i))(\varphi) \right| \\
&= \frac{1}{2} \sum_{\varphi \in \mathcal{M}[K](X)} \lim_{n_1, \dots, n_N \rightarrow \infty} \text{hg}[K](\sum_i n_i | x_i)(\varphi) \cdot \left| \frac{mn[K](\text{Flrn}(\sum_i n_i | x_i))(\varphi)}{\text{hg}[K](\sum_i n_i | x_i)(\varphi)} - 1 \right| \\
&\leq \frac{1}{2} \sum_{\varphi \in \mathcal{M}[K](X)} \left| \lim_{n_1, \dots, n_N \rightarrow \infty} \frac{mn[K](\text{Flrn}(\sum_i n_i | x_i))(\varphi)}{\text{hg}[K](\sum_i n_i | x_i)(\varphi)} - 1 \right| \\
&= 0. \quad \square
\end{aligned}$$

We may reformulate the limit results in Theorem 10.3 as ‘urn limits’ of the form:

$$\lim_{v \rightarrow \infty} d\left(\text{hg}[K](v), mn[K](\text{Flrn}(v))\right) = 0 = \lim_{v \rightarrow \infty} d\left(pl[K](v), mn[K](\text{Flrn}(v))\right).$$

The meaning of  $v \rightarrow \infty$  for  $v \in \mathcal{M}(X)$  is that each color multiplicity  $v(x)$  goes to infinity, for each element  $x$  of the finite set of colours  $X$ . We refer to the above equations as the law(s) of large urns.



## 11. THE LAW OF LARGE DRAWS

This section contains another limit property, not for large urns but for large draws. It may be seen as a metric reformulation of the law of large numbers.

But first some preliminaries. For a distribution  $\omega \in \mathcal{D}(X)$  and an observation  $p: X \rightarrow \mathbb{R}$  the variance  $\text{Var}(\omega, p) \in \mathbb{R}_{\geq 0}$  describes how much the observable is spread-out, in relation to the validity, or expected value,  $\omega \models p$ . Explicitly:

$$\text{Var}(\omega, p) := \omega \models (p - (\omega \models p) \cdot \mathbf{1})^2. \quad (11.1)$$

We recall a number of basic facts about this variance.

**Lemma 11.1.** *Let  $\omega \in \mathcal{D}(X)$  and  $p: X \rightarrow \mathbb{R}$  be given.*

(1) *The variance (11.1) can also be described as:*

$$\text{Var}(\omega, p) = (\omega \models p^2) - (\omega \models p)^2.$$

(2) *As a result,  $(\omega \models p^2) \geq (\omega \models p)^2$ .*

(3) *There is also an inequality:*

$$\omega \models |p - (\omega \models p) \cdot \mathbf{1}| \leq \sqrt{\text{Var}(\omega, p)}.$$

*Proof.* (1) Via a standard argument:

$$\begin{aligned} & \text{Var}(\omega, p) \\ & \stackrel{(11.1)}{=} \omega \models (p - (\omega \models p) \cdot \mathbf{1})^2 \\ & = \sum_{x \in X} \omega(x) \cdot (p(x) - (\omega \models p))^2 \\ & = \sum_{x \in X} \omega(x) \cdot (p(x)^2 - 2(\omega \models p) \cdot p(x) + (\omega \models p)^2) \\ & = \left( \sum_{x \in X} \omega(x) \cdot p^2(x) \right) - 2(\omega \models p) \cdot \left( \sum_{x \in X} \omega(x) \cdot p(x) \right) + \left( \sum_{x \in X} \omega(x) \cdot (\omega \models p)^2 \right) \\ & = (\omega \models p^2) - 2(\omega \models p) \cdot (\omega \models p) + (\omega \models p)^2 \\ & = (\omega \models p^2) - (\omega \models p)^2. \end{aligned}$$

(2) Obviously, by the previous point, since  $\text{Var}(\omega, p) \geq 0$ .

(3) We abbreviate  $q := |p - (\omega \models p) \cdot \mathbf{1}|$ , so that  $q(x) = |p(x) - (\omega \models p)|$ . Then:

$$\text{Var}(\omega, p) = \omega \models q^2 \geq (\omega \models q)^2, \quad \text{by the previous point.}$$

As a result,

$$\omega \models |p - (\omega \models p) \cdot \mathbf{1}| = \omega \models q \leq \sqrt{\text{Var}(\omega, p)}. \quad \square$$

Informally, the next result expresses that large multinomial draws, when normalised, are close to the urn distribution. This is intuitively clear: when we draw very many balls (in draw-replace mode), then the frequencies of the colours in the draw resemble the urn. The more formal aspect of this statement is below. It expresses that this closeness works “in probability”, that is, the probabilities of the draws must be taken into account. Indeed, a very large draw may differ significantly from the urn, for instance when all drawn balls have the same colour, but the likelihood of such draws is low.

