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Urns & Tubes

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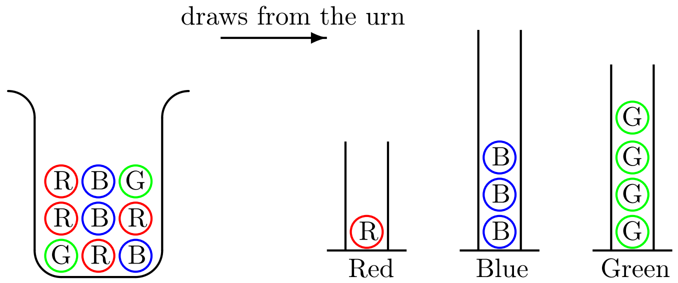
Urn models play an important role to express various basic ideas in probability theory. Here we extend this urn model with tubes. An urn contains coloured balls, which can be drawn with probabilities proportional to the numbers of balls of each colour. For each colour a tube is assumed. These tubes have different sizes (lengths). The idea is that after drawing a ball from the urn it is dropped in the tube of the corresponding colour. We consider two associated probability distributions. The *first-full* distribution on colours gives for each colour the probability that the corresponding tube is full first, before any of the other tubes. The *negative* distribution on natural numbers captures for a number k the probability that all tubes are full for the first time after k draws.

This paper uses multisets to systematically describe these first-full and negative distributions in the urns & tubes setting, in fully multivariate form, for all three standard drawing modes (multinomial, hypergeometric, and Pólya).

1 Introduction

Consider the situation sketched below (1), with an urn filled with coloured balls (on the left) and tubes of different lengths (on the right), with one tube for each colour. Below there are three colours: red (R), blue (B), and green (G), but in general there can be $N \geq 2$ many colours — and then also N tubes. We consider the following action: when a ball is drawn from the urn, it is dropped in the tube of the corresponding colour. This action is repeated.



(1)

In this paper we consider this urns & tubes setting in two scenarios, involving either *some tube* or *all tubes* being full for the first time. They both start from empty tubes.

1. The first scenario looks at the probability that some tube is completely full first, before any of the other tubes is full. As will be shown, this yields a distribution on colours, which we call the *first-full* distribution.

2. In the second scenario we consider a distribution on natural numbers, where the probability assigned to number k is the probability that all tubes are full for the first time after k draws. This means that there is some tube getting full at stage k, while all other tubes are already full — possibly with overflows. Such distributions are known in the literature as *negative* distributions. More on this at the end of this section.

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One can translate this abstract urns & tubes setting to more practical scenarios where the filling of the tubes may represent something good or bad, like hospital beds of various types becoming fully used up. Both the first-full and the negative scenarios may be relevant in risk modeling, where the fullness probabilities of tubes correspond to risks of reaching thresholds.

Intuitively, the first-full probability for a colour C decreases with the length of the C-coloured tube, and increases with the proportion of C-coloured balls in the urn. It thus involves complex dependencies. The main technical challenge is to prove that first-full is actually a distribution, with first-full probabilities for each colour adding up to one. For this purpose we reason compositionally, via certain probabilistic automata, namely Markov models with output (MOO), which terminate at some stage, after some number of compositions, producing the relevant first-full distribution. The same type of automaton can be used for negative distributions. The categorical details behind this composition are explained in the appendix

Commonly three modes of drawing balls from an urn are distinguished, see *e.g.* [14, 19, 22, 24], called *multinomial*, *hypergeometric* and *Pólya*; the last mode is also called *Pólya–Eggenberg* or *Dirichlet-multinomial*, see [15]. We use "0", "-1" and "+1" as short-hand descriptions for these different modes. Explicitly, we use:

- "0" for the multinomial mode, in which the drawn ball is returned to the urn;
- "-1" for the hypergeometric mode, where the drawn ball is not returned to the urn — so that the urn is diminishing;
- "+1" for the Pólya mode, where the drawn ball is returned to the urn, together with an additional copy, of the same colour (called a reinforcement).

The distinction between multinomial and hypergeometric modes is most familiar and is often expressed in terms of: *with* or *without* replacement. The Pólya mode is less well known. The additional ball that is added to the urn after drawing has a strengthening effect that can capture situations with a cluster dynamics, like in the spread of contagious diseases [4] or the flow of tourists [17].

In a physical explanation of the first-full distributions we need for the multinomial and Pólya modes an auxiliary box of balls on the side (with sufficiently many balls). In multinomial (resp. Pólya) mode, the ball drawn from the urn is dropped in the right tube, but one (resp. two) ball(s) of the same colour are taken from the box and added to the urn, before the next draw. In the Pólya case the urn grows in size with each draw. In the multinomial case the urn remains the same and is best described as a probability distribution (over the set of colours). In the hypergeometric mode the urn decreases in size; we thus have to assume that initially the urn contains sufficiently many balls of each colour: more than the length of each tube.

The urn & tubes set-up as introduced here generalises the famous 'problem of points', studied in the 17th century by Pierre Fermat and Blaise Pascal, that played an important role in the development of modern probability theory — in particular for the notion of expectation. See [3] for a historical and [18] for a popular account. The problem of points involves a game between two players that is terminated prematurely and where the stakes so far have to be divided between the two. The solution there is to look at the remaining number of steps for winning (and associated probabilities) for each of the players. These remaining steps translate directly into lengths of two tubes, one for each player, with multinomial draws, see Subsection 5.1 below for further details.

The current urn & tubes set-up 'inverts' the problem of points, and also generalises it in two ways: (1) urns & tubes are analysed is in fully multivariate form, and (2) the analysis covers the three drawing modes described above.

Although the same urn & tubes setting is used both for first-full and for negative distributions, these distributions are really different. First of all, negative distributions have the natural numbers $\mathbb{N}$ as sample space, with infinite support — in multinomial and Pólya mode. To $k \in \mathbb{N}$ the probability is assigned that *all* tubes are full, for the first time, after k draws — where some tubes may overflow, while others are not full yet. Such negative distributions are studied in the literature, see *e.g.* [21, 25, 26] and the textbooks [13, 15], but typically with one tube only. Still, these negative distributions are not mainstream, and are even called 'forgotten', see [20]. Here we describe negative distributions, in the general urn & tubes setting, in fully multivariate form, for all three drawing modes ("0", "-1", "+1").

In this paper we make extensive use of multisets, like in other recent publications [5, 7, 9, 11]. A multiset is like a subset, except that elements may occur multiple times. For instance, an urn is a multiset, over the set of colours. A draw of multiple balls from such an urn is a multiset. Also, the tubes of different colours are represented as a multiset. Multisets form the proper formalism for multivariate probabilities, see Section 3 below. Sending an arbitrary set X to the set of multisets over X has the structure of a monad. Similarly, taking distributions over a set forms a monad. These monad structures play an important role in the various ways that the multinomial and hypergeometric (and Pólya) operations, as Kleisli maps, can be composed, see [7] and [8]. In this paper the underlying categorical structure is kept in the background. This is a deliberate choice, in order not to limit the potential audience. For instance, in the beginning of Section 6 the composition steps for Markov models with output are spelled-out concretely; their abstract categorical form as Kleisli composition is elaborated in the appendix.

This paper is organised as follows. It starts with a concrete description of first-full distributions, for all three modes ("0", "-1", "+1"), in Section 2. Subsequently, Section 3 introduces relevant notation and terminology for multisets and distributions, and Section 4 formulates multivariate versions of the multinomial, hypergeometric and Pólya distributions, as distributions on multisets of a fixed size. For snappy formulation of the hypergeometric and Póly distributions we use binomial coefficients with multisets instead of numbers, both for ordinary binomial coefficients and for the multichoose version. We introduce suitable generalisations of Vandermonde's formula, for multisets, also in multichoose form.

The next two sections are devoted to first-full distributions. They are defined in Section 5 in a pointwise manner, as sums over multisets. These probabilities are illustrated in several bar plots. Next, Section 6 introduces three probabilistic automata, in the form of Markov models with output, which are used to show that we actually get three distributions, with probabilities adding up to one. The heart of the argument is that composition (iteration) of the steps of these automata preserves distributions.

Section 7 introduces and illustrates negative distributions in the urns & tubes setting. We pay special attention to the bivariate case, with one tube only, which is the form in which they occur in the literature. We illustrate how the probabilities add up to one, and thus yield actual distributions, vie the same compositional argument, by sketching the relevant Markov models with output.

These descriptions of the first-full distributions set the scene for two additional topics. It is known that the hypergeometric and Pólya distributions can be obtained via conditioning from binomial and from negative binomial distributions. Section 8 recalls these results in the current setting, in uniform descriptions. Finally, Section 9 concentrates on the bivariate first-full and negative distributions, with two tubes. It translates the fact that probabilities in these distributions add up to one into number-theoretic corollaries. These results seem to be new. It is left as a challenge to prove them directly.

Acknowledgments

The urn & tubes set-up in this paper was developed without awareness of the problem of points. Thanks are due to Onno Boxma for pointing out the connection.

2 Examples of first-full distributions

This section illustrates how first-full distributions come about, in the three drawing modes. We keep things simple at this stage and use only two colours, written R for red and B for blue. We assume length 2 for the red tube, and length 3 for the blue tube. We briefly describe the draw probabilities in the three modes, in this illustration.

- In the multinomial mode "0", we assume that there are three balls in the urn, one red and two blue. The probability of drawing red is thus $\frac{1}{3}$ and for blue it is $\frac{2}{3}$. These probabilities remain the same, since drawn balls are returned to the urn. This "0" case is elaborated in Example 1 below.

- In the hypergeometric "-1" mode we assume that the urn initially has three red and six blue balls. The initial probability of drawing red from this urn is thus $\frac{3}{9} = \frac{1}{3}$. It leaves an urn with two red and six blue balls. So the probability of drawing a second red ball from the resulting urn is $\frac{2}{8} = \frac{1}{4}$. Example 2 gives the first-full details in this mode.
- In our illustration of the Pólya "+1" mode we assume initially just one red and one blue ball in the urn. The probability of drawing red is thus initially $\frac{1}{2}$. Upon drawing red, not only the drawn red ball, but also an additional red ball, is added to the urn, so that it subsequently contains three balls, two red and one blue. The probability of drawing red is then $\frac{2}{3}$. The resulting dynamics is described in Example 3 below.

These three modes are elaborated below, in three separate examples.

Example 1 *As described above, in the multinomial case we assume a $\frac{1}{3}$ probability for R = red, and $\frac{2}{3}$ for B = blue. What are the possible draws for getting one tube filled first? We list the possible draws to fill the red tube (of length 2) first, on the left below, with corresponding (multinomial) probabilities, and the draws to fill the blue tube (of length 3) first on the right.*

$$\begin{array}{rr}
R,R & \frac{1}{3}\cdot\frac{1}{3} = \frac{1}{9} \\
B,R,R & \frac{2}{3}\cdot\frac{1}{3}\cdot\frac{1}{3} = \frac{2}{27} \\
R,B,R & \frac{1}{3}\cdot\frac{2}{3}\cdot\frac{1}{3} = \frac{2}{27} \\
B,B,R,R & \frac{2}{3}\cdot\frac{2}{3}\cdot\frac{1}{3}\cdot\frac{1}{3} = \frac{4}{81} \\
B,R,B,R & \frac{2}{3}\cdot\frac{1}{3}\cdot\frac{2}{3}\cdot\frac{1}{3} = \frac{4}{81} \\
R,B,B,R & \frac{1}{3}\cdot\frac{2}{3}\cdot\frac{2}{3}\cdot\frac{1}{3} = \frac{4}{81} \\
\hline
& \textit{total for } R = \frac{11}{27}
\end{array}
\qquad
\begin{array}{rr}
B,B,B & \frac{2}{3}\cdot\frac{2}{3}\cdot\frac{2}{3} = \frac{8}{27} \\
R,B,B,B & \frac{1}{3}\cdot\frac{2}{3}\cdot\frac{2}{3}\cdot\frac{2}{3} = \frac{8}{81} \\
B,R,B,B & \frac{2}{3}\cdot\frac{1}{3}\cdot\frac{2}{3}\cdot\frac{2}{3} = \frac{8}{81} \\
B,B,R,B & \frac{2}{3}\cdot\frac{2}{3}\cdot\frac{1}{3}\cdot\frac{2}{3} = \frac{8}{81} \\
\hline
& \textit{total for } B = \frac{16}{27}.
\end{array}$$

We see on the left that the two required R-draws can be mixed with at most two B-draws, but the last draw must of course be R, in order to completely fill the red tube first. Similarly, on the right, the three required B-draws can be mixed with at most one R-draw.

The probability that the blue tube is full first is the highest one. The blue tube is longer than the red one (3 versus 2), but the probability of drawing blue is higher (2 versus 1).

Example 2 *We turn to the hypergeometric mode and start with an urn with three red and six blue balls. Now each drawn ball is removed from the urn, which affects subsequent probabilities. This gives different probabilities for the same draws as in the previous example.*

$$\begin{array}{rr}
R,R & \frac{3}{9}\cdot\frac{2}{8} = \frac{1}{12} \\
B,R,R & \frac{6}{9}\cdot\frac{3}{8}\cdot\frac{2}{7} = \frac{1}{14} \\
R,B,R & \frac{3}{9}\cdot\frac{6}{8}\cdot\frac{2}{7} = \frac{1}{14} \\
B,B,R,R & \frac{6}{9}\cdot\frac{5}{8}\cdot\frac{3}{7}\cdot\frac{2}{6} = \frac{5}{84} \\
B,R,B,R & \frac{6}{9}\cdot\frac{3}{8}\cdot\frac{5}{7}\cdot\frac{2}{6} = \frac{5}{84} \\
R,B,B,R & \frac{3}{9}\cdot\frac{6}{8}\cdot\frac{5}{7}\cdot\frac{2}{6} = \frac{5}{84} \\
\hline
& \textit{total for } R = \frac{17}{42}
\end{array}
\qquad
\begin{array}{rr}
B,B,B & \frac{6}{9}\cdot\frac{5}{8}\cdot\frac{4}{7} = \frac{5}{21} \\
R,B,B,B & \frac{3}{9}\cdot\frac{6}{8}\cdot\frac{5}{7}\cdot\frac{4}{6} = \frac{5}{42} \\
B,R,B,B & \frac{6}{9}\cdot\frac{3}{8}\cdot\frac{5}{7}\cdot\frac{4}{6} = \frac{5}{42} \\
B,B,R,B & \frac{6}{9}\cdot\frac{5}{8}\cdot\frac{3}{7}\cdot\frac{4}{6} = \frac{5}{42} \\
\hline
& \textit{total for } B = \frac{25}{42}.
\end{array}$$

In this hypergeometric mode the two first-full probabilities are different from the ones in Example 1, but they still add up to one. Again, blue 'wins'.

Example 3 *Finally we consider first-full in Pólya mode, with (initial) urn containing one red and one blue ball. The probabilities for the various draws are then as follows.*

$$\begin{array}{rrcl}
R,R & \frac{1}{2}\cdot\frac{2}{3} & = & \frac{1}{3} \\
B,R,R & \frac{1}{2}\cdot\frac{1}{3}\cdot\frac{2}{4} & = & \frac{1}{12} \\
R,B,R & \frac{1}{2}\cdot\frac{1}{3}\cdot\frac{2}{4} & = & \frac{1}{12} \\
B,B,R,R & \frac{1}{2}\cdot\frac{2}{3}\cdot\frac{1}{4}\cdot\frac{2}{5} & = & \frac{1}{30} \\
B,R,B,R & \frac{1}{2}\cdot\frac{1}{3}\cdot\frac{2}{4}\cdot\frac{2}{5} & = & \frac{1}{30} \\
R,B,B,R & \frac{1}{2}\cdot\frac{1}{3}\cdot\frac{2}{4}\cdot\frac{2}{5} & = & \frac{1}{30} \\
\hline
 & \textit{total for } R & = & \frac{3}{5}
\end{array}
\qquad
\begin{array}{rrcl}
B,B,B & \frac{1}{2}\cdot\frac{2}{3}\cdot\frac{3}{4} & = & \frac{1}{4} \\
R,B,B,B & \frac{1}{2}\cdot\frac{1}{3}\cdot\frac{2}{4}\cdot\frac{3}{5} & = & \frac{1}{20} \\
B,R,B,B & \frac{1}{2}\cdot\frac{1}{3}\cdot\frac{2}{4}\cdot\frac{3}{5} & = & \frac{1}{20} \\
B,B,R,B & \frac{1}{2}\cdot\frac{2}{3}\cdot\frac{1}{4}\cdot\frac{3}{5} & = & \frac{1}{20} \\
\hline
 & \textit{total for } B & = & \frac{2}{5}.
\end{array}$$

We obtain a third first-full distribution, now with higher probability for red.

