Distributions, Continued Fractions, and the Ehrenfest Urn Model

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1. Introduction

Let f(x) be a function of a real variable and let $Lf(x) = x^{-1} \int_0^\infty f(t) e^{-tx^{-1}} dt$. As usual let

$$\frac{1}{1-a_0x} - \frac{b_0x^2}{1-a_1x} - \frac{b_1x^2}{1-a_2x} - \cdots$$

denote the continued fraction

$$\frac{1}{1 - a_0 x - b_0 x^2} \frac{1}{1 - a_1 x - b_1 x^2} \dots$$

In the classical literature on continued fractions there are many results of the form

$$Lf(x) = \frac{1}{1 - a_0 x} - \frac{b_0 x^2}{1 - a_1 x} - \frac{b_1 x^2}{1 - a_2 x} - \cdots$$
 (1)

subject to conditions on x. We are interested in results of this type for the ring $\mathbb{Q}[[x]]$ of formal power series in the indeterminate x, where \mathbb{Q} denotes the rationals. Note that if $f(x) = \sum_{i \geq 0} f_i x^i / i! \in \mathbb{Q}[[x]]$, then $L \sum_{i \geq 0} f_i x^i / i! = \sum_{i \geq 0} f_i x^i$ so in this case (1) gives a continued fraction representation of the ordinary generating function corresponding to a given exponential generating function f(x).

A number of identities of type (1) have been established on $\mathbb{Q}[[x]]$ by combinatorial means. This has been done by Flajolet [1], using continued fractions to enumerate lattice paths, and by using combinatorial bijections between these and (i) permutations (due to Françon and Viennot [2]) and (ii) "pairings" (due to Read [6], Flajolet [1]).

The following are two examples of identities in $\mathbb{Q}[[x]]$ of type (1).

$$L(\cosh^{m}(x)) = \frac{1}{1} - \frac{m \cdot 1x^{2}}{1} - \frac{(m-1) \cdot 2x^{2}}{1} - \dots - \frac{1 \cdot mx^{2}}{1}, \qquad (2)$$

$$L\left(\sum_{k \ge 0} \left\{ \frac{x^{3k}}{(3k)!} - \frac{x^{3k+1}}{(3k+1)!} \right\} \right)^{-1}$$

$$= \frac{1}{1-x} - \frac{1^{2}x^{2}}{1-2x} - \frac{2^{2}x^{2}}{1-3x} - \dots. \qquad (3)$$

The analytic version of identity (2) has been given by Rogers [8], where it is proved by means of the Stieltjes-Rogers *J*-fraction theorem. Identity (3) is given in Goulden and Jackson [3, p. 310], where it is proved by means of bijection (i), as well as the Stieltjes-Rogers *J*-fraction theorem.

In this paper we consider a third bijection, between lattice paths and distributions (i.e., ordered partitions), which enables us to obtain a combinatorial proof of Rogers' result (2). More interestingly, this leads us to a combinatorial derivation of the transition probabilities P(n, m, i, k) in the Ehrenfest urn model, originally proposed for resolving the apparent discrepancy between irreversibility and recurrence in Boltzmann's theory of gases (see Kac [5] for a discussion of this point). The model may be described as follows. There are m balls, numbered from 1 to m, distributed between two boxes (I and II). Choose an integer between 1 and m (all integers are assumed to be equally probable) and transfer the ball with this label to the other box. Let P(n, m, i, k) be the probability that box I. originally containing i balls, contains k balls after n transferences. Note that the probability that a ball is transferred from box I to box II is i/m. when I contains i balls, and the probability that a ball is transferred from box II to box I is (m-i)/m. Thus this system may be modelled as a random walk in which the state of the system is the number of balls in box I, and the single-stage transition probabilities from state i to i-1 and i+1are i/m and (m-i)/m, respectively. The *n*-stage transition probability from state i to state k is given by P(n, m, i, k). Kac [5] originally derived an expression for P(n, m, i, k), and a shorter derivation was given by Takács [9].

The Ehrenfest urn model gives a simple model of heat exchange between two isolated bodies of unequal temperatures. Temperature is represented by the numbers of balls in the boxes, and heat exchange by transference of balls.

Throughout this paper we denote the coefficient of x^n in the formal power series f(x) by $[x^n] f(x)$.