**Theorem 11.2.** *For each distribution  $\omega \in \mathcal{D}(X)$  on a metric space  $X$ ,*

$$\lim_{K \rightarrow \infty} mn[K](\omega) \models d(\omega, \text{Flrn}(-)) = 0.$$

*Proof.* Since Proposition 5.3 applies, with  $D = \text{diam}(\text{supp}(\omega))$ , it suffices to prove the limit equation for the total variation distance  $\text{tvd}$ .

$$\begin{aligned} & \lim_{K \rightarrow \infty} mn[K](\omega) \models \text{tvd}(\omega, \text{Flrn}(-)) \\ & \stackrel{(5.1)}{=} \lim_{K \rightarrow \infty} \sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot \frac{1}{2} \cdot \sum_{y \in \text{supp}(\omega)} |\text{Flrn}(\varphi)(y) - \omega(y)| \\ & = \frac{1}{2} \sum_{y \in \text{supp}(\omega)} \lim_{K \rightarrow \infty} mn[K](\omega) \models |\text{Flrn}(-)(y) - (mn[K](\omega) \models \text{Flrn}(-)(y))| \\ & \quad \text{by Proposition 7.2 (1)} \\ & \leq \frac{1}{2} \sum_{y \in \text{supp}(\omega)} \lim_{K \rightarrow \infty} \sqrt{\text{Var}(mn[K](\omega), \text{Flrn}(-)(y))} \quad \text{by Lemma 11.1 (3)} \\ & = \frac{1}{2} \sum_{y \in \text{supp}(\omega)} \lim_{K \rightarrow \infty} \sqrt{(mn[K](\omega) \models \text{Flrn}(-)(y))^2 - (mn[K](\omega) \models \text{Flrn}(-)(y))^2} \\ & \quad \text{by Lemma 11.1 (1)} \\ & = \frac{1}{2} \sum_{y \in \text{supp}(\omega)} \lim_{K \rightarrow \infty} \sqrt{\frac{(K-1) \cdot \omega(y)^2 + \omega(y)}{K} - \omega(y)^2} \quad \text{by Proposition 7.2 (5), (2)} \\ & = \frac{1}{2} \sum_{y \in \text{supp}(\omega)} \lim_{K \rightarrow \infty} \frac{\sqrt{\omega(y) \cdot (1 - \omega(y))}}{\sqrt{K}} \\ & = 0. \quad \square \end{aligned}$$

**Corollary 11.3.** *For two distributions  $\omega, \rho \in \mathcal{D}(X)$  on a metric space  $X$ ,*

$$\lim_{K \rightarrow \infty} mn[K](\omega) \models d(\text{Flrn}(-), \rho) = d(\omega, \rho).$$

*Proof.* We use the triangular inequality, both for ( $\leq$ ) and ( $\geq$ ). First, for each multiset  $\varphi$  we have  $d(\text{Flrn}(\varphi), \rho) \leq d(\text{Flrn}(\varphi), \omega) + d(\omega, \rho)$ . Hence:

$$\begin{aligned} \lim_{K \rightarrow \infty} mn[K](\omega) \models d(\text{Flrn}(-), \rho) & \leq \lim_{K \rightarrow \infty} mn[K](\omega) \models \left( d(\text{Flrn}(-), \omega) + d(\omega, \rho) \right) \\ & = \left( \lim_{K \rightarrow \infty} mn[K](\omega) \models d(\text{Flrn}(-), \omega) \right) + d(\omega, \rho) \\ & = d(\omega, \rho). \end{aligned}$$

In the other direction, we use  $d(\omega, \rho) \leq d(\omega, \text{Flrn}(\varphi)) + d(\text{Flrn}(\varphi), \rho)$ . Hence:

$$\begin{aligned} d(\omega, \rho) & = \lim_{K \rightarrow \infty} mn[K](\omega) \models d(\omega, \rho) \\ & \leq \lim_{K \rightarrow \infty} mn[K](\omega) \models \left( d(\omega, \text{Flrn}(-)) + d(\text{Flrn}(-), \rho) \right) \\ & = \left( \lim_{K \rightarrow \infty} mn[K](\omega) \models d(\omega, \text{Flrn}(-)) \right) + \left( \lim_{K \rightarrow \infty} mn[K](\omega) \models d(\text{Flrn}(-), \rho) \right) \\ & = \lim_{K \rightarrow \infty} mn[K](\omega) \models d(\text{Flrn}(-), \rho). \quad \square \end{aligned}$$

We conclude this section with some observations about large Pólya draws. Earlier in this section we have looked at large multinomial draw. Large hypergeometric draws, when the

drawsize goes to infinity, do not make sense, since the urn is finite and thus empty at some stage<sup>2</sup>. But one can ask: what happens with large Pólya draws? Does the distance between the (normalised) urn and (normalised) draws also go to zero, when the drawsize goes to infinity? That is, do large Pólya draws look very much like the urn, in probability? Recall that Pólya draws are used to capture clustering effects. Hence it is unclear what happens. The distance could go to infinity. In fact, the limit goes to a specific number.