3 Preliminaries, on multisets and distributions

We briefly describe the notation and terminology for multisets and distributions, in two separate subsections.

3.1 Multisets

As mentioned in the introduction, a multiset (or bag) is a finite 'subset' in which elements may occur multiple times. We use a 'ket' notation $|-\rangle$ borrowed from quantum theory, as convenient way of writing such multisets. For instance, the initial urn with tree red and six blue balls in Example 2 forms a multiset $3|R\rangle + 6|B\rangle$. And the three tubes in (1) form a multiset $3|R\rangle + 6|B\rangle + 5|G\rangle$. In general, a multiset over a set X is a finite formal combination $\sum_i n_i|x_i\rangle$ with $n_i \in \mathbb{N}$ and $x_i \in X$. Alternatively, a multiset is a function $\varphi\colon X \to \mathbb{N}$ with finite support $\mathrm{supp}(\varphi) = \{x \in X \mid \varphi(x) > 0\}$. The number $\varphi(x) \in \mathbb{N}$ tells how many times the element x occurs in the multiset φ. We freely switch between the formal sum and the function notation.

We shall write $\mathcal{M}(X)$ for the set of multisets over X. Notice that each multiset is finite, in our description, but the underlying set X itself need not be finite. Via pointwise addition, multisets form a commutative monoid, and in fact, $\mathcal{M}(X)$ is the free commutative monoid on X, via the unit map $\eta\colon X \to \mathcal{M}(X)$, given by $\eta(x) = 1|x\rangle$. We shall write $\mathbf{0} \in \mathcal{M}(X)$ for the empty multiset, with $\mathbf{0}(x) = 0$ for all $x \in X$.

We associate several numbers with a multiset.

Definition 1 *For a multiset $\varphi \in \mathcal{M}(X)$, write:*

1. $\|\varphi\| \coloneqq \sum_x \varphi(x)$ *for the size of φ, taking multiplicities into account;*
2. $\varphi\,! \coloneqq \prod_x \varphi(x)!$ *for the multiset factorial;*
3. $(\!(\varphi)\!) \coloneqq \dfrac{\|\varphi\|!}{\varphi\,!}$ *for the multinomial coefficient.*

We are often interested in multisets of a particular size $K \in \mathbb{N}$, so we define a subset:

$$\mathcal{M}[K](X) \coloneqq \{\varphi \in \mathcal{M}(X) \mid \|\varphi\| = K\}.$$

This $\mathcal{M}[K]$ is a functor, but not a monad.

Sequences can be turned into multisets, via 'accumulator' functions $acc\colon X^K \to \mathcal{M}[K](X)$, given by $acc(x_1,\ldots,x_K) \coloneqq 1|x_1\rangle + \cdots + 1|x_K\rangle$. Thus, for instance, $acc(a,a,b,a) = 3|a\rangle + 1|b\rangle$. The multinomial coefficient $(\!(\varphi)\!)$ is used in this paper in the following two ways.

Fact 1 1. *For a multiset φ there are $(\!(\varphi)\!)$ lists that accumulate to φ, that is, $\left|\,acc^{-1}(\varphi)\,\right| = (\!(\varphi)\!)$.*

2. *For real numbers $a_1,\ldots,a_n$, the multinomial theorem says:*

$$\big(a_1 + \cdots + a_n\big)^K = \sum_{\varphi\in\mathcal{M}[K](\{1,\ldots,n\})} (\!(\varphi)\!)\cdot \prod\nolimits_i a_i^{\varphi(i)}. \qquad \square$$

Multisets can be ordered pointwise, giving rise to some subtle distinctions.

Definition 2 *Let $\varphi, \psi \in \mathcal{M}(X)$ be given. We write:*

1. *$\varphi \leq \psi$ if $\varphi(x) \leq \psi(x)$ for all $x \in X$; in that case we define the multiset difference $\psi - \varphi$ via pointwise subtraction, as: $(\psi - \varphi)(x) = \psi(x) - \varphi(x)$;*
2. *$\varphi \leq_K \psi$ if $\|\varphi\| = K$ and $\varphi \leq \psi$;*
3. *$\varphi < \psi$ if $\varphi \leq \psi$ but $\varphi \neq \psi$;*
4. *$\varphi \prec \psi$ if $\varphi(x) < \psi(x)$ for all $x \in X$.*

The relation $\prec$ will be called *fully below*. It is different from $<$, *e.g.* in:

$$2|a\rangle + 3|b\rangle < 3|a\rangle + 3|b\rangle \qquad \text{and} \qquad 2|a\rangle + 2|b\rangle \prec 3|a\rangle + 3|b\rangle.$$

For multisets $\varphi, \psi \in \mathcal{M}(X)$ with $\varphi \leq \psi$, we define the *multiset binomial* as:

$$\begin{aligned}\binom{\psi}{\varphi} \coloneqq \frac{\psi!\!\!!}{\varphi!\!\!! \cdot (\psi - \varphi)!\!\!!} &= \frac{\prod_x \psi(x)!}{\left(\prod_x \varphi(x)!\right) \cdot \left(\prod_x (\psi(x) - \varphi(x))!\right)} \\ &= \prod_{x \in X} \frac{\psi(x)!}{\varphi(x)! \cdot (\psi(x) - \varphi(x))!} \\ &= \prod_{x \in X} \binom{\psi(x)}{\varphi(x)}.\end{aligned} \tag{2}$$

Intuitively, this is the number of ways φ can sit inside ψ.

The next result guarantees that hypergeometric draws form a distribution. It is well known, but not in this form given below, with binomials for multisets.

Proposition 1 *For a multiset $\psi \in \mathcal{M}(X)$ of size $L = \|\psi\|$ and for a number $K \leq L$,*

$$\sum_{\varphi \leq_K \psi} \binom{\psi}{\varphi} = \binom{L}{K}.$$

The binary case, when the set X has two elements, is known as Vandermonde's formula, see (4) below. The above generalisation can be obtained from it by induction on the number of elements in the support of ψ. For completeness, we include the proof. It uses Pascal's rule, which says:

$$\binom{n}{m} + \binom{n}{m+1} = \binom{n+1}{m}. \tag{3}$$

Proof. We use induction on the number of elements in the support $\mathrm{supp}(\psi)$ of the multiset ψ. We go through some initial values explicitly. If the number of elements is 0, then $\psi = \mathbf{0}$ and so $L = 0 = K$ and $\varphi \leq_K \psi$ means $\varphi = \mathbf{0}$, so that the result holds. Similarly, if $\mathrm{supp}(\psi)$ is a singleton, say $\{x\}$, then $L = \psi(x)$. For $K \leq L$ and $\varphi \leq_K \psi$ we get $\mathrm{supp}(\varphi) = \{x\}$ and $K = \varphi(x)$. The result then obviously holds.

The case where $\mathrm{supp}(\psi) = \{x, y\}$ captures the ordinary form of Vandermonde's formula. We reformulate it for numbers $B, G \in \mathbb{N}$ and $K \leq B + G$. Then:

$$\binom{B+G}{K} = \sum_{b \leq B,\, g \leq G,\, b+g=K} \binom{B}{b} \cdot \binom{G}{g}. \tag{4}$$

Intuitively: if you select K children out of B boys and G girls, the number of options is given by the sum over the options for $b \leq B$ boys times the options for $g \leq G$ girls, with $b + g = K$. The equation (4) is standard, so a proof (*e.g.* by induction on G) is skipped.

For the induction step, let $\mathrm{supp}(\psi) = \{x_1, \ldots, x_n, y\}$, for $n \geq 2$. Writing $\ell = \psi(y)$, $L' = L - \ell$ and $\psi' = \psi - \ell|y\rangle \in \mathcal{M}[L'](X)$ gives:

$$\begin{aligned}\sum_{\varphi \leq_K \psi} \binom{\psi}{\varphi} = \sum_{\varphi \leq_K \psi} \prod_x \binom{\psi(x)}{\varphi(x)} &= \sum_{n \leq \ell} \sum_{\varphi \leq_{K-n} \psi'} \binom{\ell}{n} \cdot \prod_i \binom{\psi'(x_i)}{\varphi(x_i)} \\ &\overset{\text{(IH)}}{=} \sum_{n \leq \ell,\, K-n \leq L-\ell} \binom{\ell}{n} \cdot \binom{L-\ell}{K-n} \overset{(4)}{=} \binom{L}{K}. \qquad \square\end{aligned}$$

We recall that for $n > 0$ and $m \geq 0$ there is the *multichoose* coefficient, defined for $n \geq 1$ and $m \geq 0$ as:

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

Interestingly, where $\binom{n}{m}$ is the number of *subsets* of size m of an n-element set, $\left(\!\binom{n}{m}\!\right)$ is the number of *multisets* of size m over an n-element set. It is easy to see that:

$$\left(\!\!\binom{n+1}{m+1}\!\!\right) = \left(\!\!\binom{n+1}{m}\!\!\right) + \left(\!\!\binom{n}{m+1}\!\!\right). \tag{5}$$

We extend multichoose from numbers to multisets, in line with (2):

$$\left(\!\!\binom{\psi}{\varphi}\!\!\right) := \prod_{x \in \mathrm{supp}(\psi)} \left(\!\!\binom{\psi(x)}{\varphi(x)}\!\!\right).$$

There is the following multichoose analogue of Proposition 1.

Proposition 2 *For a multiset $\psi \in \mathcal{M}(X)$ of size $L = \|\psi\| > 0$ and for any number $K \geq 0$,*

$$\sum_{\varphi \in \mathcal{M}[K](\mathrm{supp}(\psi))} \left(\!\!\binom{\psi}{\varphi}\!\!\right) = \left(\!\!\binom{L}{K}\!\!\right).$$

Proof. We start with a double-bracket analogue of (4). Fix $B \geq 1$ and $G \geq 1$. For all K one has:

$$\left(\!\!\binom{B+G}{K}\!\!\right) = \sum_{0 \leq k \leq K} \left(\!\!\binom{B}{k}\!\!\right) \cdot \left(\!\!\binom{G}{K-k}\!\!\right). \tag{6}$$

We first prove this equation by induction on $B \geq 1$. In both the base case $B = 1$ and the induction step we shall use induction on K. We shall try to keep the structure clear by using nested bullets.

- We first prove Equation (6) for $B = 1$, by induction on K.
  - When $K = 0$ both sides in (6) are equal to 1.
  - Assume Equation (6) holds for K (and $B = 1$).

$$\begin{aligned}\sum_{0 \leq k \leq K+1} \left(\!\!\binom{1}{k}\!\!\right) \cdot \left(\!\!\binom{G}{(K+1)-k}\!\!\right) &= \sum_{0 \leq k \leq K+1} \left(\!\!\binom{G}{K-(k-1)}\!\!\right) \\ &= \left(\!\!\binom{G}{K+1}\!\!\right) + \sum_{0 \leq \ell \leq K} \left(\!\!\binom{1}{\ell}\!\!\right) \cdot \left(\!\!\binom{G}{K-\ell}\!\!\right) \\ &\overset{\text{(IH)}}{=} \left(\!\!\binom{G}{K+1}\!\!\right) + \left(\!\!\binom{G+1}{K}\!\!\right) \\ &\overset{(5)}{=} \left(\!\!\binom{G+1}{K+1}\!\!\right).\end{aligned}$$

- Now assume Equation (6) holds for B (for all G, K). In order to show that it then also holds for $B + 1$ we use induction on K.

- When $K = 0$ both sides in (6) are equal to 1.
- Now assume that Equation (6) holds for K, and for B. Then:

$$\begin{aligned}
&\sum_{0\leq k\leq K+1} \left(\!\!\binom{B+1}{k}\!\!\right) \cdot \left(\!\!\binom{G}{(K+1)-k}\!\!\right) \\
&= \left(\!\!\binom{G}{K+1}\!\!\right) + \sum_{0\leq k\leq K} \left(\!\!\binom{B+1}{k+1}\!\!\right) \cdot \left(\!\!\binom{G}{K-k}\!\!\right) \\
&\stackrel{(5)}{=} \left(\!\!\binom{G}{K+1}\!\!\right) + \sum_{0\leq k\leq K} \left[\left(\!\!\binom{B}{k+1}\!\!\right) + \left(\!\!\binom{B+1}{k}\!\!\right) \right] \cdot \left(\!\!\binom{G}{K-k}\!\!\right) \\
&= \left(\!\!\binom{G}{K+1}\!\!\right) + \sum_{0\leq k\leq K} \left(\!\!\binom{B}{k+1}\!\!\right) \cdot \left(\!\!\binom{G}{K-k}\!\!\right) + \sum_{0\leq k\leq K} \left(\!\!\binom{B+1}{k}\!\!\right) \cdot \left(\!\!\binom{G}{K-k}\!\!\right) \\
&\stackrel{(\text{IH},\, K)}{=} \sum_{0\leq k\leq K+1} \left(\!\!\binom{B}{k}\!\!\right) \cdot \left(\!\!\binom{G}{(K+1)-k}\!\!\right) + \left(\!\!\binom{(B+1)+G}{K}\!\!\right) \\
&\stackrel{(\text{IH},\, B)}{=} \left(\!\!\binom{B+G}{K+1}\!\!\right) + \left(\!\!\binom{(B+1)+G}{K}\!\!\right) \\
&\stackrel{(5)}{=} \left(\!\!\binom{(B+1)+G}{K+1}\!\!\right).
\end{aligned}$$

This completes the proof of (6). We proceed with the equation in the proposition, via induction on the number of elements in the support of ψ. By assumption the support cannot be empty, so the induction starts when the support is a singleton, say $\mathrm{supp}(\psi) = \{x\}$. But then $\psi(x) = \|\psi\| = L$ and $\varphi(x) = \|\varphi\| = K$, so the result obviously holds.

Now let $\mathrm{supp}(\psi) = S \cup \{y\}$ where $y \notin S$ and S is not empty. Write:

$$L = \|\psi\| \qquad \ell = \psi(y) > 0 \qquad \psi' = \psi - \ell|y\rangle \qquad L' = L - \ell > 0.$$

By construction $S = \mathrm{supp}(\psi')$ and $L' = \|\psi'\|$. Now:

$$\begin{aligned}
\sum_{\varphi\in\mathcal{M}[K](S\cup\{y\})} \left(\!\!\binom{\psi}{\varphi}\!\!\right) &= \sum_{\varphi\in\mathcal{M}[K](S\cup\{y\})} \prod_{x\in S\cup\{y\}} \left(\!\!\binom{\psi(x)}{\varphi(x)}\!\!\right) \\
&= \sum_{0\leq k\leq K} \sum_{\varphi\in\mathcal{M}[K-k](S)} \left(\!\!\binom{\psi(y)}{k}\!\!\right) \cdot \prod_{x\in S} \left(\!\!\binom{\psi(x)}{\varphi(x)}\!\!\right) \\
&= \sum_{0\leq k\leq K} \left(\!\!\binom{\ell}{k}\!\!\right) \cdot \sum_{\varphi\in\mathcal{M}[K-k](S)} \left(\!\!\binom{\psi'}{\varphi}\!\!\right) \\
&\stackrel{(\text{IH})}{=} \sum_{0\leq k\leq K} \left(\!\!\binom{\ell}{k}\!\!\right) \cdot \left(\!\!\binom{L'}{K-k}\!\!\right) \stackrel{(6)}{=} \left(\!\!\binom{\ell+L'}{K}\!\!\right) = \left(\!\!\binom{L}{K}\!\!\right).
\end{aligned}$$

□

3.2 Probability distributions

In this paper we concentrate on finite, discrete probability distributions. Such a distribution, over a set X, is a finite formal convex combination $\sum_i r_i|x_i\rangle$ with $r_i \in [0,1]$ satisfying $\sum_i r_i = 1$ and with $x_i \in X$. Alternatively, it may be described as a function $\omega\colon X \to [0,1]$ with finite support $\mathrm{supp}(\omega) := \{x \in X \mid \omega(x) > 0\}$ and with $\sum_x \omega(x) = 1$. We shall write $\mathcal{D}(X)$ for the set of distributions on a set X. This $\mathcal{D}$ forms a monad, just like $\mathcal{M}$.