2. WEIGHTED PATHS AND THE PATH LEMMA

If $p = p_1 \cdots p_n$ is a sequence over $\{-1, 1\}$, with $n \ge 0$ and $k + p_1 + \cdots + p_i \ge 0$ for i = 0, ..., n, then we say that $(p)_k$ is a path of length n, with initial altitude k and terminal altitude $k + p_1 + \cdots + p_n$. For $i \ge 1$, p_i is a step in the path, and for $k + p_1 + \cdots + p_{i-1} = t$, then p_i is a rise or fall at altitude t, if $p_i = 1$ or -1, respectively.

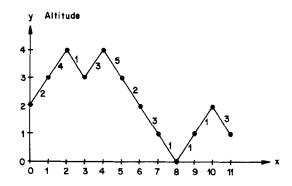
Suppose that $\pi = ((p_1 \cdots p_n)_k, w_1 \cdots w_n)$ for some $n \ge 0$, where $(p_1 \cdots p_n)_k$ is a path and $w_1 \cdots w_n$ is a sequence of positive integers such that $1 \le w_i \le \psi_{p_i}(k+p_1+\cdots+p_{i-1})$, where $\psi_{-1}(j)$, $j \ge 1$ and $\psi_1(l)$, $l \ge 0$ are fixed nonnegative integers. Then π is a weighted path of length n, with initial altitude k, and with possibility functions $\psi_{-1}(j)$ and $\psi_1(l)$. The positive integer w_i is the weight associated with the step p_i .

The weighted path $\pi = ((p_1 \cdots p_n)_k, w_1 \cdots w_n)$ may be represented geometrically in the plane by the sequence $v_0 e_1 v_1 e_2 v_2 \cdots e_n v_n$ of vertices $v_i = (i, k + p_1 + \cdots + p_i)$ and edges (steps) $e_i = v_{i-1} v_i$, with weight w_i attached as a "label" to e_i . Thus a step from altitude t is represented by an edge whose initial ordinate is t (where $t \ge 0$). The ordinate of the terminal vertex is equal to the terminal altitude of the path. The empty path at altitude k, of length 0, is represented by a single vertex at altitude k. For example, a weighted path π_1 , with possibility functions $\psi_{-1}(j) = \psi_1(j) = j+1$ is illustrated in Fig. 1.

The following enumerative result for weighted paths is well known (see, e.g., Jackson [4], Flajolet [1], or Goulden and Jackson [3]).

LEMMA 2.1. The number of weighted paths of length n, from altitude 0 to altitude 0, with possibility functions $\psi_{-1}(j)$, $j \ge 1$, and $\psi_1(l)$, $l \ge 0$, is

$$[x^n] \frac{1}{1} - \frac{\psi_1(0) \psi_{-1}(1) x^2}{1} - \frac{\psi_1(1) \psi_{-1}(2) x^2}{1} - \cdots$$



¹ = ((1 1 -1 1 -1 -1 -1 -1 11-1)₂, 2 4 1 3 5 2 3111 3)

Fig. 1. A weighted path with possibility functions $\psi_{-1}(j) = \psi_1(j) = j+1$.

3. ROGERS' RESULT AND A BIJECTION BETWEEN WEIGHTED PATHS AND DISTRIBUTIONS

We now introduce a combinatorial object which seems to have no obvious connection to weighted paths. An (n, m)-distribution of type k is an ordered partition $(\alpha_1, \alpha_2, ..., \alpha_m)$ of $\{1, 2, ..., n\}$ in which exactly k of the (possibly empty) subsets α_i have odd cardinality, where $n, m \ge k \ge 0$. For example $(\{3\}, \{1, 5\}, \{2\}, \emptyset, \{4, 6, 7\})$ is a (7, 5)-distribution of type 3. Let D(n, m) be the number of (n, m)-distributions of type 0. The following form for D(n, m) is well known (see Riordan [7]).

PROPOSITION 3.1. $D(n, m) = [x^n/n!] \cosh^m(x)$.