We sketch the background of this observation without going into all details, since it involves continuous probability theory and thus leads beyond the scope of this paper. It is well-known, see standard textbooks, like [BS00, Bil95, Fen10, Kal21, Wil62], that the Pólya distribution can be obtained via a pushforward of the multinomial channel over the Dirichlet distribution. This takes the following form, for an urn  $v \in \mathcal{M}(X)$  with  $\text{supp}(v) = X$ , for a finite set  $X$ .

$$pl[K](v)(\varphi) = \int_{\omega \in \mathcal{D}(X)} \text{Dir}(v)(\omega) \cdot mn[K](\omega)(\varphi) \, d\omega. \quad (11.2)$$

We can now formulate a Pólya analogue of Theorem 11.2.

**Proposition 11.4.** *For a non-empty urn  $v \in \mathcal{M}(X)$ ,*

$$\begin{aligned} \lim_{K \rightarrow \infty} pl[K](v) \models d(\text{Flrn}(-), \text{Flrn}(v)) &= \int_{\omega \in \mathcal{D}(X)} \text{Dir}(v)(\omega) \cdot d(\omega, \text{Flrn}(v)) \, d\omega \\ &= \text{Dir}(v) \models d(-, \text{Flrn}(v)). \end{aligned} \quad (11.3)$$

*The latter formulation uses validity  $\models$  in a continuous setting.*

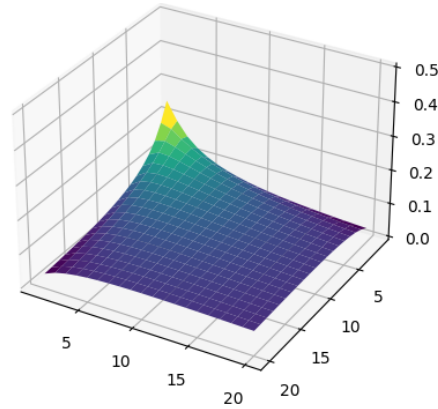
The integral in (11.3) is a special number associated with the urn / multiset  $v$ . It remains an open question to compute this integral more concretely.

*Proof.* We apply the formula (11.2) in:

$$\begin{aligned} &\lim_{K \rightarrow \infty} pl[K](v) \models d(\text{Flrn}(-), \text{Flrn}(v)) \\ &= \lim_{K \rightarrow \infty} \sum_{\varphi \in \mathcal{M}[K](X)} pl[K](v)(\varphi) \cdot d(\text{Flrn}(\varphi), \text{Flrn}(v)) \\ &= \lim_{K \rightarrow \infty} \sum_{\varphi \in \mathcal{M}[K](X)} \left( \int_{\omega \in \mathcal{D}(X)} \text{Dir}(v)(\omega) \cdot mn[K](\omega)(\varphi) \, d\omega \right) \cdot d(\text{Flrn}(\varphi), \text{Flrn}(v)) \\ &= \int_{\omega \in \mathcal{D}(X)} \text{Dir}(v)(\omega) \cdot \lim_{K \rightarrow \infty} \sum_{\varphi \in \mathcal{M}[K](X)} mn[K](\omega)(\varphi) \cdot d(\text{Flrn}(\varphi), \text{Flrn}(v)) \, d\omega \\ &= \int_{\omega \in \mathcal{D}(X)} \text{Dir}(v)(\omega) \cdot \lim_{K \rightarrow \infty} \left( mn[K](\omega) \models d(\text{Flrn}(-), \text{Flrn}(v)) \right) \, d\omega \\ &= \int_{\omega \in \mathcal{D}(X)} \text{Dir}(v)(\omega) \cdot d(\omega, \text{Flrn}(v)) \, d\omega \quad \text{by Corollary 11.3} \\ &= \text{Dir}(v) \models d(-, \text{Flrn}(v)). \end{aligned} \quad \square$$

<sup>2</sup>In a theory with negative probabilities one can have hypergeometric overdrawing, see [JS23].

The plot below gives an impression of the numbers (11.3) in the binary case with total variation distance, for urns  $i|a) + j|b)$  for the 400 cases  $1 \leq i, j \leq 20$ .



## 12. CONCLUDING REMARKS

Category theory provides a fresh look at the area of probability theory, see *e.g.* [Fri20] or [Jac25] for an overview. This paper demonstrates that draw operations, viewed as (Kleisli) maps, are remarkably well-behaved: they exactly preserve Kantorovich distances. Such distances on urns filled with coloured balls are relatively simple, starting from a ‘ground’ metric on the set of colours. But on draw distributions, the distances involve Kantorovich-over-Kantorovich. In addition, well-known limit behaviour, for large urns and large draws, is formulated in terms of Kantorovich distances.

This paper arose from a fresh categorical perspective on classical urn models, in line with earlier work [Jac21, Jac22b, Jac22c] of the author. Is category theory necessary to obtain (or prove) these results? No, one can strip all categorical language from what has been described above and formulate and prove the isometry results in traditional probabilistic language. But it is a fact that these results have not appeared within the traditional, non-categorical setting. We do not argue that category theory is necessary, but we do believe that its new, fresh perspective is helpful and leads to new ideas and results. More generally, category theory often helps in a particular mathematical setting to organise the material in a structured manner and to ask relevant questions: does this category have limits or colimits? Is this operation functorial, and if so, what does it preserve, does it have adjoints, *etc.* This paper uses category theory in a light-weight manner and is not a hard-core paper in categorical probability theory, using for instance Markov categories [Fri20]. Hopefully it works as invitation to invest efforts to learn the new categorically-inspired approach and what it brings.