Distributions on a product set $X \times Y$ are often called *joint* distributions. One way to obtains such distributions is to put $\omega \in \mathcal{D}(X)$ and $\rho \in \mathcal{D}(Y)$ in parallel as $\omega \otimes \rho \in \mathcal{D}(X \times Y)$, where:

$$\omega \otimes \rho = \sum_{x\in X, y\in Y} \omega(x) \cdot \rho(y) \,\big|\, x, y \big\rangle.$$

We then write $\omega^K = \omega \otimes \cdots \otimes \omega \in \mathcal{D}(X^K)$, for numbers $K \geq 1$.

Each non-empty multiset can be turned into a distribution, via normalisation. We shall call this operation *frequentist learning*, written as *Flrn*, since it involves learning by counting. Explicitly:

$$Flrn\Big(\sum_i n_i|x_i\rangle\Big) \coloneqq \sum_i \frac{n_i}{n}|x_i\rangle \qquad \text{where} \qquad n = \sum_i n_i.$$

Alternatively, $Flrn(\varphi)(x) = \dfrac{\varphi(x)}{\|\varphi\|}$, or simply, $Flrn(\varphi) = \dfrac{1}{\|\varphi\|} \cdot \varphi$.

Multisets and distributions as defined above have finite support. We shall also need (discrete) distributions with infinite support. Therefore we define, for an arbitrary set X,

$$\mathcal{D}_\infty(X) \coloneqq \{\omega \colon X \to [0,1] \mid \sum_x \omega(x) = 1\}.$$

It can be shown that the support of $\omega \in \mathcal{D}_\infty(X)$ is necessarily countable or finite. In practice one typically encounters $X = \mathbb{N}$. For instance, the Poisson distribution can be described as an element of $\mathcal{D}_\infty(\mathbb{N})$. Later on we shall describe negative distributions that also live in $\mathcal{D}_\infty(\mathbb{N})$.

4 Multinomial, hypergeometric, and Pólya distributions

This section introduces the multinomial, hypergeometric and Pólya distributions, in multivariate form. This is most conveniently done via (binomial / multichoose) coefficients for multisets, which is non-standard. The formulations that are used below can be derived in a compositional manner via iterated drawing of single elements, using a suitable form of Kleisli composition, see [9, 10] for details.

4.1 Multinomial distributions

Since the urn remains unchanged for multinomial draws, it is most appropriate to describe it as a distribution $\omega \in \mathcal{D}(X)$, for a set of colours X. The multinomial distribution $mn[K](\omega)$ is a distribution on draws of size K, and thus an element of the set $\mathcal{D}\big(\mathcal{M}[K](X)\big)$. Explicitly,

$$mn[K](\omega) \coloneqq \sum_{\varphi \in \mathcal{M}[K](X)} (\varphi) \cdot \prod_{x \in X} \omega(x)^{\varphi(x)} \,\big|\varphi\big\rangle. \tag{7}$$

The probabilities in this multinomial distribution add up to one by the Multinomial Theorem, see Fact 1 (2). For instance,

$$\begin{aligned} mn[3]\big(\tfrac{1}{3}|a\rangle + \tfrac{1}{2}|b\rangle + \tfrac{1}{6}|c\rangle\big) \;=\; & \tfrac{1}{27}\Big|3|a\rangle\Big\rangle + \tfrac{1}{6}\Big|2|a\rangle + 1|b\rangle\Big\rangle + \tfrac{1}{4}\Big|1|a\rangle + 2|b\rangle\Big\rangle + \tfrac{1}{8}\Big|3|b\rangle\Big\rangle \\ & + \tfrac{1}{18}\Big|2|a\rangle + 1|c\rangle\Big\rangle + \tfrac{1}{6}\Big|1|a\rangle + 1|b\rangle + 1|c\rangle\Big\rangle + \tfrac{1}{8}\Big|2|b\rangle + 1|c\rangle\Big\rangle \\ & + \tfrac{1}{36}\Big|1|a\rangle + 2|c\rangle\Big\rangle + \tfrac{1}{24}\Big|1|b\rangle + 2|c\rangle\Big\rangle + \tfrac{1}{216}\Big|3|c\rangle\Big\rangle \end{aligned}$$

Notice that the right-hand-side is a distribution over multisets. The multisets are written inside the 'big' kets $\Big| - \Big\rangle$ using 'small' ket $| - \rangle$ for the individual colours a, b, c. The probabilities of these multisets, as draws, are written before the big kets. This may require some parsing if you see this notation style for the first time.

The next result expresses multinomial probabilities in terms of sequences (of drawn balls).

Lemma 3 *For $\omega \in \mathcal{D}(X)$ and $\varphi \in \mathcal{M}[K](X)$ one has:*

$$mn[K](\omega)(\varphi) = \sum_{\vec{x} \in acc^{-1}(\varphi)} \omega^K(\vec{x}) = \sum_{\vec{x} \in acc^{-1}(\varphi)} \prod_i \omega(x_i). \qquad \square$$

The bivariate (or binary) form of these multinomial distributions involves a map $\mathcal{D}(2) \to \mathcal{D}\big(\mathcal{M}[K](2)\big)$, where $2 = \{0,1\}$. Via the isomorphisms $\mathcal{D}(2) \cong [0,1]$ and $\mathcal{M}[K](2) \cong \{0,1,2,\ldots,K\}$ this map is often described as a *binomial* $bn[K]\colon [0,1] \to \mathcal{D}\big(\{0,1,\ldots,K\}\big)$, given on $r \in [0,1]$ as:

$$\begin{aligned} bn[K](r) &\coloneqq \sum_{0\leq k\leq K} \binom{K}{k} \cdot r^k \cdot (1-r)^{K-k}\,\big|\,k\,\big\rangle \\ &= \sum_{0\leq k\leq K} mn[K]\Big(r|0\rangle + (1-r)|1\rangle\Big)\Big(k|0\rangle + (K-k)|1\rangle\Big)\,\big|\,k\,\big\rangle \end{aligned} \tag{8}$$

4.2 Hypergeometric distributions

Proposition 1 guarantees that the probabilities add up to one in the following multivariate definition of the hypergeometric distribution, again on multisets of size K. It assumes an urn υ of size $L = \|\upsilon\| \geq K$.

$$hg[K](\upsilon) \coloneqq \sum_{\varphi\leq_K \upsilon} \frac{\binom{\upsilon}{\varphi}}{\binom{L}{K}}\,\big|\,\varphi\,\big\rangle. \tag{9}$$

For instance,

$$hg[3]\big(4|a\rangle + 6|b\rangle\big) = \tfrac{1}{30}\Big|3|a\rangle\Big\rangle + \tfrac{3}{10}\Big|2|a\rangle + 1|b\rangle\Big\rangle + \tfrac{1}{2}\Big|1|a\rangle + 2|b\rangle\Big\rangle + \tfrac{1}{6}\Big|3|b\rangle\Big\rangle.$$

Lemma 4 *For an urn $u \in \mathcal{M}(X)$ and a draw $\varphi \leq_K \upsilon$,*

$$hg[K](\upsilon)(\varphi) = \sum_{\vec{x}\in acc^{-1}(\varphi)} \prod_{0\leq i<K} Flrn\Big(\upsilon - acc(x_1,\ldots,x_i)\Big)(x_{i+1}). \qquad \square$$

4.3 Pólya distributions

The Pólya distribution can be described in a similar way, using the multichoose binomial coefficients. It yields a distribution on multisets of size K, for a non-empty urn υ, via:

$$pl[K](\upsilon) \coloneqq \sum_{\varphi\in\mathcal{M}[K](\mathrm{supp}(\upsilon))} \frac{\left(\!\binom{\upsilon}{\varphi}\!\right)}{\left(\!\binom{L}{K}\!\right)}\,\big|\,\varphi\,\big\rangle. \tag{10}$$

This is well-defined by Proposition 2. A subtle point is that the draws φ must be restricted to elements that occur in the urn υ. That's achieved by summing over $\varphi \in \mathcal{M}[K](\mathrm{supp}(\upsilon))$, so that $\mathrm{supp}(\varphi) \subseteq \mathrm{supp}(\upsilon)$.

The Pólya distribution is known [19], sometimes as Dirichlet-multinomial. Its formulation in terms of multichoose multinomial coefficients of multisets (10), in analogy with the multinomial coefficients of multisets in the hypergeometric distribution (9), seems new. Formulation that come close are [26, Eqn. (A.1)] or [15, Eqn. (40.7)]. The details that this captures the Pólya urn — where a drawn ball is returned together with an additional copy of the same colour — are elaborated in [10].

Here is an example of a Pólya distribution, for the same urn as above, in the hypergeometric illustration.

$$pl[3]\big(4|a\rangle + 6|b\rangle\big) = \tfrac{1}{11}\Big|3|a\rangle\Big\rangle + \tfrac{3}{11}\Big|2|a\rangle + 1|b\rangle\Big\rangle + \tfrac{21}{55}\Big|1|a\rangle + 2|b\rangle\Big\rangle + \tfrac{14}{55}\Big|3|b\rangle\Big\rangle.$$

Lemma 5 *For an urn $\upsilon \in \mathcal{M}(X)$ and a draw $\varphi \in \mathcal{M}[K](X)$ with* $\mathrm{supp}(\varphi) \subseteq \mathrm{supp}(\upsilon)$,

$$pl[K](\upsilon)(\varphi) = \sum_{\vec{x}\in acc^{-1}(\varphi)} \prod_{0\leq i<K} Flrn\Big(\upsilon + acc(x_1,\ldots,x_i)\Big)(x_{i+1}). \qquad \square$$

5 First-full definitions

From the illustrations in Section 2 we can extract the general formulations for the first-full probabilities. They use the fully-below relation $\prec$ between multisets from Definition 2, given by $\varphi \prec \psi$ iff $\varphi(x) < \psi(x)$ for all x. At this stage we only give the probabilities pointwise. Proving that they add up to one, and thus form a probability distribution, is achieved later, in Theorems 7, 9 and 11.

We write $\mathbf{1} = \sum_{x\in X} 1|x\rangle$ for the multiset of singletons on a finite set X of colours. The tubes in our urns & tubes setting are represented as a multiset $\tau \in \mathcal{M}(X)$. We require $\tau \geq \mathbf{1}$, so that each tube has at least length 1. Empty tubes are irrelevant and can be ignored.

The definitions below involve draws $\varphi \prec \tau$, so that none of the tubes is full yet. For colour x we take those draws φ with $\varphi(x) = \tau(x) - 1$, so that only one ball is missing in tube x. The probability of this last ball is included in the three formulations below, resp. as $\omega(x)$, as $\mathit{Flrn}(\psi - \varphi)(x)$ and as $\mathit{Flrn}(\psi + \varphi)(x)$.

Definition 3 *Let X be a finite set of colours with a multiset of tubes $\tau \geq \mathbf{1}$ over X, and let $x \in X$ be an arbitrary element.*

1. *Let $\omega \in \mathcal{D}(X)$ be a distribution with full support. The* multinomial first-full *probabilities are given via the function $\mathit{mnff}(\omega, \tau) \colon X \to [0, 1]$ determined by:*

$$\mathit{mnff}(\omega, \tau)(x) \coloneqq \sum_{\substack{\varphi \prec \tau, \\ \varphi(x) = \tau(x) - 1}} \mathit{mn}(\omega)(\varphi) \cdot \omega(x).$$

2. *Let $\upsilon \in \mathcal{M}(X)$ be an urn / multiset with $\upsilon \geq \tau$. The* hypergeometric first-full *probabilities $\mathit{hgff}(\upsilon, \tau) \colon X \to [0, 1]$ are defined as:*

$$\mathit{hgff}(\upsilon, \tau)(x) \coloneqq \sum_{\substack{\varphi \prec \tau, \\ \varphi(x) = \tau(x) - 1}} \mathit{hg}(\upsilon)(\varphi) \cdot \mathit{Flrn}(\upsilon - \varphi)(x).$$

3. *Let $\upsilon \in \mathcal{M}(X)$ be an urn with $\upsilon \geq \mathbf{1}$. The* Pólya first-full *probabilities $\mathit{plff}(\upsilon, \tau) \colon X \to [0, 1]$ are:*

$$\mathit{plff}(\upsilon, \tau)(x) \coloneqq \sum_{\substack{\varphi \prec \tau, \\ \varphi(x) = \tau(x) - 1}} \mathit{pl}(\upsilon)(\varphi) \cdot \mathit{Flrn}(\upsilon + \varphi)(x).$$

Earlier we have written multinomial, hypergeometric and Pólya distributions as $\mathit{mn}[K]$, $\mathit{hg}[K]$ and $\mathit{pl}[K]$, with explicit parameter $K \in \mathbb{N}$ for the size of the draw. For convenience we have omitted this K in the above formulations. It may be added as $K = \|\varphi\|$, but that makes the notation unnecessarily heavy.

In the above definition we require full support of the urn/distribution ω, for convenience. We could have been more relaxed and required only $\mathrm{supp}(\omega) \subseteq \mathrm{supp}(\tau)$ and $\mathrm{supp}(\upsilon) \subseteq \mathrm{supp}(\tau)$. When these are proper inclusions, there are tubes that will never receive any balls. Then we might as well exclude them altogether.

Figure 1 presents illustrations of these different first-full probabilities, for two different multisets of tubes, at the top of the second and third column. In the second column the three tubes have the same length; the corresponding first-full plots then resemble the urns. In the third column the tubes differ; the highest first-full probabilities are determined not only by the lowest tubes, but also by the highest numbers in the urns. The bar plots are based on distributions that are computed via the formulations in Definition 3.

5.1 The problem of points

We briefly elaborate the connection between (multinomial) first-full distributions and the ancient problem of points, as discussed in the introduction. We do so via an example in [18], with two players, called A and B, playing a game that ends when one of the players has won 4 times. The winner then gets 64 coins. Each time, the probability of winning for A is $\frac{6}{10}$ and is $\frac{4}{10}$ for B.

Figure 1: First-full distributions on space of colours $\{a, b, c\}$ arising from the two tube configurations in the top row, and from the three urns in the left column. The inner distributions are the results, for the multinomial, hypergeometric and Pólya modes.

A particular game is terminated abruptly at a stage where A has won $a < 4$ times and B has won $b < 4$ times. The question that has occupied Fermat and Pascal is how to fairly divide the stake of 64 coins at such an unfinished stage. Their solution is to look at the chances of A and B to win, if they were to continue from where the game was terminated. One then looks at the number of times $4 - a$ and $4 - b$ that A and B still need to win. This can be reformulated in terms of tubes to be filled.

Thus, the distribution capturing the chances for A and B to still win in this (aborted) situation of the game — if the game would be continued — is a multinomial first-full:

$$\rho(a, b) := \mathit{mnff}\big(\tfrac{6}{10}|A\rangle + \tfrac{4}{10}|B\rangle,\ (4-a)|A\rangle + (4-b)|B\rangle\big). \tag{11}$$

For instance, $\rho(1, 2) = \frac{297}{625}|A\rangle + \frac{328}{625}|B\rangle$. The division of stakes from the problem of points can now be formulated in terms of such first-full distributions. Figure 3 in [18], reconstructed here in Figure 2, contains, for $a = 1$ and $b = 2$, as fair share for A:

$$\rho(1, 2)(A) \cdot 64 = \tfrac{297}{625} \cdot 64 \approx 30.4128 \quad \text{coins.}$$

In this way all numbers in Figure 3 of [18] can be reconstructed, for all numbers $0 \le a < 4$ and $0 \le b < 4$, see Figure 3.