Proof. Clearly

$$D(n, m) = \sum_{\substack{i_1, \dots, i_m \text{ even} \\ i_1 + \dots + i_m = n}} \frac{n!}{i_1! \cdots i_m!}$$

and multiplying both sides by $x^n/n!$ and summing for $n \ge 0$ yields

$$\sum_{n\geq 0} D(n, m) \frac{x^n}{n!} = \left(\sum_{i \text{ even }} \frac{x^i}{i!}\right)^m = \cosh^m(x).$$

Alternatively, an (n, m)-distribution of type 0 consists of an ordered collection of m even subsets that form a partition of $\{1, 2, ..., n\}$. The exponential generating function for even sets is $\sum_{i \text{ even }} 1 \cdot x^i / i! = \cosh(x)$, so by the product lemma for exponential generating functions (Goulden and Jackson [3, p. 163]), the exponential generating function for (n, m)-distributions of type 0 is $\cosh^m(x)$.

The second method of proof in Proposition 3.1 will be used in Proposition 4.2, for a generalized distribution problem.

Next we establish a bijection Π between these distributions and a set of weighted paths. For an arbitrary (n, m)-distribution d of type 0 let $\Gamma(d) = (\gamma_0(d), \gamma_1(d), ..., \gamma_n(d))$, where $\gamma_i(d)$ is the unique (i, m)-distribution formed by deleting elements i+1,...,n from d. Thus $\gamma_0(d) = (\varnothing,...,\varnothing)$ and $\gamma_n(d) = d$. For example, if $d_0 = (\{4,6\},\{1,5\},\{2,3\})$, a (6,3)-distribution of type 0, then $\Gamma(d_0) = ((\varnothing,\varnothing,\varnothing),(\varnothing,\{1\},\varnothing),(\varnothing,\{1\},\{2\}),(\varnothing,\{1\},\{2,3\}),(\{4\},\{1\},\{2,3\}),(\{4\},\{1\},\{2,3\}),(\{4\},\{1,5\},\{2,3\}),(\{4,6\},\{1,5\},\{2,3\}))$.

Let the type of $\gamma_i(d)$ be denoted by t_i , so that $\gamma_i(d)$ consists of t_i odd subsets and $m - t_i$ even subsets for i = 0, ..., n. Then $\Pi(d) = ((r_1 \cdots r_n)_0, s_1 \cdots s_n)$ is the weighted path formed as follows. If $\gamma_{i+1}(d)$ is formed from $\gamma_i(d)$ by inserting i + 1 into the kth, from the left, of the t_i odd subsets in $\gamma_i(d)$, then

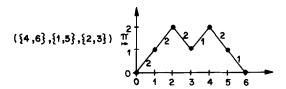


Fig. 2. The weighted path corresponding to $(\{4,6\},\{1,5\},\{2,3\})$.

 $r_{i+1} = -1$ and $s_{i+1} = k$. If $\gamma_{i+1}(d)$ is formed from $\gamma_i(d)$ by inserting i+1 into the kth, from the left, of the $m-t_i$ even subsets in $\gamma_i(d)$, then $r_{i+1} = 1$ and $s_{i+1} = k$. For example, if $d_0 = (\{4, 6\}, \{1, 5\}, \{2, 3\})$ then $\Pi(d_0) = ((1 \ 1 \ -1 \ 1 \ -1 \ -1)_0, 2 \ 2 \ 2 \ 1 \ 2 \ 1)$, which is illustrated in Fig. 2.

Now $r_1 + \cdots + r_i = t_i$, since inserting i into an odd subset reduces the number of odd subsets by one, and inserting i into an even subset increases the number of odd subsets by one. Thus r_{i+1} is a step at altitude t_i and $\psi_{-1}(t_i) = t_i$, $\psi_1(t_i) = m - t_i$, i = 0,..., n-1, so $\Pi(d)$ is a path of length n from altitude 0 to altitude 0, with possibility functions $\psi_{-1}(j) = j$ and $\psi_1(j) = m - j$. Let W(n, m) be the number of weighted paths of length n, from altitude 0 to altitude 0, with possibility functions $\psi_{-1}(j) = j$ and $\psi_1(j) = m - j$. The following result is now immediate.

Correspondence 3.2. D(n, m) = W(n, m) for $n, m \ge 0$.

Proof. The construction of $\Pi(d)$, given above, is clearly reversible, so Π is a bijection between the set of (n, m)-distributions of type 0, and the set of weighted paths of length n, from altitude 0 to altitude 0, with possiblity functions $\psi_{-1}(j) = j$ and $\psi_1(j) = m - j$. The result follows by the definitions of D(n, m) and W(n, m).