This paper concentrates on drawing from an urn using finite discrete probability distributions. A natural question is whether other operations, especially involving infinite discrete and continuous probability, also preserve distance. This question is solved in [AG21, Prop. 3.2] for parameterised distributions  $\omega[\theta]$  on (subsets of) the reals: the Kantorovich distance equals the (real-number) distance between the expected values:

$$d(\omega[\theta_1], \omega[\theta_2]) = | \mathbb{E}(\omega[\theta_1]) - \mathbb{E}(\omega[\theta_2]) |. \quad (12.1)$$

As special cases, one has, for instance for the Kantorovich distances between Poisson and exponential distributions (on  $\mathbb{N}$  and  $\mathbb{R}_{>0}$ ):

$$d(\text{Pois}[\lambda_1], \text{Pois}[\lambda_2]) = |\lambda_1 - \lambda_2| \quad d(\text{Exp}[\lambda_1], \text{Exp}[\lambda_2]) = \left| \frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right|.$$

This equation (12.1) is very powerful. However, the isometry results for draw distributions in this paper are not instances of (12.1) since these draw distributions are not distributions on real numbers, but on multisets.

Another question that may be asked is if the (isometry) results for draw distributions, with respect to the Kantorovich distance, also hold for Kullback-Leibler divergence (see [CT06] for extensive information). This is largely an open question. What we can offer is the following result for multinomial distributions. We write  $D_{KL}$  for this Kullback-Leibler divergence and use its definition implicitly in the proof below.

**Proposition 12.1.** *Let distributions  $\omega, \omega' \in \mathcal{D}(X)$  be given with a draw-size number  $K \in \mathbb{N}$ . Then:*

$$D_{KL}\left(\text{mn}[K](\omega), \text{mn}[K](\omega')\right) = K \cdot D_{KL}(\omega, \omega').$$

*Proof.* We may assume  $\text{supp}(\omega) \subseteq \text{supp}(\omega')$  and write  $\text{supp}(\omega') = \{x_1, \dots, x_n\} \subseteq X$ .

$$\begin{aligned} D_{KL}\left(\text{mn}[K](\omega), \text{mn}[K](\omega')\right) &= \sum_{\varphi \in \mathcal{M}[K](X)} \text{mn}[K](\omega)(\varphi) \cdot \ln \left( \frac{\text{mn}[K](\omega)(\varphi)}{\text{mn}[K](\omega')(\varphi)} \right) \\ &= \sum_{\varphi \in \mathcal{M}[K](X)} \text{mn}[K](\omega)(\varphi) \cdot \ln \left( \frac{(\varphi) \cdot \prod_i \omega(x_i)^{\varphi(x_i)}}{(\varphi) \cdot \prod_i \omega'(x_i)^{\varphi(x_i)}} \right) \\ &= \sum_{\varphi \in \mathcal{M}[K](X)} \text{mn}[K](\omega)(\varphi) \cdot \ln \left( \prod_i \left( \frac{\omega(x_i)}{\omega'(x_i)} \right)^{\varphi(x_i)} \right) \\ &= \sum_{\varphi \in \mathcal{M}[K](X)} \text{mn}[K](\omega)(\varphi) \cdot \sum_i \varphi(x_i) \cdot \ln \left( \frac{\omega(x_i)}{\omega'(x_i)} \right) \\ &= \sum_i \left( \sum_{\varphi \in \mathcal{M}[K](X)} \text{mn}[K](\omega)(\varphi) \cdot \varphi(x_i) \right) \cdot \ln \left( \frac{\omega(x_i)}{\omega'(x_i)} \right) \\ &= \sum_i K \cdot \omega(x_i) \cdot \ln \left( \frac{\omega(x_i)}{\omega'(x_i)} \right) \quad \text{by Proposition 7.2 (1)} \\ &= K \cdot D_{KL}(\omega, \omega'). \quad \square \end{aligned}$$

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#### APPENDIX A. PROOF OF THE EQUATIONS IN (4.1)

We recall the three formulations (4.1) of the Kantorovich distance.

$$d(\omega, \omega') := \bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models d_X \stackrel{(*)}{=} \bigvee_{\substack{p, p' \in \text{Obs}(X), p \oplus p' \leq d_X \\ (**) \\ q \in \text{Fact}_S(X)}} \omega \models p + \omega' \models p' \quad (\text{A.1})$$

The observation  $p \oplus p' \in \text{Obs}(X \times X)$  is defined as  $(p \oplus p')(x, x') = p(x) + p'(x')$ . The minimum given by the meet  $\bigwedge$  exists since there is at least one coupling of  $\omega, \omega'$ , namely the product  $\omega \otimes \omega'$ . The two joins  $\bigvee$  are also taken over non-empty domains since one can instantiate with the zero observation / factor  $\mathbf{0}$ .