#points remaining for B	#points already won by B						
0	4	0	0	0	0		
1	3	8.2944	13.824	23.04	38.4	64	
2	2	21.56544	30.4128	41.472	53.76	64	
3	1	34.83648	43.68384	52.5312	59.904	64	
4	0	45.453312	52.5312	58.42944	62.3616	64	
		0	1	2	3	4	#points already won by A
		4	3	2	1	0	#points remaining for A

Figure 2: The stakes for player A in the problem of points illustration copied from [18], see Subsection 5.1.

b					
3	$\frac{5184}{625}\lvert A\rangle + \frac{34816}{625}\lvert B\rangle = 8.2944\lvert A\rangle + 55.7056\lvert B\rangle$	$\frac{1728}{125}\lvert A\rangle + \frac{6272}{125}\lvert B\rangle = 13.824\lvert A\rangle + 50.176\lvert B\rangle$	$\frac{576}{25}\lvert A\rangle + \frac{1024}{25}\lvert B\rangle = 23.04\lvert A\rangle + 40.96\lvert B\rangle$	$\frac{192}{5}\lvert A\rangle + \frac{128}{5}\lvert B\rangle = 38.4\lvert A\rangle + 25.6\lvert B\rangle$	
2	$\frac{67392}{3125}\lvert A\rangle + \frac{132608}{3125}\lvert B\rangle = 21.56544\lvert A\rangle + 42.43456\lvert B\rangle$	$\frac{19008}{625}\lvert A\rangle + \frac{20992}{625}\lvert B\rangle = 30.4128\lvert A\rangle + 33.5872\lvert B\rangle$	$\frac{5184}{125}\lvert A\rangle + \frac{2816}{125}\lvert B\rangle = 41.472\lvert A\rangle + 22.528\lvert B\rangle$	$\frac{1344}{25}\lvert A\rangle + \frac{256}{25}\lvert B\rangle = 53.76\lvert A\rangle + 10.24\lvert B\rangle$	
1	$\frac{108864}{3125}\lvert A\rangle + \frac{91136}{3125}\lvert B\rangle = 34.83648\lvert A\rangle + 29.16352\lvert B\rangle$	$\frac{136512}{3125}\lvert A\rangle + \frac{63488}{3125}\lvert B\rangle = 43.68384\lvert A\rangle + 20.31616\lvert B\rangle$	$\frac{32832}{625}\lvert A\rangle + \frac{7168}{625}\lvert B\rangle = 52.5312\lvert A\rangle + 11.4688\lvert B\rangle$	$\frac{7488}{125}\lvert A\rangle + \frac{512}{125}\lvert B\rangle = 59.904\lvert A\rangle + 4.096\lvert B\rangle$	
0	$\frac{710208}{15625}\lvert A\rangle + \frac{289792}{15625}\lvert B\rangle = 45.453312\lvert A\rangle + 18.546688\lvert B\rangle$	$\frac{32832}{625}\lvert A\rangle + \frac{7168}{625}\lvert B\rangle = 52.5312\lvert A\rangle + 11.4688\lvert B\rangle$	$\frac{182592}{3125}\lvert A\rangle + \frac{17408}{3125}\lvert B\rangle = 58.42944\lvert A\rangle + 5.57056\lvert B\rangle$	$\frac{38976}{625}\lvert A\rangle + \frac{1024}{625}\lvert B\rangle = 62.3616\lvert A\rangle + 1.6384\lvert B\rangle$	
	0	1	2	3	a

Figure 3: The stakes for both players A and B in the problem of points illustration from [18], reconstructed as $64 \cdot \rho(a, b)$ via first-full multinomials (11), where $a = \#$points already won by A and $b = \#$points already won by B. This table corresponds to the numbers in the central 4×4 part of Figure 2.

Fermat and Pascal solved the problem of points in binary form, for two players. Our multivariate formulation of the first-full multinomial distribution in Definition 3 (1) can be used when there are multiple (finitely many) players.

6 First-full yields distributions

Our goal in this section is to prove that the probabilities in the three pointwise first-full formulations in Definition 3 all add up to one, and thus form proper probability distributions. The trick is to use the multiset of tubes as a position in a probabilistic automaton that changes with every draw-and-drop action. The automaton precisely records the relevant probabilities and terminates after a finite number of iterations, with a first-full distribution on colours as result. This works because in each composition step distributions are preserved. Hence, if we start with a distribution, we will also end up with a distribution, namely a first-full one.

We use Markov models with output (MOOs) as probabilistic automata. They can be described as functions (coalgebras) of the form:

$$Y \xrightarrow{c} \mathcal{D}(Y + X) \tag{12}$$

where Y is a set of positions and X is a set of outputs. The $+$ is a coproduct (disjoint union).

We will not use separate 'coprojection' functions for these coproducts; the types of the elements will make it clear whether they live in the left or right component of a coproduct $Y + X$. What's important is that a function c as above can be composed with itself, giving the required iterations (or transitions) of the automaton: with a successor position in Y the automaton can continue, and with an output in X, the automaton halts.

A compositional argument underlying the next iterations (13) of an automaton (12) is provided in the appendix. At this stage we use such iterations $c^n : Y \to \mathcal{D}(Y+X)$, for $n \in \mathbb{N}$, via the concrete formulations given below, where $y \in Y$ is a start position.

$$\begin{aligned} c^0(y) &\coloneqq 1\big|y\big\rangle \\ c^{n+1}(y) &\coloneqq \sum_{z\in Y+X} \Big(\textstyle\sum_{y'\in Y} c(y)(y')\cdot c^n(y')(z)\Big)\,\big|z\big\rangle \;+\; \displaystyle\sum_{x\in X} c(y)(x)\big|x\big\rangle. \end{aligned} \tag{13}$$

The first sum defines the transitions and the second sum the outputs. Notice that these are defined as proper distributions. Hence via iterated composition only distributions arise. This fact will be crucial.

In the next three subsections we define three appropriate Markov models with output (12) with transitions that incorporate the first-full steps.

6.1 Multinomial first-full distributions

In multinomial mode an urn is represented as a distribution $\omega \in \mathcal{D}(X)$, with full support. We shall write as set of tubes:

$$\mathcal{M}_{\geq 1}(X) \coloneqq \{\tau \in \mathcal{M}(X) \mid \tau \geq \mathbf{1}\} \qquad \text{where} \qquad \mathbf{1} = \sum_{x\in X} 1|x\rangle.$$

Associated with urn/distribution ω we define the following multinomial Markov model with output $MN(\omega)$, with tubes in $\mathcal{M}_{\geq 1}(X)$ as positions.

$$\begin{array}{ccc} \mathcal{M}_{\geq 1}(X) & \xrightarrow{\quad MN(\omega)\quad} & \mathcal{D}\Big(\mathcal{M}_{\geq 1}(X) + X\Big) \\ \tau & \longmapsto & \displaystyle\sum_{x,\,\tau(x)>1} \omega(x)\big|\tau-1|x\rangle\big\rangle \;+\; \sum_{x,\,\tau(x)=1} \omega(x)\big|x\big\rangle. \end{array}$$

The aim is to iterate this Markov model with output $MN(\omega)$, using composition for such models, as described in (13). We illustrate the resulting dynamics by redoing Example 1, with state $\omega = \frac{1}{3}|a\rangle + \frac{2}{3}|b\rangle$ and tubes $\tau = 2|a\rangle + 3|b\rangle$. Then:

$$\begin{aligned} MN(\omega)(\tau) &= \tfrac{1}{3}\Big|1|a\rangle + 3|b\rangle\Big\rangle + \tfrac{2}{3}\Big|2|a\rangle + 2|b\rangle\Big\rangle \\ MN(\omega)^2(\tau) &= \tfrac{1}{3}\cdot\tfrac{1}{3}\big|a\big\rangle + \tfrac{1}{3}\cdot\tfrac{2}{3}\Big|1|a\rangle + 2|b\rangle\Big\rangle + \tfrac{2}{3}\cdot\tfrac{1}{3}\Big|1|a\rangle + 2|b\rangle\Big\rangle + \tfrac{2}{3}\cdot\tfrac{2}{3}\Big|2|a\rangle + 1|b\rangle\Big\rangle \\ &= \tfrac{1}{9}\big|a\big\rangle + \tfrac{4}{9}\Big|1|a\rangle + 2|b\rangle\Big\rangle + \tfrac{4}{9}\Big|2|a\rangle + 1|b\rangle\Big\rangle \\ MN(\omega)^3(\tau) &= \tfrac{1}{9}\big|a\big\rangle + \tfrac{4}{9}\cdot\tfrac{1}{3}\big|a\big\rangle + \tfrac{4}{9}\cdot\tfrac{2}{3}\Big|1|a\rangle + 1|b\rangle\Big\rangle + \tfrac{4}{9}\cdot\tfrac{1}{3}\Big|1|a\rangle + 1|b\rangle\Big\rangle + \tfrac{4}{9}\cdot\tfrac{2}{3}\big|b\big\rangle \\ &= \tfrac{7}{27}\big|a\big\rangle + \tfrac{12}{27}\Big|1|a\rangle + 1|b\rangle\Big\rangle + \tfrac{8}{27}\big|b\big\rangle \\ MN(\omega)^4(\tau) &= \tfrac{7}{27}\big|a\big\rangle + \tfrac{12}{27}\cdot\tfrac{1}{3}\big|a\big\rangle + \tfrac{12}{27}\cdot\tfrac{2}{3}\big|b\big\rangle + \tfrac{8}{27}\big|b\big\rangle \\ &= \tfrac{11}{27}\big|a\big\rangle + \tfrac{16}{27}\big|b\big\rangle. \end{aligned}$$

This is precisely the outcome that we obtained in Example 1 by manually checking all options.

We formulate at a more general level what's happening via iteration.

Lemma 6 *Consider the above Markov model with output $MN(\omega)$ for a distribution $\omega \in \mathcal{D}(X)$.*

1. *For a multiset $\varphi \in \mathcal{M}_{\geq 1}(X)$,*

$$\begin{aligned} MN(\omega)^n(\tau)(\varphi) &= \sum \Big\{ \omega^n(\ell) \,\Big|\, \ell = \langle x_1, \ldots, x_n\rangle \in X^n \text{ with } \varphi = \tau - 1|x_1\rangle - \cdots - 1|x_n\rangle \Big\} \\ &= \sum \Big\{ mn[n](\omega)(\chi) \,\Big|\, \chi \leq \tau - \mathbf{1} \text{ with } \|\chi\| = n \text{ and } \varphi = \tau - \chi \Big\}. \end{aligned}$$

2. *For an element $x \in X$,*

$$\begin{aligned} MN(\omega)^{n+1}(\tau)(x) = \sum \Big\{ mn[K](\omega)(\chi) \cdot \omega(x) \,\Big|\, & K \leq n \text{ and } \chi \leq \tau - \mathbf{1} \\ & \text{with } \|\chi\| = K \text{ and } (\tau - \chi)(x) = 1 \Big\}. \end{aligned}$$

Proof. 1. We first prove the first equation, by induction on n. The case $n = 0$ is trivial since we have on the left-hand-side $MN(\omega)^0(\tau) = 1|\tau\rangle$, and on the right-hand-side a sum over the empty sequence $\ell = \langle\rangle$ for which by definition $\omega^0(\ell) = 1$. Next,

$$\begin{aligned} MN(\omega)^{n+1}(\tau)(\varphi) &= \sum_{x \in X} \omega(x) \cdot MN(\omega)^n(\tau - 1|x\rangle))(\varphi) \\ &\overset{\text{(IH)}}{=} \sum_{x \in X} \omega(x) \cdot \sum \Big\{ \omega^n(\ell) \,\Big|\, \ell = \langle x_1, \ldots, x_n\rangle \in X^n \\ &\qquad\qquad \text{with } \varphi = \tau - 1|x\rangle - 1|x_1\rangle - \cdots - 1|x_n\rangle \Big\} \\ &= \sum \Big\{ \omega^{n+1}(\ell) \,\Big|\, \ell = \langle x_1, \ldots, x_n, x_{n+1}\rangle \in X^{n+1} \\ &\qquad\qquad \text{with } \varphi = \tau - 1|x_1\rangle - \cdots - 1|x_n\rangle - 1|x_{n+1}\rangle \Big\}. \end{aligned}$$

The second equation in point (1) follows from Lemma 3.

2. Using the previous point:

$$\begin{aligned} MN(\omega)^{n+1}(\tau)(x) &= \sum \Big\{ MN(\omega)^K(\tau)(\varphi) \cdot MN(\omega)(\varphi)(x) \,\Big|\, K \leq n \text{ and } \varphi \in \mathcal{M}_{\geq 1}(X) \Big\} \\ &= \sum \Big\{ MN(\omega)^K(\tau)(\varphi) \cdot \omega(x) \,\Big|\, K \leq n,\, \varphi \in \mathcal{M}_{\geq 1}(X) \text{ with } \varphi(x) = 1 \Big\} \\ &= \sum \Big\{ mn[K](\omega)(\chi) \cdot \omega(x) \,\Big|\, K \leq n \text{ and } \chi \leq \tau - \mathbf{1} \\ &\qquad\qquad \text{with } \|\chi\| = K \text{ and } (\tau - \chi)(x) = 1 \Big\}. \end{aligned}$$ □

We now show that after suitably many iterations of the Markov model with output $MN(\omega)$ a multinomial first-full distribution remains, see Definition 3.

Theorem 7 *Let set X have N elements and let tubes $\tau \in \mathcal{M}_{\geq 1}(X)$ have size (combined length) $L = \|\tau\| \geq N$. For $\omega \in \mathcal{D}(X)$ one has:*

$$\mathrm{supp}\Big(MN(\omega)^{L-N+1}(\tau)\Big) \subseteq X, \qquad \textit{and then} \qquad MN(\omega)^{L-N+1}(\tau) = \mathit{mnff}(\omega, \tau).$$

In particular, this shows that multinomial first-full $\mathit{mnff}(\omega, \tau)$ is a probability distribution, with probabilities adding up to one.

Proof. Since $\tau \geq \mathbf{1}$, we have $L = \|\tau\| \geq \|\mathbf{1}\| = N$. With each transition of the Markov model $MN(\omega)$, say going from multiset φ to φ', one has $\|\varphi'\| = \|\varphi\| - 1$. Hence after $L - N$ steps, starting from τ, at most a multiset of singletons remains. It transitions to single elements in one step. Hence after at most $L - N + 1$ steps, $MN(\omega)(\tau)$ stabilises as distribution over elements $x \in X$, in the X-component of $\mathcal{M}_{\geq 1}(X) + X$. By Lemma 6 (2) we then get:

$$\begin{aligned} MN(\omega)^{L-N+1}(\tau)(x) &= \sum \Big\{ mn[K](\omega)(\chi) \cdot \omega(x) \,\Big|\, K \leq L - N \text{ and } \chi \in \mathcal{M}[K](X) \\ &\qquad\qquad \text{with } \chi \leq \tau - \mathbf{1} \text{ and } (\tau - \chi)(x) = 1 \Big\} \\ &= \sum \Big\{ mn(\omega)(\chi) \cdot \omega(x) \,\Big|\, \chi \prec \tau \text{ with } \chi(x) = \tau(x) - 1 \Big\} \\ &= \mathit{mnff}(\omega, \tau)(x), \qquad \text{see Definition 3 (1).} \end{aligned}$$

We use that $\chi \leq \tau - \mathbf{1}$ iff $\chi \prec \tau$, where, recall, $\prec$ is the fully-below order. □

6.2 Hypergeometric first-full distributions

Recall that for a hypergeometric first-full distribution we use an urn as a multiset υ, from which each drawn ball is actually removed, and then dropped in the right tube. Thus, the probability of drawing a particularly coloured ball changes throughout the filling of the tubes. Hence, if we wish to turn the situation into a Markov model with output, we have to carry the urn along. This leads to the following set-up.