But we have another way of determining W(n, m).

Proposition 3.3.

$$W(n, m) = [x^{n}] \frac{1}{1} - \frac{m \cdot 1 \cdot x^{2}}{1} - \frac{(m-1) \cdot 2 \cdot x^{2}}{1}$$
$$- \cdots \frac{2 \cdot (m-1) \cdot x^{2}}{1} - \frac{1 \cdot m \cdot x^{2}}{1}.$$

Proof. Direct from Lemma 2.1, with $\psi_{-1}(j) = j$ and $\psi_1(j) = m - j$. The continued fraction is finite since $\psi_1(m) = 0$.

Combining the previous three results, we obtain a combinatorial proof of Rogers' result (stated as identity (2) in Sect. 1).

Proof of Rogers' Result. From Proposition 3.1 we have

$$\sum_{n>0} D(n, m) \frac{x^n}{n!} = \cosh^m(x)$$

so

$$\sum_{n \ge 0} D(n, m) x^n = L \left\{ \sum_{n \ge 0} D(n, m) \frac{x^n}{n!} \right\} = L \{ \cosh^m(x) \}.$$

But from Proposition 3.3

$$\sum_{n \ge 0} W(n, m) x^n = \frac{1}{1} - \frac{m \cdot 1 \cdot x^2}{1} - \cdots \frac{1 \cdot m \cdot x^2}{1},$$

and the result follows by Correspondence 3.2.

The numbers D(n, m) and W(n, m) have been introduced to enable us to prove the power series identity between $\cosh^m(x)$ and its corresponding continued fraction. If we were interested in obtaining a closed-form expression for W(n, m), then the direct use of Proposition 3.3 seems difficult. However, combining Proposition 3.1 and Correspondence 3.2 give the following expression for W(n, m).

Proposition 3.4.

$$W(n, m) = D(n, m) = \frac{1}{2^m} \sum_{j=0}^m {m \choose j} (m - 2j)^n.$$

Proof. From Correspondence 3.2 and Proposition 3.1,

$$W(n, m) = D(n, m) = \left[\frac{x^n}{n!}\right] \cosh^m(x) = \frac{1}{2^m} \left[\frac{x^n}{n!}\right] (e^x + e^{-x})^m$$
$$= \frac{1}{2^m} \sum_{j=0}^m {m \choose j} \left[\frac{x^n}{n!}\right] e^{(m-2j)x}$$

and the result follows.

4. THE EHRENFEST TRANSITION PROBABILITIES AND DISTRIBUTIONS

Let W(n, m, i, k) be the number of weighted paths of length n, from altitude i to altitude k, with possibility functions $\psi_{-1}(j) = j$ and $\psi_{1}(j) = j$

m-j. We wish to evaluate W(n, m, i, k) because of its close connection with the Ehrenfest transition probability P(n, m, i, k), defined in Section 1.

Proposition 4.1.

$$P(n, m, i, k) = \frac{1}{m^n} W(n, m, i, k).$$

Proof. Let $a(b_0, b_1,...; c_1, c_2,...)$ be the number of paths of length n from altitude i to altitude k with b_j rises and c_j falls at altitude j, where $b_0 + b_1 + \cdots + c_1 + c_2 + \cdots = n$. Then

$$P(n, m, i, k) = \sum a(b_0, ...; c_1, ...) \prod_{j \ge 0} \left(1 - \frac{j}{m}\right)^{b_j} \prod_{l \ge 1} \left(\frac{l}{m}\right)^{c_l}$$

$$= \frac{1}{m^n} \sum a(b_0, ...; c_1, ...) \prod_{j \ge 0} (m - j)^{b_j} \prod_{l \ge 0} l^{c_l}$$

$$= \frac{1}{m^n} W(n, m, i, k). \quad \blacksquare$$

In Proposition 3.4 we evaluated $W(n, m, 0, 0) \equiv W(n, m)$ indirectly, by establishing a bijection between paths from altitude 0 to altitude 0 and (n, m)-distributions of type 0. The number of such distributions is denoted by D(n, m), and has a simple exponential generating function, given in Proposition 3.1. We did not evaluate W(n, m) directly by extracting the appropriate coefficient from the continued fraction.