We first concentrate on equation  $(*)$  in (A.1). The inequality  $(\geq)$  is easy: let  $p, p' \in \text{Obs}(X)$  satisfy  $p \oplus p' \leq d_X$ . Then for each coupling  $\tau \in \mathcal{D}(X \times X)$  of  $\omega, \omega'$  one has:

$$\begin{aligned} \tau \models d_X \geq \tau \models p \oplus p' &= \sum_{x, x' \in X} \tau(x, x') \cdot (p \oplus p')(x, x') \\ &= \sum_{x, x' \in X} \tau(x, x') \cdot (p(x) + p'(x')) \\ &= \sum_{x, x' \in X} \tau(x, x') \cdot p(x) + \sum_{x, x' \in X} \tau(x, x') \cdot p'(x') \\ &= \sum_{x \in X} \left( \sum_{x' \in X} \tau(x, x') \right) \cdot p(x) + \sum_{x' \in X} \left( \sum_{x \in X} \tau(x, x') \right) \cdot p'(x') \\ &= \sum_{x \in X} \omega(x) \cdot p(x) + \sum_{x' \in X} \omega'(x') \cdot p'(x') \\ &= \omega \models p + \omega' \models p'. \end{aligned}$$

As a result, since this inequality holds for all couplings  $\tau$ ,

$$\bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models d_X \geq \omega \models p + \omega' \models p'.$$

And since the latter holds for all  $p, p'$  we get the  $(\geq)$  part of  $(*)$ .

$$\bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models d_X \geq \bigvee_{p, p' \in \text{Obs}(X) \text{ with } p \oplus p' \leq d_X} \omega \models p + \omega' \models p'.$$

This inequality shows in particular that this join  $\bigvee$  exists.

For the  $(\leq)$  part of  $(*)$  in (A.1) we have to do more work and exploit Farkas Lemma, which we formulate first. It captures a separation property that plays a central role in the duality theorem in linear programming, see *e.g.* [MG06] for further details and discussion.

**Lemma A.1** (Farkas Lemma). *For a matrix  $A \in \mathbb{R}^{m \times n}$  and a vector  $b \in \mathbb{R}^m$  there are equivalences of the following form.*

- (1)  $\exists v \in (\mathbb{R}_{\geq 0})^n. A \cdot v = b \iff \neg \exists u \in \mathbb{R}^m. u^T \cdot A \geq \mathbf{0} \text{ and } u^T \cdot b < 0.$
- (2)  $\exists v \in (\mathbb{R}_{\geq 0})^n. A \cdot v \leq b \iff \neg \exists u \in (\mathbb{R}_{\geq 0})^m. u^T \cdot A \geq \mathbf{0} \text{ and } u^T \cdot b < 0.$

*Proof.* A (short) proof of the first item may be found in [Kag24]. Next, [MG06, Prop. 6.4.3] contains a derivation of the second item from the first.  $\square$

We are going to apply this lemma in the Kantorovich context, in order to prove the  $(\leq)$  part of  $\stackrel{(*)}{=}$  in (A.1). Let  $\omega, \omega' \in \mathcal{D}(X)$  be given, where  $X = \{x_1, \dots, x_n\}$ . We take  $m = 2n$  in Lemma A.1 with vector  $b \in \mathbb{R}^{2n}$  given by the sequence of probabilities:

$$b := (\omega(x_1), \dots, \omega(x_n), \omega'(x_1), \dots, \omega'(x_n)).$$

For convenience we write  $t$  for the minimum validity  $\bigwedge_{\tau \in \text{dcp}l^{-1}(\omega, \omega')} \tau \models d_X$ .

We use the matrix  $A \in \mathbb{R}^{2n \times n^2}$  that captures marginalisation, when applied to distributions, giving a mapping  $\mathcal{D}(X \times X) \rightarrow \mathcal{D}(X) \times \mathcal{D}(X)$ .

$$A := \underbrace{\begin{pmatrix} 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & \cdots & 0 & 0 & \cdots & 0 \\ & & & \vdots & & & & \vdots & & & & & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 1 & 1 & \cdots & 1 \\ 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & 1 & \cdots & 0 & \cdots & 0 & 1 & \cdots & 0 \\ & & & \vdots & & & & \vdots & & & & & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 & \cdots & 0 & 0 & \cdots & 1 \end{pmatrix}}_{n^2 \text{ columns}} \left. \begin{array}{l} \right\} n \text{ rows} \\ \left. \right\} n \text{ rows} \end{array}$$

We turn the matrix  $A \in \mathbb{R}^{2n \times n^2}$  into a matrix  $A' \in \mathbb{R}^{(4n+1) \times n^2}$  in the following manner.

- On top of  $A$  we add the row  $d_X(x_1, x_1), d(x_1, x_2), \dots, d_X(x_n, x_n)$  containing the  $n^2$  distance values.
- Below  $A$  we add the matrix  $-A$ , with all numbers in  $A$  negated.