Let's use the *ad-hoc* notation:

$$\mathcal{M}_{\geq\geq 1}(X) \coloneqq \{(\upsilon, \tau) \in \mathcal{M}(X) \times \mathcal{M}(X) \mid \upsilon \geq \tau \geq \mathbf{1}\}.$$

It is the set of positions in the following hypergeometric MMO.

$$\begin{array}{rcl} \mathcal{M}_{\geq\geq 1}(X) & \xrightarrow{\qquad\qquad HG \qquad\qquad} & \mathcal{D}\Big(\mathcal{M}_{\geq\geq 1}(X) + X\Big) \\ (\upsilon,\tau) & \longmapsto & \displaystyle\sum_{x,\,\tau(x)>1} Flrn(\upsilon)(x)\Big|\,\upsilon - 1|x\rangle,\ \tau - 1|x\rangle\,\Big\rangle + \sum_{x,\,\tau(x)=1} Flrn(\upsilon)(x)\big|\,x\,\big\rangle. \end{array}$$

We now redo Example 2, with urn $\upsilon = 3|a\rangle + 6|b\rangle$ and tubes $\tau = 2|a\rangle + 3|b\rangle$. Then:

$$\begin{array}{rcl} HG(\upsilon,\tau) & = & \frac{3}{9}\Big|2|a\rangle + 6|b\rangle, 1|a\rangle + 3|b\rangle\Big\rangle + \frac{6}{9}\Big|3|a\rangle + 5|b\rangle, 2|a\rangle + 2|b\rangle\Big\rangle \\ HG^2(\upsilon,\tau) & = & \frac{1}{3}\cdot\frac{2}{8}\big|a\big\rangle + \frac{1}{3}\cdot\frac{6}{8}\Big|2|a\rangle + 5|b\rangle, 1|a\rangle + 2|b\rangle\Big\rangle \\ & & \quad + \frac{2}{3}\cdot\frac{3}{8}\Big|2|a\rangle + 5|b\rangle, 1|a\rangle + 2|b\rangle\Big\rangle + \frac{2}{3}\cdot\frac{5}{8}\Big|3|a\rangle + 4|b\rangle, 2|a\rangle + 1|b\rangle\Big\rangle \\ HG^3(\upsilon,\tau) & = & \frac{1}{12}\big|a\big\rangle + \frac{1}{2}\cdot\frac{2}{7}\big|a\big\rangle + \frac{1}{2}\cdot\frac{5}{7}\Big|2|a\rangle + 4|b\rangle, 1|a\rangle + 1|b\rangle\Big\rangle \\ & & \quad + \frac{5}{12}\cdot\frac{3}{7}\Big|2|a\rangle + 4|b\rangle, 1|a\rangle + 1|b\rangle\Big\rangle + \frac{5}{12}\cdot\frac{4}{7}\big|b\big\rangle \\ HG^4(\upsilon,\tau) & = & \frac{19}{84}\big|a\big\rangle + \frac{15}{28}\cdot\frac{2}{6}\big|a\big\rangle + \frac{15}{28}\cdot\frac{4}{6}\big|b\big\rangle + \frac{5}{21}\big|b\big\rangle \\ & = & \frac{17}{42}\big|a\big\rangle + \frac{25}{42}\big|b\big\rangle. \end{array}$$

The next lemma makes explicit what's going on.

Lemma 8 *Let $\upsilon, \tau \in \mathcal{M}(X)$ be multisets with $\upsilon \geq \tau \geq \mathbf{1}$.*

1. *For $\upsilon', \tau' \in \mathcal{M}(X)$ with $\upsilon' \geq \tau' \geq \mathbf{1}$,*

$$\begin{array}{rl} HG^n(\upsilon,\tau)(\upsilon',\tau') & = \sum\Big\{\displaystyle\prod_{0\leq i<n} Flrn\Big(\upsilon - acc(x_1,\ldots,x_i)\Big)(x_{i+1})\,\Big|\,\ell = \langle x_1,\ldots,x_n\rangle \in X^n \\ & \qquad\qquad \text{with } \upsilon' = \upsilon - acc(\ell) \text{ and } \tau' = \tau - acc(\ell)\Big\} \\ & = \sum\Big\{hg[n](\upsilon)(\chi)\,\Big|\,\chi \leq \tau - \mathbf{1} \text{ with } \|\chi\| = n,\ \upsilon' = \upsilon - \chi,\ \tau' = \tau - \chi\Big\}. \end{array}$$

2. *For an element $x \in X$,*

$$\begin{array}{rl} HG^{n+1}(\upsilon,\tau)(x) = \sum\Big\{hg[K](\upsilon)(\chi)\cdot Flrn(\upsilon - \chi)(x)\,\Big|\, & K \leq n \text{ and } \chi \leq \tau - \mathbf{1} \\ & \text{with } \|\chi\| = K \text{ and } (\tau - \chi)(x) = 1\Big\}. \end{array}$$

Proof. 1. We first prove the first equation by induction on n. The case $n = 0$ is trivial, so we proceed with the induction step:

$$\begin{array}{l} HG^{n+1}(\upsilon,\tau)(\upsilon',\tau') \\ = \displaystyle\sum_{x\in X} Flrn(\upsilon)(x)\cdot HG^n(\upsilon - 1|x\rangle, \tau - 1|x\rangle)(\upsilon',\tau') \end{array} \tag{14}$$

$$
\begin{aligned}
&\overset{\text{(IH)}}{=} \sum_{x\in X} \mathit{Flrn}(\upsilon)(x)\cdot \sum \Big\{ \prod_{0\le i<n} \mathit{Flrn}\Big(\upsilon - 1|x\rangle - \mathit{acc}(x_1,\ldots,x_i)\Big)(x_{i+1}) \;\Big|\; \\
&\qquad\qquad \ell = \langle x_1,\ldots,x_n\rangle \in X^n \text{ with } \upsilon' = \upsilon - 1|x\rangle - \mathit{acc}(\ell) \\
&\qquad\qquad \text{and } \tau' = \tau - 1|x\rangle - \mathit{acc}(\ell) \Big\} \\
&= \sum \Big\{ \prod_{0\le i<n+1} \mathit{Flrn}\Big(\upsilon - \mathit{acc}(x_1,\ldots,x_i))(x_{i+1})\Big) \;\Big|\; \\
&\qquad\qquad \ell = \langle x_1,\ldots,x_n,x_{n+1}\rangle \in X^{n+1} \text{ with } \upsilon' = \upsilon - \mathit{acc}(\ell) \\
&\qquad\qquad \text{and } \tau' = \tau - \mathit{acc}(\ell) \Big\}.
\end{aligned}
$$

The second equation follows from Lemma 4.

2. Via the previous point:

$$
\begin{aligned}
\mathit{HG}^{n+1}(\upsilon,\tau)(x) &= \sum \Big\{ \mathit{HG}^K(\upsilon,\tau)(\upsilon',\tau')\cdot \mathit{HG}(\upsilon',\tau')(x) \;\Big|\; K \le n \text{ and } \tau'(x)=1 \Big\} \\
&= \sum \Big\{ \mathit{hg}[K](\upsilon)(\chi)\cdot \mathit{Flrn}(\upsilon')(x) \;\Big|\; K\le n,\ \|\chi\| = K, \tau'(x) = 1, \\
&\qquad\qquad \chi \le \tau - \mathbf{1} \text{ and } \upsilon' = \upsilon - \chi \text{ and } \tau' = \tau - \chi \Big\} \\
&= \sum \Big\{ \mathit{hg}[K](\upsilon)(\chi)\cdot \mathit{Flrn}(\upsilon - \chi)(x) \;\Big|\; K \le n \text{ and } \chi \le \tau - \mathbf{1} \\
&\qquad\qquad \text{with } \|\chi\| = K \text{ and } (\tau-\chi)(x) = 1 \Big\}.
\end{aligned}
$$

□

We now obtain that the hypergeometric first-full probabilities form a distribution, in the same way as in Theorem 7 for the multinomial mode.

Theorem 9 *Let set X have N elements and let tubes $\tau \in \mathcal{M}_{\ge 1}(X)$ have size $L = \|\tau\|$. For urn $\upsilon \ge \tau$ one has:*

$$
\mathrm{supp}\Big(\mathit{HG}^{L-N+1}(\upsilon,\tau)\Big) \subseteq X \qquad \text{and} \qquad \mathit{HG}^{L-N+1}(\upsilon,\tau) = \mathit{hgff}(\upsilon,\tau).
$$

As a result, hypergeometric first-full $\mathit{hgff}(\upsilon,\tau)$ is a probability distribution. □

6.3 Pólya first-full distributions

The Pólya first-full mode is very similar to the hypergeometric first-full mode, except that the drawn ball is not removed from the urn ("-1"), but it is returned together with another ball of the same colour ("+1"). In this case the urn is a multiset υ with as only requirement $\upsilon \ge \mathbf{1}$ so that at least one ball of each colour is present. We thus use a Pólya MMO of the following form.

$$
\begin{array}{ccc}
\mathcal{M}_{\ge 1}(X)\times\mathcal{M}_{\ge 1}(X) & \xrightarrow{\quad PL \quad} & \mathcal{D}\Big(\mathcal{M}_{\ge 1}(X)\times\mathcal{M}_{\ge 1}(X) + X\Big) \\
(\upsilon,\tau) & \longmapsto & \displaystyle\sum_{x,\,\tau(x)>1} \mathit{Flrn}(\upsilon)(x)\Big|\upsilon{+}1|x\rangle,\ \tau{-}1|x\rangle\Big\rangle + \sum_{x,\,\tau(x)=1} \mathit{Flrn}(\upsilon)(x)\Big|x\Big\rangle.
\end{array}
$$

We recalculate the outcome of Example 3 as illustration, with urn $\upsilon = 1|a\rangle + 1|b\rangle$ and tubes $\tau = 2|a\rangle + 3|b\rangle$. Then:

$$
\begin{aligned}
PL(\upsilon,\tau) &= \frac{1}{2}\Big|2|a\rangle + 1|b\rangle, 1|a\rangle + 3|b\rangle\Big\rangle + \frac{1}{2}\Big|1|a\rangle + 2|b\rangle, 2|a\rangle + 2|b\rangle\Big\rangle \\
PL^2(\upsilon,\tau) &= \frac{1}{2}\cdot\frac{2}{3}\Big|a\Big\rangle + \frac{1}{2}\cdot\frac{1}{3}\Big|2|a\rangle + 2|b\rangle, 1|a\rangle + 2|b\rangle\Big\rangle \\
&\quad + \frac{1}{2}\cdot\frac{1}{3}\Big|2|a\rangle + 2|b\rangle, 1|a\rangle + 2|b\rangle\Big\rangle + \frac{1}{2}\cdot\frac{2}{3}\Big|1|a\rangle + 3|b\rangle, 2|a\rangle + 1|b\rangle\Big\rangle
\end{aligned}
$$

$$\begin{aligned}
PL^3(\upsilon,\tau) &= \frac{1}{3}\big|\,a\,\big\rangle + \frac{1}{3}\cdot\frac{1}{2}\big|\,a\,\big\rangle + \frac{1}{3}\cdot\frac{1}{2}\Big|\,2|\,a\,\rangle + 3|\,b\,\rangle, 1|\,a\,\rangle + 1|\,b\,\rangle\Big\rangle \\
&\quad + \frac{1}{3}\cdot\frac{1}{4}\Big|\,2|\,a\,\rangle + 3|\,b\,\rangle, 1|\,a\,\rangle + 1|\,b\,\rangle\Big\rangle + \frac{1}{3}\cdot\frac{3}{4}\big|\,b\,\big\rangle \\
PL^4(\upsilon,\tau) &= \frac{1}{2}\big|\,a\,\big\rangle + \frac{1}{4}\cdot\frac{2}{5}\big|\,a\,\big\rangle + \frac{1}{4}\cdot\frac{3}{5}\big|\,b\,\big\rangle + \frac{1}{4}\big|\,b\,\big\rangle \\
&= \frac{3}{5}\big|\,a\,\big\rangle + \frac{2}{5}\big|\,b\,\big\rangle.
\end{aligned}$$

We proceed with a pattern that is by now familiar. That's why we only state the results and leave the proofs to the interested reader.

Lemma 10 *Let $\upsilon, \tau \in \mathcal{M}(X)$ be multisets with $\upsilon \geq \tau \geq \mathbf{1}$.*

1. *For $\upsilon', \tau' \in \mathcal{M}(X)$ with $\upsilon', \tau' \geq \mathbf{1}$,*

$$\begin{aligned}
PL^n(\upsilon,\tau)(\upsilon',\tau') &= \sum \Big\{ \prod_{0\leq i<n} \mathit{Flrn}\Big((\upsilon + acc(x_1,\ldots,x_i)\Big)(x_{i+1}) \,\Big|\, \ell = \langle x_1,\ldots,x_n\rangle \in X^n \\
&\qquad\qquad \text{with } \upsilon' = \upsilon + acc(\ell) \text{ and } \tau' = \tau - acc(\ell) \Big\} \\
&= \sum \Big\{ pl[n](\upsilon)(\chi) \,\Big|\, \chi \leq \tau - \mathbf{1} \text{ with } \|\chi\| = n,\ \upsilon' = \upsilon + \chi,\ \tau' = \tau - \chi \Big\}.
\end{aligned}$$

2. *For an element $x \in X$,*

$$\begin{aligned}
PL^{n+1}(\upsilon,\tau)(x) \;=\; \sum \Big\{ pl[K](\upsilon)(\chi)\cdot \mathit{Flrn}(\upsilon+\chi)(x) \,\Big|\, & K \leq n \text{ and } \chi \leq \tau - \mathbf{1} \\
& \text{with } \|\chi\| = K \text{ and } (\tau-\chi)(x) = 1 \Big\}.
\end{aligned}$$

□

Theorem 11 *Let set X have N elements and let tubes $\tau \in \mathcal{M}_{\geq 1}(X)$ have size $L = \|\tau\| \geq N$. For urn $\upsilon \geq \mathbf{1}$ one gets:*

$$\mathrm{supp}\Big(PL^{L-N+1}(\upsilon,\tau)\Big) \subseteq X \qquad \text{and} \qquad PL^{L-N+1}(\upsilon,\tau) \;=\; \mathit{plff}(\upsilon,\tau).$$

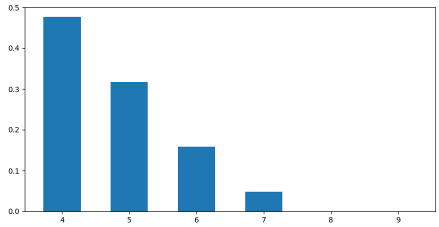
In particular, Pólya first-full $\mathit{plff}(\upsilon,\tau)$ is a probability distribution. □

Remark 1 In the end we have two (equivalent) ways to compute first-full distributions, namely via their pointwise formulations (in Definition 3) and via their three MMO's, as described above. The latter can easily be turned into recursive definitions. Experiments with both implementations show that the recursive approach is slower than the one based on the definitions. This is not surprising since the recursive approach computes probabilities for sequences, with much duplication, instead of for multisets (as accumulations of those sequences). In contrast, reasoning with sequences is easier than with multisets. In the end that is the whole reason why we use the MMO-approach — for proving that combined first-full probabilities form a distribution.

7 Negative distributions

The urns & tubes set-up that we have used to introduce first-full distributions can also be used to describe 'negative' distributions. The latter are known from the literature, in bivariate form, with one tube only. Here we use our multiset-based approach to describe them systematically, in multivariate form, for all three modes (multinomial, hypergeometric and Pólya). We concentrate on the definitions and on illustrations. The fact that these definitions lead to actual probability distributions is addressed, by giving the corresponding Markov models with output, but without all the mathematical details. After all, these distributions are not new.

We start with an example. Consider a group of people consisting of five males (M) and four females (F). From this group we like to form a committee with two male and two female members. Iteratively we choose members from the group, at random, until the committee is formed. How many choices are needed? More precisely, what is the probability — that the committee is first formed — for each number of choices. We might be done after four choices, if they immediately involve two males and two females. But we may also first pick three men, and then two females, which involves five choices. What is the highest possible number of choices? It is seven, when all five men are chosen, before the two females. Hence this situation involves a distribution on the set $\{4, 5, 6, 7\}$. It is:

$\frac{10}{21}|4\rangle + \frac{20}{63}|5\rangle + \frac{10}{63}|6\rangle + \frac{1}{21}|7\rangle$ in 

How does it come about? We can see the group of people as an urn $\upsilon = 5|M\rangle + 4|F\rangle$ from which we 'draw' candidate committee members, in hypergeometric mode: after drawing a member from the urn/group, this person is either put in the committee, or is skipped, when there are already two committee members with this person's gender in the committee.