In a similar way, we can express W(n, m, i, k) as a coefficient in an expression involving the above continued fraction and its numerator and denominator polynomials. This expression is not given here, since the coefficient is difficult to extract directly, so we consider a generalization of the above distributions that will allow us to evaluate W(n, m, i, k) indirectly.

An (n, m, i)-distribution of type k is an ordered partition $(\alpha_1, \alpha_2, ..., \alpha_m)$ of $\{0_1, 0_2, ..., 0_i, 1, 2, ..., n\}$ in which $0_j \in \alpha_j$ for j = 1, ..., i, and in which exactly k of the (possibly empty) subsets α_j have odd cardinality, where $m \ge i, k \ge 0$, $i + n \ge k, n \ge 0$. For example, $(\{0_1, 2, 6\}, \{0_2\}, \emptyset, \{1, 3, 5, 7\}, \{4\})$ is a (7, 5, 2)-distribution of type 3. Let D(n, m, i, k) be the number of (n, m, i)-distributions of type k. With an arbitrary (n, m, i)-distribution $d = (\alpha_1, ..., \alpha_m)$ we associate the unique (n, m)-distribution $\Omega(d) = (\beta_1, ..., \beta_m)$, where $\beta_j = \alpha_j - \{0_j\}$ for j = 1, ..., i, and $\beta_j = \alpha_j$ for j = i + 1, ..., m. We now enumerate (n, m, i)-distributions by considering the (n, m)-distributions which result from the application of Ω .

Proposition 4.2.

$$D(n, m, i, k) = \left[y^k \frac{x^n}{n!} \right] (\sinh(x) + y \cosh(x))^i (\cosh(x) + y \sinh(x))^{m-i}.$$

Proof. Let d be an arbitrary (n, m, i)-distribution. Then $\Omega(d)$ is an (n, m)-distribution, consisting of m ordered subsets. The type of d equals the sum of the number of even subsets in the first i subsets of $\Omega(d)$ plus the number of odd subsets in the last m-i subsets of $\Omega(d)$. Following the proof of Proposition 3.1, the exponential generating function for even sets is $\cosh(x)$ and for odd sets is $\sinh(x)$, and the result follows.

The equality of W(n, m, i, k) and D(n, m, i, k) is now established by suitably modifying the mapping Π of Section 3. If d is an (n, m, i)-distribution of type k, then let $\Gamma'(d) = (\gamma'_0(d), \gamma'_1(d), ..., \gamma'_n(d))$, where $\gamma'_j(d)$ is the unique (j, m, i)-distribution formed by deleting elements j+1,..., n from d. Thus $\gamma'_0(d) = (\{0_1\}, ..., \{0_i\}, \emptyset, ..., \emptyset)$ and $\gamma'_n(d) = d$. Let t'_j be the type of $\gamma'_j(d)$, for j=0,..., n, so $t'_0=i$ and $t'_n=k$. Define $\Pi'(d) = ((r'_1 \cdots r'_n)_i, s'_1 \cdots s'_n)$ to be the weighted path defined as follows. If $\gamma'_{j+1}(d)$ is formed from $\gamma'_j(d)$ by inserting j+1 into the lth, from the left, of the t'_j odd subsets in $\gamma'_j(d)$, then $r'_{j+1}=-1$ and $s'_{j+1}=l$. If $\gamma'_{j+1}(d)$ is formed from $\gamma'_j(d)$ by inserting j+1 into the lth, from the left of the $m-t'_j$ even subsets in $\gamma'_j(d)$, then $r'_{j+1}=1$ and $s'_{j+1}=l$.

For example, if $d_0 = (\{0_1, 2, 6\}, \{0_2\}, \emptyset, \{1, 3, 5, 7\}, \{4\})$, a (7, 5, 2)-distribution of type 3, then $\Pi'(d_0) = ((1 -1 -1 1 1 1 -1)_2, 2 1 2 4 3 1 3)$, which is illustrated in Fig. 3.

But $i + r'_1 + \cdots + r'_j = t'_j$, so r'_{j+1} is a step at altitude t'_j , and $\psi_{-1}(t'_j) = t'_j$, $\psi_1(t'_j) = m - t'_j$, so $\Pi'(d)$ is a path of length n from altitude i to altitude k, with possibility functions $\psi_{-1}(j) = j$ and $\psi_1(j) = m - j$.