For each  $\varepsilon > 0$  we form a similar sequence  $b_\varepsilon \in \mathbb{R}^{4n+1}$  of the form  $(t - \varepsilon, b_1, \dots, b_{2n}, -b_1, \dots, -b_{2n})$ . In this way the following statement holds.

$$\neg \exists v \in (\mathbb{R}_{\geq 0})^{n^2}. A' \cdot v \leq b_\varepsilon.$$

Indeed,  $v = (v_1, \dots, v_{n^2})$  with  $A' \cdot v \leq b_\varepsilon$  would give a multiset  $\sigma \in \mathcal{M}(X \times X)$ , namely  $\sigma = \sum_{i,j} v_{(i-1)n+j} |x_i, x_j\rangle$ . It is a coupling of  $\omega, \omega'$  since  $A \cdot v = b = (\omega, \omega')$  via the inequalities  $A \cdot v \leq b$  and  $-A \cdot v \leq -b$ . Therefore,  $\sigma$  is a distribution. Moreover, it satisfies  $\sigma \models d_X \leq t - \varepsilon$ . The latter contradicts the minimality of  $t$ .

By applying item (2) of Farkas Lemma A.1 we get a vector  $u \in \mathbb{R}^{4n+1}$  with  $u \geq \mathbf{0}$  satisfying:

$$\begin{aligned} u_0 \cdot d_X + (u_1, \dots, u_{2n}) \cdot A - (u_{2n+1}, \dots, u_{4n}) \cdot A &\geq \mathbf{0} \\ u_0 \cdot (t - \varepsilon) + (u_1, \dots, u_{2n}) \cdot b - (u_{2n+1}, \dots, u_{4n}) \cdot b &< 0. \end{aligned} \tag{A.2}$$

We first cover the case  $u_0 = 0$ . The vector  $u$  is then a solution in (A.2) for  $\varepsilon = t$ , so that applying the direction  $(\Leftarrow)$  in Lemma A.1 (2) gives a coupling  $\sigma$  with  $\sigma \models d_X = 0$ . This gives  $t = 0$ . But then we are done, since trivially:

$$\begin{aligned} \bigvee_{p, p' \in \text{Obs}(X) \text{ with } p \oplus p' \leq d_X} \omega \models p + \omega' \models p' &\geq \omega \models \mathbf{0} + \omega' \models \mathbf{0} \\ &= 0 = t = \bigwedge_{\tau \in \text{dcp}l^{-1}(\omega, \omega')} \tau \models d_X. \end{aligned}$$



We may now assume  $u_0 > 0$ , so we can form two observations  $p, p' \in \text{Obs}(X)$  via the definitions:

$$p(x_i) := \frac{u_{2n+i} - u_i}{u_0} \quad \text{and} \quad p'(x_i) := \frac{u_{3n+i} - u_{n+i}}{u_0}.$$

The first of the inequalities (A.2) translates to  $p(x_i) + p'(x_j) \leq d_X(x_i, x_j)$  for each  $i, j$ , that is, to  $p \oplus p' \leq d_X$ . The second inequality gives us  $\omega \models p + \omega' \models p' > t - \varepsilon$ . We thus get:

$$\bigvee_{p, p' \in \text{Obs}(X) \text{ with } p \oplus p' \leq d_X} \omega \models p + \omega' \models p' > t - \varepsilon.$$

Since this holds for each  $\varepsilon > 0$  we obtain:

$$\bigvee_{p, p' \in \text{Obs}(X) \text{ with } p \oplus p' \leq d_X} \omega \models p + \omega' \models p' \geq t = \bigwedge_{\tau \in \text{dcpl}^{-1}(\omega, \omega')} \tau \models d_X.$$

This proves the  $(\leq)$  part of  $\stackrel{(*)}{=}$  in (A.1).

We now turn to the second equation  $\stackrel{(**)}{=}$  in (A.1), again starting from two distributions  $\omega, \omega' \in \mathcal{D}(X)$ . Its proof is more elementary. For  $(\geq)$ , let  $q \in \text{Fact}_S(X)$  be given. Without loss of generality we assume  $\omega \models q \leq \omega' \models q$ . We take as observations  $p = -q$  and  $p' = q$ . Then, because  $q$  is short:

$$(p \oplus p')(x, x') = p(x) + p'(x') = q(x') - q(x) \leq |q(x') - q(x)| \leq d_X(x, x').$$

Moreover,

$$\begin{aligned} |\omega \models q - \omega' \models q| &= \omega' \models q - \omega \models q \\ &= \omega \models p + \omega' \models p' \\ &\leq \bigvee_{p, p' \in \text{Obs}(X) \text{ with } p \oplus p' \leq d_X} \omega \models p + \omega' \models p'. \end{aligned}$$

Since this holds for all  $q \in \text{Fact}_S(X)$  we get:

$$\bigvee_{q \in \text{Fact}_S(X)} |\omega \models q - \omega' \models q| \leq \bigvee_{p, p' \in \text{Obs}(X) \text{ with } p \oplus p' \leq d_X} \omega \models p + \omega' \models p'.$$

For  $(\leq)$  let  $p, p' \in \text{Obs}(X)$  be given with  $p \oplus p' \leq d_X$ . We form  $q: X \rightarrow \mathbb{R}$  as:

$$q(x) := \bigwedge_{y \in X} d_X(x, y) - p(y)$$

We make a few points explicit.