- The probability of being done in four steps is given by the hypergeometric distribution at multiset $2|M\rangle + 2|F\rangle$. Indeed,

$$hg[4](\upsilon)\Big(2|M\rangle + 2|F\rangle\Big) = \frac{10}{21}.$$

- We may need five steps in two cases: (1) when we first choose three men and one woman, in any order, and finally a woman, or (2) when we first choose three women and one man, in any order, and finally a man. This leads to the probability:

$$hg[4](\upsilon)\Big(3|M\rangle + 1|F\rangle\Big) \cdot \frac{3}{5} + hg[4](\upsilon)\Big(1|M\rangle + 3|F\rangle\Big) \cdot \frac{4}{5} = \frac{20}{63} \cdot \frac{3}{5} + \frac{10}{63} \cdot \frac{4}{5} = \frac{20}{63}.$$

- We need six steps when we first choose four men and one woman, and then one woman, or when we first choose one man and four women. In the latter case we are done at the next selection, because we can only choose a male. The associated probability is thus obtained as:

$$hg[5](\upsilon)\Big(4|M\rangle + 1|F\rangle\Big) \cdot \frac{3}{4} + hg[5](\upsilon)\Big(1|M\rangle + 4|F\rangle\Big) = \frac{10}{63} \cdot \frac{3}{4} + \frac{5}{126} = \frac{10}{63}.$$

- Finally, there is only one possibility that requires the maximum number of seven steps, namely when we first choose five men and one woman. The associated probability is simply:

$$hg[6](\upsilon)\Big(5|M\rangle + 1|F\rangle\Big) = \frac{1}{21}.$$

In this example we may consider the committee that needs to be filled with two males and two females as a pair of tubes, both of length two. Thus, the urns & tubes model can be used here as well, but with a different question, namely what is the probability of filling *all* tubes in a certain number of steps.

Thus, abstractly, our starting point is the same as in the previous section, see Picture 1: we have an urn filled with coloured balls, together with coloured tubes. The question that we now look at is as follows.

> Suppose we draw k balls from the urn, to fill the tubes, for $k \in \mathbb{N}$. What is the probability that all tubes are full for the first time after drawing these k balls? This means that there is one tube that becomes full with the k-th ball, while sufficiently many balls — typically more than needed — have already been drawn to fill all other tubes.

The filling of all tubes can be seen as a desired condition, or as a risk. The probability distribution that we are after gives for each $k \in \mathbb{N}$ the probability of reaching this threshold condition for the first time.

- Historically the distributions that arise in this manner are called *negative*. They are not very well known, and are even called 'forgotten' in [20]. These negative distributions may occur in different forms, depending on the mode of drawing ("-1", "0", or "+1"). Accordingly, we shall speak of *negative hypergeometric*, *negative multinomial*, and *negative Pólya* distributions. Below we cover all three modes.

- The negative hypergeometric distribution has finite support, since at some stage the urn is empty. In multinomial mode the urn does not change, and in Pólya mode the urn grows in size. Hence in these last two cases the support of the negative distributions are infinite subsets of the natural numbers. Recall that we write $\mathcal{D}_\infty(\mathbb{N})$ for set of discrete distributions on $\mathbb{N}$ with (possibly) infinite support.

- In the literature (see *e.g.* [13, 20, 21, 25, 26]) negative distributions are studied only for the (simple) case with a single tube and usually with only two colours. Here we deal with the general, multivariate and multi-tube, scenario, where there are multiple colours and as many tubes as colours. Like before, we shall write τ for the tubes and $L := \|\tau\|$ for the sum of the lengths of all tubes. We assume that $L > 0$ so that there is at least one non-empty tube that can be filled. We shall write $\mathcal{M}_*(X) \hookrightarrow \mathcal{M}(X)$ for the subset of *non-empty* multisets; we thus require $\tau \in \mathcal{M}_*(X)$. The negative distributions on $\mathbb{N}$ that we are after will 'start at L': they are zero at $k < L$, since one needs to draw at least L balls to fill all tubes.

- As in the first-fill case, in Section 5, there is a challenge to show that negative probabilities add up to one, and thus form a proper distribution. Again we use Markov models with output, like in the previous section, but without elaborating all details. Previously, we only had finitely many possible transitions. Here, in the negative setting, there may be infinitely many transitions, leading to infinite supports.

Definition 4 *Let X be a finite set (of colours) with $|X| \geq 2$ and let $\tau \in \mathcal{M}_*(X)$ be an X-indexed collection of tubes.*

1. *For $\omega \in \mathcal{D}(X)$, we define at $k > 0$ the* negative multinomial *probability as:*

$$nmn(\omega,\tau)(k) := \sum_{x\in\mathrm{supp}(\tau)} \; \sum_{\substack{\varphi\in\mathcal{M}[k-1](X),\\ \tau-1|x\rangle \leq \varphi,\, \varphi(x)=\tau(x)-1}} mn[k-1](\omega)(\varphi)\cdot\omega(x).$$

2. *For an urn $\upsilon \in \mathcal{M}(X)$ with $\upsilon \geq \tau$, we define the* negative hypergeometric *probability at $k > 0$ as:*

$$nhg(\upsilon,\tau)(k) := \sum_{x\in\mathrm{supp}(\tau)} \; \sum_{\substack{\varphi\leq_{k-1}\upsilon,\\ \tau-1|x\rangle \leq \varphi,\, \varphi(x)=\tau(x)-1}} hg[k-1](\upsilon)(\varphi)\cdot Flrn(\upsilon-\varphi)(x).$$

3. *Finally, for an urn $\upsilon \in \mathcal{M}(X)$ with $\upsilon \geq \mathbf{1}$, and for $k > 0$ we define the* negative Pólya *probability as:*

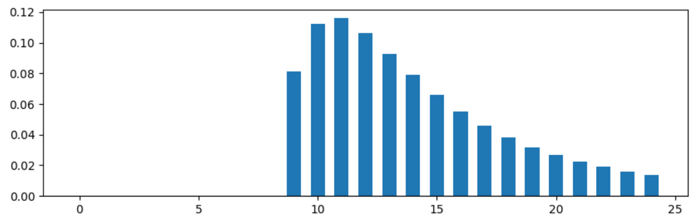
$$npl(\upsilon,\tau)(k) := \sum_{x\in\mathrm{supp}(\tau)} \; \sum_{\substack{\varphi\in\mathcal{M}[k-1](X),\\ \tau-1|x\rangle \leq \varphi,\, \varphi(x)=\tau(x)-1}} pl[k-1](\upsilon)(\varphi)\cdot Flrn(\upsilon+\varphi)(x).$$

These distributions may be extended to $k = 0$ by setting them to zero there.

In each of the above three cases we sum over draws φ satisfying $\tau-1|x\rangle \leq \varphi$ and $\varphi(x) = \tau(x)-1$. The inequality $\leq$ implies that $\tau(y) \leq \varphi(y)$ for all $y \neq x$, so that all tubes are full (possibly with overflow) after drawing φ, except for colour x. The equality $\varphi(x) = \tau(x) - 1$ says that there is precisely one ball of colour x missing to ensure that all tubes are full. The probability of additionally drawing this missing ball of colour x is multiplied in each of the above three cases with the probability of the draw φ, as $\omega(x)$ in item (1), as $Flrn(\upsilon - \varphi)(x)$ in item (2), and as $Flrn(\upsilon + \varphi)(x)$ in item (3). In the first-fill probabilities in Definition 3 this is done analogously.

Computing negative distributions by hand is laborious because it involves summing over all colours and over all draws, of a certain size. However, this can be automated without too much effort.

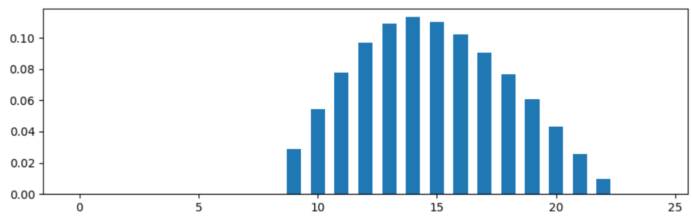
Example 4 *Take $X = \{a, b, c\}$ with tubes $\tau = 2|a\rangle + 4|b\rangle + 3|c\rangle$, having total length $L = \|\tau\| = 9$. For a state $\omega = \frac{1}{6}|a\rangle + \frac{1}{2}|b\rangle + \frac{1}{3}|c\rangle$. A first part of the resulting negative multinomial distribution $nmn(\omega, \tau)$ on $\mathbb{N}$ looks as follows.*



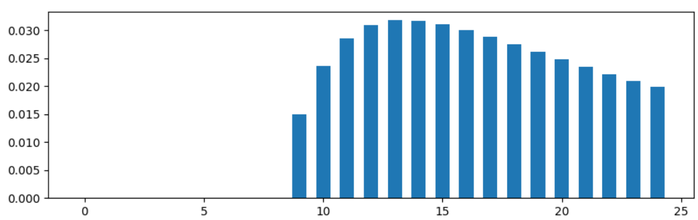
The sum of the probabilities in this picture is approximately 0.92. The remaining 0.08 is in the long tail. An exact description of the first four probabilities is:

$$nmn(\omega, \tau) = \tfrac{35}{432}|9\rangle + \tfrac{875}{7776}|10\rangle + \tfrac{3605}{31104}|11\rangle + \tfrac{1243}{11664}|12\rangle + \cdots \tag{15}$$

With urn $\upsilon = 10|a\rangle + 6|b\rangle + 8|c\rangle$ the negative hypergeometric distribution $nhg(\upsilon, \tau)$ runs from $L = \|\tau\| = 9$ to $\|\upsilon\| - 1 = 23$ and looks in its entirety as follows.



Using urn $\upsilon = 3|a\rangle + 2|b\rangle + 1|c\rangle$ the negative Pólya distribution $npl(\upsilon, \tau)$ on $\mathbb{N}$ starts as described below.



This pictures only contains about 0.42 of all probabilities. This negative Pólya is thus heavy-tailed and its probabilities are less concentrated at the beginning than in the negative multinomial.

7.1 The common one-tube situation

In the introduction to this section we mentioned that the negative distributions that are commonly considered in the literature involve one tube only. We describe what happens then, as special case of the above formulations in Definition 4, and recover familiar formulations. It turns out, in all three drawing modes, that the relevant probabilities can also be described via the 'non-negative' bivariate distribution.

Theorem 12 *Let X be a set of colours, with a special fixed element $y \in X$, and with single-tube multiset $\tau = m|y\rangle$ for $m > 0$.*

1. *Let $\omega \in \mathcal{D}(X)$ satisfy $0 < \omega(y) < 1$. For $k \geq 0$,*

$$\begin{aligned} nmn\big(\omega, m|y\rangle\big)(m+k) &= \frac{m}{m+k} \cdot mn[m+k]\Big(\omega(y)|0\rangle + (1-\omega(y))|1\rangle\Big)\Big(m|0\rangle + k|1\rangle\Big) \\ &= nbn[m]\big(\omega(y)\big)(m+k). \end{aligned}$$

The latter expression involves the negative binomial distribution, of the form:

$$nbn[m](s) \coloneqq \sum_{i \geq 0} \left(\!\!\binom{m}{i}\!\!\right) \cdot s^m \cdot (1-s)^i \, \big| m+i \big\rangle \in \mathcal{D}_\infty(\mathbb{N}). \tag{16}$$

2. *Similarly, for an urn $\upsilon \in \mathcal{M}[L](X)$ with $\upsilon(y) \geq m$, one has, for $k \geq 0$,*

$$\begin{aligned} nhg\big(\upsilon, m|y\rangle\big)(m+k) &= \frac{m}{m+k} \cdot hg[m+k]\big(\upsilon(y)|0\rangle + (L-\upsilon(y))|1\rangle\big)\big(m|0\rangle + k|1\rangle\big) \\ &= \frac{m}{m+k} \cdot \frac{\binom{\upsilon(y)}{m} \cdot \binom{L-\upsilon(y)}{k}}{\binom{L}{m+k}}. \end{aligned}$$

3. *Also negative Pólya with one tube reduces to bivariate non-negative form. For an urn $\upsilon \in \mathcal{M}[K](X)$ with $\upsilon(y) > 0$ one has:*

$$\begin{aligned} npl\big(\upsilon, m|y\rangle\big)(m+k) &= \frac{m}{m+k} \cdot pl[m+k]\big(\upsilon(y)|0\rangle + (L-\upsilon(y))|1\rangle\big)\big(m|0\rangle + k|1\rangle\big) \\ &= \frac{m}{m+k} \cdot \frac{\left(\!\binom{\upsilon(y)}{m}\!\right) \cdot \left(\!\binom{L-\upsilon(y)}{k}\!\right)}{\left(\!\binom{L}{m+k}\!\right)}. \end{aligned}$$

Proof. 1. In presence of a single tube the negative multinomial becomes a single sum over multisets:

$$\begin{aligned} nmn\big(\omega, m|y\rangle\big)(m+k) &= \sum_{\varphi \in \mathcal{M}[m+k-1](X),\, \varphi(y)=m-1} mn[m+k-1](\omega)(\varphi) \cdot \omega(y) \\ &= \sum_{\varphi \in \mathcal{M}[k](X-y)} mn[m+k-1](\omega)\big((m-1)|y\rangle + \varphi\big) \cdot \omega(y) \\ &= \sum_{\varphi \in \mathcal{M}[k-m](X-y)} \frac{(m+k-1)!}{(m-1)! \cdot \varphi!!} \cdot \omega(y)^m \cdot \prod_{x \neq y} \omega(x)^{\varphi(x)} \\ &= \binom{m+k-1}{m-1} \cdot \omega(y)^m \cdot \sum_{\varphi \in \mathcal{M}[k](X-y)} \frac{k!}{\varphi!!} \cdot \prod_{x \neq y} \omega(x)^{\varphi(x)} \\ &= \left(\!\!\binom{m}{k}\!\!\right) \cdot \omega(y)^m \cdot \big(\textstyle\sum_{x \neq y} \omega(x)\big)^k \qquad \text{by Fact 1 (2)} \\ &= \left(\!\!\binom{m}{k}\!\!\right) \cdot \omega(y)^m \cdot (1-\omega(y))^k \\ &= nbn[m]\big(\omega(y)\big)(m+k). \end{aligned}$$

At the same time we can write:

$$\begin{aligned} \left(\!\!\binom{m}{k}\!\!\right) \cdot \omega(y)^m \cdot (1-\omega(y))^k &= \frac{m}{m+k} \cdot \binom{m+k}{k} \cdot \omega(y)^m \cdot (1-\omega(y))^k \\ &= \frac{m}{m+k} \cdot mn[m+k]\Big(\omega(y)|0\rangle + (1-\omega(y))|1\rangle\Big)\Big(m|0\rangle + k|1\rangle\Big). \end{aligned}$$

2. We write $\upsilon' = \upsilon - \upsilon(y)|y\rangle$ for the urn from which all balls of colour y have been removed.

$$\begin{aligned}
& nhg\big(\upsilon, m|y\rangle\big)(m+k) \\
&= \sum_{\varphi \leq_{m+k-1} \upsilon,\, \varphi(y)=m-1} hg[m+k-1](\upsilon)(\varphi) \cdot \mathit{Flrn}\big(\upsilon - \varphi\big)(y) \\
&= \sum_{\varphi \leq_k \upsilon'} hg[m+k-1](\upsilon)\big((m-1)|y\rangle + \varphi\big) \cdot \mathit{Flrn}\Big(\upsilon - (m-1)|y\rangle - \varphi\Big)(y) \\
&= \sum_{\varphi \leq_k \upsilon'} \frac{\binom{\upsilon(y)}{m-1} \cdot \prod_{x \neq y} \binom{\upsilon(x)}{\varphi(x)}}{\binom{L}{m+k-1}} \cdot \frac{\upsilon(y) - (m-1)}{L - (m+k-1)} \qquad \text{where } L = \|\upsilon\| \\
&= \frac{m \cdot \binom{\upsilon(y)}{m} \cdot \sum_{\varphi \leq_k \upsilon'} \binom{\upsilon'}{\varphi}}{(m+k) \cdot \binom{L}{m+k}} \qquad \text{since } \binom{n}{m} \cdot (n-m) = (m+1) \cdot \binom{n}{m+1} \\
&= \frac{m}{m+k} \cdot \frac{\binom{\upsilon(y)}{m} \cdot \binom{L-\upsilon(y)}{k}}{\binom{L}{m+k}} \qquad \text{by Proposition 1} \\
&= \frac{m}{m+k} \cdot hg[m+k]\big(\upsilon(y)|0\rangle + (L-\upsilon(y))|1\rangle\big)\big(m|0\rangle + k|1\rangle\big).
\end{aligned}$$

3. In the Pólya case we proceed in a similar manner, for $\upsilon \in \mathcal{M}[L](X)$.

$$\begin{aligned}
& npl\big(\upsilon, m|y\rangle\big)(m+k) \\
&= \sum_{\varphi \in \mathcal{M}[m+k-1](X),\, \varphi(y)=m-1} pl[m+k-1](\upsilon)(\varphi) \cdot \mathit{Flrn}(\upsilon + \varphi)(y) \\
&= \sum_{\varphi \in \mathcal{M}[k](X-y)} pl[m+k-1](\upsilon)\big((m-1)|y\rangle + \varphi\big) \\
&\qquad\qquad \cdot \mathit{Flrn}\Big(\upsilon + (m-1)|y\rangle + \varphi\Big)(y) \\
&= \sum_{\varphi \in \mathcal{M}[k](X-y)} \frac{\left(\!\binom{\upsilon(y)}{m-1}\!\right) \cdot \prod_{x \neq y} \left(\!\binom{\upsilon(x)}{\varphi(x)}\!\right)}{\left(\!\binom{L}{m+k-1}\!\right)} \cdot \frac{\upsilon(y) + (m-1)}{L + (m+k-1)} \\
&= \frac{m \cdot \left(\!\binom{\upsilon(y)}{m}\!\right) \cdot \sum_{\varphi \in \mathcal{M}[k](X-y)} \left(\!\binom{\upsilon'}{\varphi}\!\right)}{(m+k) \cdot \left(\!\binom{L}{m+k}\!\right)} \qquad \text{where } \upsilon' = \upsilon - \upsilon(y)|y\rangle \\
&= \frac{m}{m+k} \cdot \frac{\left(\!\binom{\upsilon(y)}{m}\!\right) \cdot \left(\!\binom{L-\upsilon(y)}{k}\!\right)}{\left(\!\binom{L}{m+k}\!\right)} \qquad \text{by Proposition 2} \\
&= \frac{m}{m+k} \cdot pl[m+k]\big(\upsilon(y)|0\rangle + (L-\upsilon(y))|1\rangle\big)\big(m|0\rangle + k|1\rangle\big).
\end{aligned}$$

□

7.2 Negatives yield distributions

We will illustrate that the probabilities in the 'negative' formulations in Definition 4 yield actual distributions. We shall proceed as in Section 6 and introduce appropriate Markov models with output (MMO). The positions in these MMOs are tuples involving a 'stage' number $i \in \mathbb{N}$. Each step involves one of the following three options.