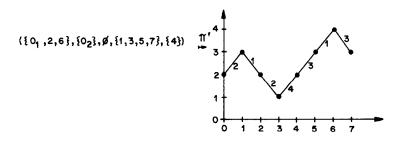


Fig. 3. The weighted path corresponding to $(\{0_1, 2, 6\}, \{0_2\}, \emptyset, \{1, 3, 5, 7\}, \{4\})$.

CORRESPONDENCE 4.3. D(n, m, i, k) = W(n, m, i, k).

Proof. The mapping Π' described above is a bijection between the set of (n, m, i)-distributions of type k and the set of weighted paths of length n, from altitude i to altitude k, with possibility functions $\psi_{-1}(j) = j$ and $\psi_1(j) = m - j$. The result follows immediately.

By combining the above results, we may obtain the transition probabilities for the Ehrenfest urn model. The following form for these probabilities is given in Kac [5] and Takács [9].

THEOREM 4.4.

$$P(n, m, i, k) = \frac{1}{2^m} \sum_{j=0}^m a_{ij} a_{jk} \left(1 - \frac{2j}{m}\right)^n$$

where $\sum_{j=0}^{m} a_{ij} z^{j} = (1-z)^{i} (1+z)^{m-i}$.

Proof. From Propositions 4.1, 4.2 and Correspondence 4.3, we have

$$P(n, m, i, k) = \frac{1}{m^n} \left[y^k \frac{x^n}{n!} \right] (\sinh(x) + y \cosh(x))^i$$

$$\times (\cosh x + y \sinh(x))^{m-i}$$

$$= \frac{1}{m^n} \left[y^k \frac{x^n}{n!} \right] \frac{1}{2^m} ((1+y) e^x - (1-y) e^{-x})^i$$

$$\times ((1+y) e^x + (1-y) e^{-x})^{m-i}$$

$$= \frac{1}{2^m} \frac{1}{m^n} \left[y^k \frac{x^n}{n!} \right] \sum_{i=0}^m a_{ij} \{ (1+y) e^x \}^{m-j} \{ (1-y) e^{-x} \}^j$$

and the result follows, since $[y^k](1-y)^j(1+y)^{m-j} = a_{jk}$ and $m^{-n}[x^n/n!]$ $e^{(m-2j)x} = (1-2j/m)^n$.

Let $E(n, m, i) = \sum_{k=0}^{m} k \cdot P(n, m, i, k)$ be the expected value of the state which the system is in n stages after starting in stage i. It is straightforward to determine E(n, m, i) from the given generating function.

Proposition 4.5.

$$E(n, m, i) = \frac{m}{2} \left\{ 1 - \left(1 - \frac{2i}{m} \right) \left(1 - \frac{2}{m} \right)^n \right\}.$$

Proof. From Propositions 4.1, 4.2 and Correspondence 4.3, we have

$$E(n, m, i) = \frac{1}{m^n} \left[\frac{x^n}{n!} \right] \frac{\partial}{\partial y} \left(\sinh(x) + y \cosh(x) \right)^i$$

$$\times \left(\cosh(x) + y \sinh(x) \right)^{m-i} |_{y=1}$$

$$= \frac{1}{m^n} \left[\frac{x^n}{n!} \right] \left(i \cosh(x) + (m-i) \sinh(x) \right) e^{(m-1)x}$$

$$= \frac{1}{2m^n} \left[\frac{x^n}{n!} \right] \left(me^x - (m-2i) e^{-x} \right) e^{(m-1)x}$$

$$= \frac{1}{2m^n} \left(m^{n+1} - (m-2i)(m-2)^n \right),$$

and the result follows.

This is equivalent to a result (Eq. (64)) of Kac [5], which in the limit yields Newton's law of cooling.

Finally, we give an explicit example of the correspondence between the Ehrenfest model of moving one of m balls between two boxes n times, and the distribution problem of partitioning n objects into m sets. For m = 6, n = 11, Correspondence 4.3 tells us that if we start with balls 1, 2 in box 1, and transfer balls 3, 1, 3, 6, 2, 5, 5, 3, 5, 6, 1, leaving 3 balls in box 1, then the corresponding (11, 6, 2)-distribution of type 3 is $(\{0_1, 2, 11\}, \{0_2, 5\}, \{1, 3, 8\}, \emptyset, \{6, 7, 9\}, \{4, 10\})$.

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