- By using  $x$  in place of  $y$  in the range of the above meet  $\bigwedge$  we get  $q(x) \leq -p(x)$ . Further, since  $p(x) + p'(x') \leq d_X(x, x')$  we have  $p'(x') \leq d_X(x, x') - p(x) \leq q(x')$ . Thus,  $p \leq -q$  and  $p' \leq q$ .
- Next,  $q$  is short. Indeed, for  $x, x' \in X$ , and arbitrary  $y \in X$  we have, by the triangular inequality,

$$q(x) \leq d_X(x, y) - p(y) \leq d_X(x, x') + d_X(x', y) - p(y).$$

Since this holds for each  $y$  we get:

$$\begin{aligned} q(x) &\leq \bigwedge_{y \in X} d_X(x, x') + d_X(x', y) - p(y) \\ &= d_X(x, x') + \bigwedge_{y \in X} d_X(x', y) - p(y) = d_X(x, x') + q(x'). \end{aligned}$$

Thus:  $q(x) - q(x') \leq d_X(x, x')$ . By symmetry also:  $q(x') - q(x) \leq d_X(x, x')$ , and thus  $|q(x) - q(x')| = \max(q(x) - q(x'), q(x') - q(x)) \leq d_X(x, x')$ .

- Let  $M$  be the minimum value of  $q$ , which exists, since we assume that  $X$  is a finite set. We take  $q' = q + M \cdot \mathbf{1}$ . This is a factor, that is, a function  $X \rightarrow \mathbb{R}_{\geq 0}$  taking non-negative values. Moreover,  $q'$  is short since  $q$  is short.

We can now put things together.

$$\begin{aligned} \omega \models p + \omega' \models p' \leq \omega \models -q + \omega' \models q & \quad \text{since } p \leq -q \text{ and } p' \leq q \\ & \leq |\omega \models q - \omega' \models q| \\ & = |\omega \models q' - \omega' \models q'| \quad \text{since } q' = q + M \cdot \mathbf{1} \\ & \leq \bigvee_{q \in \text{Fact}_S(X)} |\omega \models q - \omega' \models q|. \end{aligned}$$

Because this holds for all  $p, p'$  we get, as required, the inequality ( $\leq$ ) for  $\stackrel{**}{=}$  in (A.1):

$$\bigvee_{p, p' \in \text{Obs}(X) \text{ with } p \oplus p' \leq d_X} \omega \models p + \omega' \models p' \leq \bigvee_{q \in \text{Fact}_S(X)} |\omega \models q - \omega' \models q|.$$

## APPENDIX B. PROOF OF THE EQUATIONS IN (6.1)

We start with a basic result about coupling and decoupling (2.1) of multisets.

**Lemma B.1.** *Consider sets  $X, Y$  and a number  $K \in \mathbb{N}$ .*

- (1) *There is a commuting triangle of the form:*

$$\begin{array}{ccc} X^K \times Y^K & \xrightarrow[\cong]{\text{zip}} & (X \times Y)^K & \xrightarrow{\text{acc}} & \mathcal{M}[K](X \times Y) \\ & \searrow & & \swarrow & \\ & \text{acc} \times \text{acc} & \mathcal{M}[K](X) \times \mathcal{M}[K](Y) & \xleftarrow{\text{dcpl}} & \end{array} \quad (\text{B.1})$$

*As a result, the decouple function  $\text{dcpl} = \langle \mathcal{M}(\pi_1), \mathcal{M}(\pi_2) \rangle: \mathcal{M}[K](X \times Y) \rightarrow \mathcal{M}[K](X) \times \mathcal{M}[K](Y)$  is surjective.*

- (2) *There is the following equality of subsets of  $\mathcal{M}[K](X \times Y)$ , for multisets  $\varphi \in \mathcal{M}[K](X)$  and  $\psi \in \mathcal{M}[K](Y)$ .*

$$\text{dcpl}^{-1}(\varphi, \psi) = \{ \text{acc}(\text{zip}(\vec{x}, \vec{y})) \mid \vec{x} \in \text{acc}^{-1}(\varphi), \vec{y} \in \text{acc}^{-1}(\psi) \}.$$

*In particular, the subset  $\text{dcpl}^{-1}(\varphi, \psi) \subseteq \mathcal{M}[K](X \times Y)$  is finite.*