1. For colour x with already full tube, so $\tau(x) = 0$, one can draw another ball of colour x and move to a next position in the MMO. We then have an overflow situation for colour x so this next position has the same tubes τ and an incremented stage, which change from i to $i + 1$.

2. In case colour x is the last one whose tube needs to be filled, we have $\tau(x) > 0$ and $\|\tau\| = 1$, or equivalently $\tau(x) = 1$ and $\tau(y) = 0$ for all $y \neq x$. Then we can draw this last ball and move to the output $i + 1$, from which no further transitions are possible.

3. When colour x's tube is not full yet, and there are other non-full tubes as well — so when $\tau(x) > 0$ and $\|\tau\| > 1$ — we can draw a ball of colour x and drop it in the tube of colour x. The next position then involves new tubes $\tau - 1|x\rangle$, where the number of missing balls of colour x is reduced by 1, with incremented stage $i + 1$.

Negative multinomial distributions

The MMO for negative multinomials has pairs (τ, i) as positions, with tubes $\tau \in \mathcal{M}_*(X)$ and stage $i \in \mathbb{N}$. The above three options are captured as follows.

$$\begin{array}{l} \mathcal{M}_*(X) \times \mathbb{N} \xrightarrow{\quad NMN(\omega) \quad} \mathcal{D}\Big(\mathcal{M}_*(X) \times \mathbb{N} \,+\, \mathbb{N}\Big) \\ (\tau, i) \longmapsto \displaystyle\sum_{x,\, \tau(x)=0} \omega(x)\big|\tau, i{+}1\big\rangle + \sum_{x,\, \tau(x)>0,\, \|\tau\|=1} \omega(x)\big|i{+}1\big\rangle \\ \qquad\qquad + \displaystyle\sum_{x,\, \tau(x)>0,\, \|\tau\|>1} \omega(x)\big|\tau - |x\rangle, i{+}1\big\rangle. \end{array} \tag{17}$$

Starting from initial position $(\tau, 0)$ one eventually ends up with an output in $\mathbb{N}$. We reason informally from the contrapositive: an infinite sequences $(\rho, k) \to (\rho, k+1) \to (\rho, k+2) \to \cdots$ exists only if the colours $x \in \mathrm{supp}(\rho)$ are never drawn when the size of the draws goes to infinity. This is impossible.

Negative hypergeometric distributions

In the hypergeometric (and Pólya) mode the urn changes with every draw, so we have to incorporate not only the tubes τ but also the urn υ in the positions of our MMO. For convenience, we introduce the following special notation.

$$\mathcal{M}_{\geq *}(X) \coloneqq \{(\upsilon, \tau) \in \mathcal{M}_*(X) \times \mathcal{M}_*(X) \mid \upsilon \geq \tau\}.$$

The inequality $\upsilon \geq \tau$ expresses that the urn contains sufficiently many balls of each colour to fill the tubes. This inequality acts as an invariant for the following negative hypergeometric MMO.

$$\begin{array}{l} \mathcal{M}_{\geq *}(X) \times \mathbb{N} \xrightarrow{\quad NHG \quad} \mathcal{D}\Big(\mathcal{M}_{\geq *}(X) \times \mathbb{N} + \mathbb{N}\Big) \\ (\upsilon, \tau, i) \longmapsto \displaystyle\sum_{x,\, \tau(x)=0,\, \upsilon(x)>0} \mathit{Flrn}(\upsilon)(x)\big|\upsilon - 1|x\rangle, \tau, i{+}1\big\rangle \\ \qquad\qquad + \displaystyle\sum_{x,\, \tau(x)>0,\, \|\tau\|=1} \mathit{Flrn}(\upsilon)(x)\big|i{+}1\big\rangle \\ \qquad\qquad + \displaystyle\sum_{x,\, \tau(x)>0,\, \|\tau\|>1} \mathit{Flrn}(\upsilon)(x)\big|\upsilon - 1|x\rangle, \tau - |x\rangle, i{+}1\big\rangle. \end{array} \tag{18}$$

It is obvious that there are no infinite transitions starting from $(\upsilon, \tau, 0)$ since in each non-output step the urn υ decreases in size.

Negative Pólya

We now require that initially, the urn υ contains for all colours of the tubes τ at least one ball. This can expressed as inclusion of supports. Hence we define:

$$\mathcal{M}_{\supseteq *}(X) \coloneqq \{(\upsilon, \tau) \in \mathcal{M}_*(X) \times \mathcal{M}_*(X) \mid \mathrm{supp}(\upsilon) \supseteq \mathrm{supp}(\tau)\}.$$

This is used in the following negative Pólya MMO. It looks very much like the hypergeometric one in (18), with removal of balls from the urn replaced by addition.

$$
\begin{array}{rcl}
\mathcal{M}_{\supseteq *}(X) \times \mathbb{N} & \xrightarrow{\qquad NPL \qquad} & \mathcal{D}\Big(\mathcal{M}_{\supseteq *}(X) \times \mathbb{N} + \mathbb{N}\Big) \\
(\upsilon, \tau, i) & \longmapsto & \displaystyle\sum_{x,\, \tau(x)=0} \mathit{Flrn}(\upsilon)(x)\big|\,\upsilon{+}1|x\rangle, \tau, i{+}1\,\big\rangle \\
& & \displaystyle\quad + \sum_{x,\, \tau(x)>0,\, \|\tau\|=1} \mathit{Flrn}(\upsilon)(x)\big|\,i{+}1\,\big\rangle \\
& & \displaystyle\quad + \sum_{x,\, \tau(x)>0,\, \|\tau\|>1} \mathit{Flrn}(\upsilon)(x)\big|\,\upsilon{+}1|x\rangle, \tau{-}|x\rangle, i{+}1\,\big\rangle.
\end{array}
\tag{19}
$$

Also in this case there are no infinite transitions from an initial position $(\upsilon, \tau, 0)$, because the probability that certain colours do not occur in Pólya draws becomes zero as the size of draws goes to infinity.

8 Hypergeometric and Pólya distributions via (negative) binomials

In Section 4 we have have introduced the (ordinary, non-negative) hypergeometric and Pólya distributions $hg[K](\upsilon)$ and $pl[K](\upsilon)$, for an urn υ. It is known that these distributions can also be obtained via conditioning, namely of parallel binomials in the hypergeometric case, and of parallel negative binomials in the Pólya case (see *e.g.* [26], for the bivariate, and also [12] for the multivariate case). These conditionings build on Propositions 1, 2 and fit very well in the current account, and are therefore included here, in fully multivariate form. In order to do so we need to recall the basics of probabilistic conditioning, see *e.g.* [5, 6, 10, 7, 9] for more information.

Let $\omega \in \mathcal{D}(X)$ be distribution and $p\colon X \to [0,1]$ be a (fuzzy) predicate. We write $\omega \models p := \sum_x \omega(x) \cdot p(x)$ for the validity (expected value) of p in ω. If this validity is non-zero, we can define the updated distribution $\omega|_p \in \mathcal{D}(X)$ as the normalised product:

$$
\omega|_p(x) \coloneqq \frac{\omega(x) \cdot p(x)}{\omega \models p}.
$$

See *e.g.* [5, 6, 9] for more information.

The two propositions below describe the two conditioning results for hypergeometric and Pólya distributions. They both use the following sum predicate $sum_K\colon \mathbb{N}^\ell \to [0,1]$, for $K \in \mathbb{N}$.

$$
sum_K(n_1, \ldots, n_\ell) \coloneqq \begin{cases} 1 & \text{if } n_1 + \cdots + n_\ell = K \\ 0 & \text{otherwise.} \end{cases} \tag{20}
$$

Proposition 13 *Conditioning parallel binomials with this sum predicate (20) yields the hypergeometric distribution: for $K \leq \sum_i k_i$,*

$$
\big(bn[k_1](r) \otimes \cdots \otimes bn[k_\ell](r)\big)\big|_{sum_K} = hg[K]\big(\textstyle\sum_i k_i|i\rangle\big).
$$

This works for any number $r \in [0,1]$.

Proof. We first compute the validity:

$$
\begin{array}{l}
bn[k_1](r) \otimes \cdots \otimes bn[k_\ell](r) \models sum_K \\
\displaystyle = \sum_{n_i \leq k_i} \big(bn[k_1](r) \otimes \cdots \otimes bn[k_\ell](r)\big)(n_1, \ldots, n_\ell) \cdot sum_K(n_1, \ldots, n_\ell) \\
\displaystyle = \sum_{n_i \leq k_i,\, \sum_i n_i = K} bn[k_1](r)(n_1) \cdot \ldots \cdot bn[k_\ell](r)(n_\ell) \\
\displaystyle = \sum_{n_i \leq k_i,\, \sum_i n_i = K} \binom{k_1}{n_1} \cdot r^{n_1} \cdot (1{-}r)^{k_1 - n_1} \cdot \ldots \cdot \binom{k_\ell}{n_\ell} \cdot r^{n_\ell} \cdot (1{-}r)^{k_\ell - n_\ell}
\end{array}
\tag{21}
$$

$$
\begin{aligned}
&= \sum_{n_i \leq k_i,\, \sum_i n_i = K} \binom{\sum_i k_i|i\rangle}{\sum_i n_i|i\rangle} \cdot r^K \cdot (1-r)^{(\sum_i k_i)-K} \\
&= \binom{\sum_i k_i}{K} \cdot r^K \cdot (1-r)^{(\sum_i k_i)-K} \qquad \text{by Proposition 1} \\
&= bn[\textstyle\sum_i k_i](r)(K).
\end{aligned}
$$

Now we can move on to the conditioning itself. We see that the probability $r \in [0,1]$ drops out of the calculation.

$$
\begin{aligned}
&\big(bn[k_1](r) \otimes \cdots \otimes bn[k_\ell](r)\big)\big|_{sum_K} \\
&= \sum_{n_i \leq k_i} \frac{\big(bn[k_1](r) \otimes \cdots \otimes bn[k_\ell](r)\big)(\vec{n}) \cdot sum_K(\vec{n})}{bn[k_1](r) \otimes \cdots \otimes bn[k_\ell](r) \models sum_K} \big| n_1, \ldots, n_\ell \big\rangle \\
&= \sum_{n_i \leq k_i,\, \sum_i n_i = K} \frac{\binom{k_1}{n_1} \cdot r^{n_1} \cdot (1-r)^{k_1 - n_1} \cdot \ldots \cdot \binom{k_\ell}{n_\ell} \cdot r^{n_\ell} \cdot (1-r)^{k_\ell - n_\ell}}{\binom{\sum_i k_i}{K} \cdot r^K \cdot (1-r)^{(\sum_i k_i)-K}} \big| n_1, \ldots, n_\ell \big\rangle \\
&= \sum_{n_i \leq k_i,\, \sum_i n_i = K} \frac{\prod_i \binom{k_i}{n_i} \cdot r^K \cdot (1-r)^{(\sum_i k_i)-K}}{\binom{\sum_i k_i}{K} \cdot r^K \cdot (1-r)^{(\sum_i k_i)-K}} \big| n_1, \ldots, n_\ell \big\rangle \\
&= \sum_{n_i \leq k_i,\, \sum_i n_i = K} \frac{\prod_i \binom{k_i}{n_i}}{\binom{\sum_i k_i}{K}} \big| n_1, \ldots, n_\ell \big\rangle \\
&\overset{(9)}{=} hg[K]\Big(\textstyle\sum_i k_i|i\rangle\Big).
\end{aligned}
$$

In the last line we implicitly identify the sequence $n_1, \ldots, n_\ell$ with the multiset $n_1|1\rangle + \cdots + n_\ell|\ell\rangle$. □

There is a similar result for Pólya distributions, using negative binomials. It requires some care since it involves a shift of arguments, since negative distributions (on $\mathbb{N}$) start only after a certain number of steps.

Proposition 14 *The multivariate Pólya distribution can be described as conditioning of negative binomials: for $K \geq \sum_i k_i$,*

$$
\begin{aligned}
&\big(nbn[k_1](r) \otimes \cdots \otimes nbn[k_\ell](r)\big)\big|_{sum_K}(k_1 + n_1, \ldots, k_\ell + n_\ell) \\
&= \begin{cases} pl[K - \sum_i k_i]\big(\sum_i k_i|i\rangle\big)\big(\sum_i n_i|i\rangle\big) & \text{if } \sum_i k_i + n_i = K \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}
$$

The number $r \in [0,1]$ is arbitrary, and the predicate sum_K is from (20).