- (3) *If  $\tau = \text{acc}(\text{zip}(\vec{x}, \vec{y})) \in \mathcal{M}[K](X \times X)$ , where  $X$  is a metric space, then:*

$$\text{Flrn}(\tau) \models d_X = \frac{1}{K} \cdot d_{X^K}(\vec{x}, \vec{y}).$$

*Proof.* (1) Via the naturality of  $\text{acc}: (-)^K \Rightarrow \mathcal{M}[K]$ , we get for  $\vec{x} \in \text{acc}^{-1}(\varphi)$  and  $\vec{y} \in \text{acc}^{-1}(\psi)$ ,

$$\begin{aligned} \text{dcpl}\left(\text{acc}(\text{zip}(\vec{x}, \vec{y}))\right) &= \langle \mathcal{M}(\pi_1)\left(\text{acc}(\text{zip}(\vec{x}, \vec{y}))\right), \mathcal{M}(\pi_2)\left(\text{acc}(\text{zip}(\vec{x}, \vec{y}))\right) \rangle \\ &= \langle \text{acc}\left((\pi_1)^K(\text{zip}(\vec{x}, \vec{y}))\right), \text{acc}\left((\pi_2)^K(\text{zip}(\vec{x}, \vec{y}))\right) \rangle \\ &= \langle \text{acc}(\pi_1(\vec{x}, \vec{y})), \text{acc}(\pi_2(\vec{x}, \vec{y})) \rangle \\ &= \langle \text{acc}(\vec{x}), \text{acc}(\vec{y}) \rangle \\ &= \langle \varphi, \psi \rangle. \end{aligned}$$

This allows us to show that  $dcpl: \mathcal{M}[K](X \times Y) \rightarrow \mathcal{M}[K](X) \times \mathcal{M}[K](Y)$  is a surjective function: let a pair  $\langle \varphi, \psi \rangle \in \mathcal{M}[K](X) \times \mathcal{M}[K](Y)$  be given. Using the surjectivity of accumulation we can find  $\vec{x} \in X^K$  and  $\vec{y} \in Y^K$  with  $acc(\vec{x}) = \varphi$  and  $acc(\vec{y}) = \psi$ . The above argument shows that  $\chi := acc(zip(\vec{x}, \vec{y})) \in \mathcal{M}[K](X \times Y)$  satisfies  $dcpl(\chi) = \langle acc(\vec{x}), acc(\vec{y}) \rangle = \langle \varphi, \psi \rangle$ .

- (2) The previous point gives the inclusion  $(\supseteq)$ . For  $(\subseteq)$ , let  $\chi \in dcpl^{-1}(\varphi, \psi)$  be given. There is a sequence  $\vec{z} \in (X \times Y)^K$  with  $acc(\vec{z}) = \chi$ . Write  $\vec{z} = zip(\vec{x}, \vec{y})$ , for  $\vec{x} = (\pi_1)^K(\vec{z})$  and  $\vec{y} = (\pi_2)^K(\vec{z})$ . We claim that  $acc(\vec{x}) = \varphi$  and  $acc(\vec{y}) = \psi$ . We elaborate only the first equation, since the second one is obtained in the same way. By assumption,  $\chi$  is coupling of  $\varphi, \psi$ , so:

$$\varphi = \mathcal{M}(\pi_1)(\chi) = \mathcal{M}(\pi_1)(acc(zip(\vec{x}, \vec{y}))) = acc(\vec{x}).$$

The last equation is obtained as in the previous point.

- (3) Let  $\tau = acc(zip(\vec{x}, \vec{y})) \in \mathcal{M}[K](X \times X)$ , for  $\vec{x}, \vec{y} \in X^K$ . Then:

$$\begin{aligned} Flrn(\tau) \models d_X &= \frac{1}{K} \cdot \sum_{(u,v) \in X^2} acc(zip(\vec{x}, \vec{y}))(u, v) \cdot d_X(u, v) \\ &= \frac{1}{K} \cdot \sum_{1 \leq i \leq K} d_X(x_i, y_i) \stackrel{(3.1)}{=} \frac{1}{K} \cdot d_{X^K}(\vec{x}, \vec{y}). \quad \square \end{aligned}$$

**Theorem B.2.** Equation (6.1) holds, that is, for a metric space  $X$  with multisets  $\varphi, \varphi' \in \mathcal{M}[K](X)$ ,

$$\bigwedge_{\tau \in dcpl^{-1}(\varphi, \varphi')} Flrn(\tau) \models d_X = \frac{1}{K} \cdot \bigwedge_{\vec{x} \in acc^{-1}(\varphi), \vec{y} \in acc^{-1}(\varphi')} d_{X^K}(\vec{x}, \vec{y})$$

*Proof.* By Lemma B.1. For  $(\leq)$  we notice that for each pair of vectors  $\vec{x} \in acc^{-1}(\varphi), \vec{y} \in acc^{-1}(\varphi')$  we have that  $\tau = acc(zip(\vec{x}, \vec{y}))$  is a coupling of  $\varphi, \varphi'$  with  $Flrn(\tau) \models d_X = \frac{1}{K} \cdot d_{X^K}(\vec{x}, \vec{y})$ . For  $(\geq)$  we notice that each coupling  $\tau$  is of the form  $\tau = acc(zip(\vec{x}, \vec{y}))$ , for some vectors  $\vec{x} \in acc^{-1}(\varphi), \vec{y} \in acc^{-1}(\varphi')$ . Then again,  $Flrn(\tau) \models d_X = \frac{1}{K} \cdot d_{X^K}(\vec{x}, \vec{y})$ .  $\square$