Proof. We start with the validity:

$$
\begin{aligned}
&\big(nbn[k_1](r) \otimes \cdots \otimes nbn[k_\ell](r)\big) \models sum_K \qquad (22) \\
&= \sum_{n_1, \ldots, n_\ell} \big(nbn[k_1](r) \otimes \cdots \otimes nbn[k_\ell](r)\big)(n_1, \ldots, n_\ell) \cdot sum_K(n_1, \ldots, n_\ell) \\
&= \sum_{n_i,\, \sum_i k_i + n_i = K} bn[k_1](r)(k_1 + n_1) \cdot \ldots \cdot bn[k_\ell](r)(k_\ell + n_\ell) \\
&\overset{(16)}{=} \sum_{n_i,\, \sum_i k_i + n_i = K} \prod_i \left(\!\binom{k_i}{n_i}\!\right) \cdot r^{k_i} \cdot (1-r)^{n_i} \\
&= \sum_{n_i,\, \sum_i n_i = K - \sum_i k_i} \prod_i \left(\!\binom{\sum_i k_i|i\rangle}{\sum_i n_i|i\rangle}\!\right) \cdot r^{\sum_i k_i} \cdot (1-r)^{\sum_i n_i}
\end{aligned}
$$

$$
\begin{aligned}
&= \left(\!\!\binom{\sum_i k_i}{K - \sum_i k_i}\!\!\right) \cdot r^{\sum_i k_i} \cdot (1-r)^{K-\sum_i k_i} \qquad \text{by Proposition 2} \\
&= nbn[\textstyle\sum_i k_i](r)(K).
\end{aligned}
$$

Conditioning yields, when $\sum_i k_i + n_i = K$,

$$
\begin{aligned}
&\big(nbn[k_1](r) \otimes \cdots \otimes nbn[k_\ell](r)\big)\big|_{sum_K}(k_1+n_1, \ldots, k_\ell+n_\ell) \\
&= \frac{\big(bn[k_1](r) \otimes \cdots \otimes bn[k_\ell](r)\big)\big((k_1+n_1, \ldots, k_\ell+n_\ell\big)}{nbn[k_1](r) \otimes \cdots \otimes nbn[k_\ell](r) \models sum_K} \\
&= \frac{\prod_i \left(\!\binom{k_i}{n_i}\!\right) \cdot r^{k_i} \cdot (1-r)^{n_i}}{\left(\!\binom{\sum_i k_i}{K-\sum_i k_i}\!\right) \cdot r^{\sum_i k_i} \cdot (1-r)^{K-\sum_i k_i}} \\
&= \frac{\prod_i \left(\!\binom{k_i}{n_i}\!\right)}{\left(\!\binom{\sum_i k_i}{K-\sum_i k_i}\!\right)} \\
&\overset{(10)}{=} pl[K-\textstyle\sum_i k_i]\big(\sum_i k_i|i\rangle\big)\big(\sum_i n_i|i\rangle\big).
\end{aligned}
$$

□

9 Number-theoretic corollaries

In this final section we extract several number-theoretic equations from the fact that first-full and negative probabilities form distributions and thus add up to one. These equations are obtained from the bivariate case, with two tubes. Recall, that the bivariate situation studied in the literature involves one tube only. As far as we know, the equations given below are new (or at least, not very familiar). For some of them — like Corollaries 15 (1) and 16 (1) — the author has direct proofs, but not for the others.

We first look at what follows from the bivariate first-full distributions.

Corollary 15 *Fix numbers $n > 0$ and $m > 0$.*

1. *For $r, s \in [0, 1]$ with $r + s = 1$ one has:*

$$
r^n \cdot \sum_{j<m} \left(\!\!\binom{n}{j}\!\!\right) \cdot s^j \;+\; s^m \cdot \sum_{i<n} \left(\!\!\binom{m}{i}\!\!\right) \cdot r^i \;=\; 1.
$$

2. *For $N \geq n$ and $M \geq m$ one has:*

$$
\sum_{j<m} \left(\!\!\binom{n}{j}\!\!\right) \cdot \binom{N-n+M-j}{N-n} \;+\; \sum_{i<n} \left(\!\!\binom{m}{i}\!\!\right) \cdot \binom{N-i+M-m}{M-m} \;=\; \binom{N+M}{N}.
$$

3. *For $N > 0$ and $M > 0$,*

$$
n \cdot \left(\!\!\binom{N}{n}\!\!\right) \cdot \sum_{j<m} \frac{\left(\!\binom{M}{j}\!\right)}{\left(\!\binom{n+j}{N+M}\!\right)} \;+\; m \cdot \left(\!\!\binom{M}{m}\!\!\right) \cdot \sum_{i<n} \frac{\left(\!\binom{N}{i}\!\right)}{\left(\!\binom{i+m}{N+M}\!\right)} \;=\; N+M.
$$

Proof. Take a binary space $X = \{a, b\}$ with tubes $\tau = n|a\rangle + m|b\rangle$.

1. The numbers r, s form a state $\omega = r|a\rangle + s|b\rangle$. Since $mnff(\omega, \tau)$ is a distribution on X we get $mnff(\omega, \tau)(a) + mnff(\omega, \tau)(b) = 1$. According to Definition 3 (1) this means:

$$
1 = \sum_{j<m} mn(\omega)((n-1)|a\rangle + j|b\rangle) \cdot \omega(a)
$$

$$
\begin{aligned}
&\quad + \sum_{i<n} mn(\omega)(i|a\rangle + (m-1)|b\rangle) \cdot \omega(b) \\
&= \sum_{j<m} \binom{n-1+j}{n-1} \cdot r^{n-1} \cdot s^j \cdot r \; + \; \sum_{i<n} \binom{i+m-1}{i} \cdot r^i \cdot s^{m-1} \cdot s \\
&= r^n \cdot \sum_{j<m} \left(\!\binom{n}{j}\!\right) \cdot s^j \; + \; s^m \cdot \sum_{i<n} \left(\!\binom{m}{i}\!\right) \cdot r^i.
\end{aligned}
$$

2. For urn $\upsilon = N|a\rangle + M|b\rangle$ we have a hypergeometric first-fill distribution $hgff(\upsilon, \tau)$, so that by Definition 3 (2):

$$
\begin{aligned}
1 \;&=\; hgff(\upsilon,\tau)(a) + hgff(\upsilon,\tau)(b) \\
&= \sum_{j<m} hg(\upsilon)((n-1)|a\rangle + j|b\rangle) \cdot Flrn\big(\upsilon - (n-1)|a\rangle - j|b\rangle\big)(a) \\
&\qquad + \sum_{i<n} hg(\upsilon)(i|a\rangle + (m-1)|b\rangle) \cdot Flrn\big(\upsilon - i|a\rangle - (m-1)|b\rangle\big)(b) \\
&= \sum_{j<m} \frac{\binom{N}{n-1} \cdot \binom{M}{j}}{\binom{N+M}{n-1+j}} \cdot \frac{N-n+1}{N+M-n+1-j} \\
&\qquad + \sum_{i<n} \frac{\binom{N}{i} \cdot \binom{M}{m-1}}{\binom{N+M}{i+m-1}} \cdot \frac{M-m+1}{N+M-i-m+1} \\
&= \sum_{j<m} \frac{N! \cdot M! \cdot (n-1+j)! \cdot (N+M-n+1-j)!}{(n-1)! \cdot (N-n+1)! \cdot j! \cdot (M-j)! \cdot (N+M)!} \cdot \frac{N-n+1}{N+M-n+1-j} \\
&\qquad + \sum_{i<n} \frac{N! \cdot M! \cdot (i+m-1)! \cdot (N+M-i-m+1)!}{i! \cdot (N-i)! \cdot (m-1)! \cdot (M-m+1)! \cdot (N+M)!} \cdot \frac{M-m+1}{N+M-i-m+1} \\
&= \frac{1}{\binom{N+M}{N}} \cdot \left(\sum_{j<m} \left(\!\binom{n}{j}\!\right) \cdot \binom{N-n+M-j}{N-n} \; + \; \sum_{i<n} \left(\!\binom{m}{i}\!\right) \cdot \binom{N-i+M-m}{M-m} \right).
\end{aligned}
$$

3. By rewriting the equation $plff(\upsilon,\tau)(a) + plff(\upsilon,\tau)(b) = 1$ in a similar manner. □

Next we look at the consequences of having (bivariate) negative distributions.

Corollary 16 *Let arbitrary numbers $n > 0$ and $m > 0$ be given.*

1. *For probabilities $r, s \in (0,1)$ with $r + s = 1$ one has:*

$$
\sum_{i\geq 0} \left(\!\binom{n}{m+i}\!\right) \cdot s^i \; + \; \left(\!\binom{m}{n+i}\!\right) \cdot r^i \;=\; \frac{1}{r^n \cdot s^m}.
$$

2. *For $N \geq n$ and $M \geq m$,*

$$
\begin{aligned}
&\sum_{j \leq M-m} \left(\!\binom{n}{m+j}\!\right) \cdot \binom{N-n+M-m-j}{N-n} \\
&\qquad + \sum_{i \leq N-n} \left(\!\binom{m}{n+i}\!\right) \cdot \binom{N-n-i+M-m}{M-m} \;=\; \binom{N+M}{N}.
\end{aligned}
$$

3. *For $N > 0$ and $M > 0$ we have:*

$$
n \cdot \left(\!\binom{N}{n}\!\right) \cdot \sum_{j\geq m} \frac{\left(\!\binom{M}{j}\!\right)}{\left(\!\binom{n+j}{N+M}\!\right)} \; + \; m \cdot \left(\!\binom{M}{m}\!\right) \cdot \sum_{i \geq n} \frac{\left(\!\binom{N}{i}\!\right)}{\left(\!\binom{i+m}{N+M}\!\right)} \;=\; N+M.
$$

Proof. We only do the first and third item and leave the second one to the interested reader. Like in the proof of Corollary 15 we fix a space $X = \{a, b\}$ with tubes $\tau = n|a\rangle + m|b\rangle$. For state $\omega = r|a\rangle + s|b\rangle$ we use that the negative multinomial $nmn(\omega, \tau)$ is a distribution on $\mathbb{N}$ and unpack its description from Definition 4 (1).

$$\begin{aligned}
1 &= \sum_{i\geq 0} nmn(\omega,\tau)(i) \\
&= \sum_{i\geq 0} mn(\omega)((n-1)|a\rangle + (m+i)|b\rangle)\cdot\omega(a) \;+\; mn(\omega)((n+i)|a\rangle + (m-1)|b\rangle)\cdot\omega(b) \\
&= \sum_{i\geq 0} \binom{n+i+m-1}{n-1}\cdot r^{n-1}\cdot s^{m+i}\cdot r \;+\; \binom{n+i+m-1}{n+i}\cdot r^{n+i}\cdot s^{m-1}\cdot s \\
&= r^n\cdot s^m\cdot\sum_{i\geq 0}\left(\!\!\binom{n}{m+i}\!\!\right)\cdot s^i \;+\; \left(\!\!\binom{m}{n+i}\!\!\right)\cdot r^i.
\end{aligned}$$

For item (3) we use:

$$\begin{aligned}
1 &= \sum_{i\geq 0} pl(\upsilon)((n-1)|a\rangle + (m+j)|b\rangle)\cdot Flrn(\upsilon + (n-1)|a\rangle + (m+j)|b\rangle)(a) \\
&\qquad + pl(\upsilon)((n+i)|a\rangle + (m-1)|b\rangle)\cdot Flrn(\upsilon + (n+i)|a\rangle + (m-1)|b\rangle)(b) \\
&= \sum_{i\geq 0}\frac{\left(\!\binom{N}{n-1}\!\right)\cdot\left(\!\binom{M}{m+i}\!\right)}{\left(\!\binom{N+M}{n-1+m+i}\!\right)}\cdot\frac{N+n-1}{N+M+n-1+m+i} \\
&\qquad + \frac{\left(\!\binom{N}{n+i}\!\right)\cdot\left(\!\binom{M}{m-1}\!\right)}{\left(\!\binom{N+M}{n+i+m-1}\!\right)}\cdot\frac{M+m-1}{N+M+n+i+m-1} \\
&= \sum_{i\geq 0}\frac{n\cdot\left(\!\binom{N}{n}\!\right)\cdot\left(\!\binom{M}{m+i}\!\right)\cdot(n-1+m+i)!\cdot(N+M-1)!}{(N+M+n-2+m+i)!}\cdot\frac{1}{N+M+n-1+m+i} \\
&\qquad + \frac{\left(\!\binom{N}{n+i}\!\right)\cdot m\cdot\left(\!\binom{M}{m}\!\right)\cdot(n+i+m-1)!\cdot(N+M-1)!}{(N+M+n+i+m-2)!}\cdot\frac{1}{N+M+n+i+m-1} \\
&= \frac{1}{N+M}\cdot\left(n\cdot\left(\!\!\binom{N}{n}\!\!\right)\cdot\sum_{j\geq m}\frac{\left(\!\binom{M}{j}\!\right)}{\left(\!\binom{n+j}{N+M}\!\right)} + m\cdot\left(\!\!\binom{M}{m}\!\!\right)\cdot\sum_{i\geq n}\frac{\left(\!\binom{N}{i}\!\right)}{\left(\!\binom{i+m}{N+M}\!\right)}\right).
\end{aligned}$$

□

10 Conclusions

This paper extends the familiar urn model to an urn & tubes model. It raises several research questions, with possible applications in risk modeling. The extension is first used to introduce first-full distributions, which have a historical basis in the 'problem of points' of Pascal and Fermat. Next, the urn & tubes models is used for negative distributions. The contribution of this paper lies in systematisation, via a clear model, formalised via multisets (for urns, draws, tubes), covering the three main drawing modes (multinomial, hypergeometric, Pólya).

This paper concentrates on the conceptual basis, formalisation, and illustration of first-full and negative distributions. There is more to say, for instance about associated statistical properties like mean and (co)variance. They exist in the literature for the single tube case. Extension to general tubes is a challenge that is left open here.

The urn & tubes model may be generalised, for instance to multiple urns, where there is a choice from which urn one wishes to draw a ball. When the contents of the urns are known, one can consider different strategies for such choices, in different drawing modes, via Markov decision processes (see *e.g.* [1, 23]). When the contents are unknown, the setting may be used for reinforcement learning [16, 27]: jointly learning these contents and developing a strategy.

Appendix

Section 6 and Subsection 7.2 use a compositional approach for showing that first-full and negative probabilities add up to one, and thus form proper distributions. The distributions appear after iteratively self-composing a Markov model with output, in the form of a coalgebra $c\colon Y \to \mathcal{D}(Y + X)$, see (12). There is a little bit of category theory underlying this composition, which we make explicit in this appedix.

It is well known that the mapping $A \mapsto \mathcal{D}(A)$, sending a set A to the set of (discrete, finite) probability distributions on A is a monad, on the category **Sets** of sets and functions. The unit η and multiplication μ of this monad $\mathcal{D}$ are:

$$\begin{array}{ccc} A \xrightarrow{\;\eta\;} \mathcal{D}(A) & \qquad & \mathcal{D}\big(\mathcal{D}(A)\big) \xrightarrow{\qquad\mu\qquad} \mathcal{D}(A) \\ a \longmapsto 1\big|a\big\rangle & & \sum_i r_i\big|\omega_i\big\rangle \longmapsto \displaystyle\sum_{a\in A}\Big(\sum_i r_i\cdot\omega_i(a)\Big)\big|a\big\rangle. \end{array}$$

We write $A + B$ for the coproduct (disjoint union) of two sets A, B, with coprojections $A \xrightarrow{\kappa_1} A + B \xleftarrow{\kappa_2} B$, and cotuple $[f, g]\colon A + B \to C$, for $f\colon A \to C$, $g\colon B \to C$. For a fixed set X, the mapping $A \mapsto A + X$ is also a monad with unit $\kappa_1\colon A \to A + X$ and multiplication $[\mathrm{id}, \kappa_2]\colon (A + X) + X \to A + X$.

These two monads $\mathcal{D}$ and $(-) + X$ are connected via a distributive law, of the form:

$$\mathcal{D}(A) + X \xrightarrow{\;\lambda\;} \mathcal{D}(A + X) \qquad \text{namely} \qquad \lambda = \big[\mathcal{D}(\kappa_1),\, \eta \circ \kappa_2\big].$$

A general categorical result, see *e.g.* [2], now says that the composite $\mathcal{D}\big((-) + X\big)$ is then also a monad. In particular, if we have maps $c\colon A \to \mathcal{D}\big(B + X\big)$ and $d\colon B \to \mathcal{D}\big(C + X\big)$ we can form a composition $d \bullet c\colon A \to \mathcal{D}\big(C + X\big)$ as:

$$\begin{array}{rl} d \bullet c \;=\; \Big(A \xrightarrow{c} \mathcal{D}\big(B{+}X\big) \xrightarrow{\mathcal{D}(d+\mathrm{id})} & \mathcal{D}\big(\mathcal{D}\big(C{+}X\big){+}X\big) \\ & \Big\downarrow{\scriptstyle \mathcal{D}(\lambda)} \\ & \mathcal{D}\big(\mathcal{D}\big((C{+}X){+}X\big)\big) \xrightarrow{\mathcal{D}(\mathcal{D}([\mathrm{id},\kappa_2]))} \mathcal{D}\big(\mathcal{D}\big(C{+}X\big)\big) \xrightarrow{\mu} \mathcal{D}\big(C{+}X\big)\Big) \end{array}$$

Now assume that we have a Markov model with output (MMO) $c\colon Y \to \mathcal{D}\big(Y + X\big)$. We can form self-composites $c^n\colon Y \to \mathcal{D}\big(Y + X\big)$, for $n \in \mathbb{N}$, in the following manner:

$$c^0 = \eta \circ \kappa_1 \qquad \text{and} \qquad c^{n+1} = c^n \bullet c.$$

By elaborating the details we get the self-composition formulas (13) used for MMOs.

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