# PÓLYA URN MODELS UNDER GENERAL REPLACEMENT SCHEMES

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In this paper, we consider a Pólya urn model containing balls of m different labels under a general replacement scheme, which is characterized by an  $m \times m$  addition matrix of integers without constraints on the values of these  $m^2$  integers other than non-negativity. This urn model includes some important urn models treated before. By a method based on the probability generating functions, we consider the exact joint distribution of the numbers of balls with particular labels which are drawn within n draws. As a special case, for m=2, the univariate distribution, the probability generating function and the expected value are derived exactly. We present methods for obtaining the probability generating functions and the expected values for all n exactly, which are very simple and suitable for computation by computer algebra systems. The results presented here develop a general workable framework for the study of Pólya urn models and attract our attention to the importance of the exact analysis. Our attempts are very useful for understanding non-classical urn models. Finally, numerical examples are also given in order to illustrate the feasibility of our results.

Key words and phrases: Pólya urn, replacement scheme, addition matrix, probability generating functions, double generating functions, expected value.

## 1. Introduction

Urn models have been among the most popular probabilistic schemes and have received considerable attention in the literature (see Johnson *et al.* (1997), Feller (1968)). The Pólya urn was originally applied to problems dealing with the spread of a contagious disease (see Johnson and Kotz (1977), Marshall and Olkin (1993)).

We describe the Pólya urn scheme briefly. From an urn containing  $\alpha_1$  balls labeled 1 and  $\alpha_2$  balls labeled 2, a ball is drawn, its label is noted and the ball is returned to the urn along with additional balls depending on the label of the ball drawn; If a ball labeled i (i = 1, 2) is drawn,  $a_{ij}$  balls labeled j (j = 1, 2) are added. This scheme is characterized by the following  $2 \times 2$  addition matrix of integers,  $\binom{a_{11}}{a_{12}} \binom{a_{21}}{a_{22}}$ ; whose rows are indexed by the label selected and whose columns are indexed by the label of the ball added.

Several Pólya urn models have been studied by many authors in the various addition matrices, which generate many fruitful results. The case of the classical Pólya urn model ( $a_{11} = a_{22}, a_{12} = a_{21} = 0$ ) was studied earlier and a detailed discussion can be found in Johnson and Kotz (1977). In the case of  $a_{11} = a_{22}$ ,  $a_{12} = a_{21} = 0$ , Aki and Hirano (1988) obtained the Pólya distribution of order

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k. In the case of  $a_{ii} = c$ ,  $a_{ij} = 0$  for  $i \neq j$  (i, j = 0, 1, ..., m), Inoue and Aki (2000) considered the waiting time problem for the first occurrence of a pattern in the sequence obtained by an  $(m + 1) \times (m + 1)$  Pólya urn scheme. In the case of  $a_{11} = a_{22}$ ,  $a_{12} = a_{21}$ , Friedman (1949) obtained the moment generating function of the total number of balls with a particular label remaining in the urn after n draws; Friedman's urn can be used to model the growth of leaves in recursive trees (see also Mahmoud and Smythe (1991)). In the case of  $a_{11} + a_{12} = a_{21} + a_{22}$ , Bagchi and Pal (1985) showed an interesting example of Pólya urn scheme applied to data structures in computer. (Gouet (1989, 1993) corrected some of the statements made by Bagchi and Pal (1985)). In a  $p \times p$  Pólya urn scheme (constant row sums allowing negative entries on the diagonal, but having several constraints on the eigenvalue structure), Smythe (1996) considered a central limit theorem.

One interest has been focused on the exact distribution of the total numbers of balls with particular labels remaining in the urn after n draws, or the exact distribution of the numbers of balls with particular labels which are drawn within n draws from the urn. Their derivation involves a combinatorial method of counting paths representing a realization of the urn development.

For a long time, most investigations have been made under the special structure of the constant addition matrix with constant row sums, which implies a steady linear growth of the urn size. The reason for the imposition of this constraint is mathematical convenience; Urn schemes where the constraint is imposed are generally much simpler to analyze than those where it was not imposed.

Recently, Kotz et al. (2000) attempted to treat a Pólya urn model containing 2 different labels according to a general replacement scheme, and pointed out that no constraint case is considerably more challenging even in  $2 \times 2$  case. That is, the exact distribution of the number of balls with a particular label which are drawn within n draws is rather convoluted and such an exact distribution is rather unwieldy for large n for numerical computation.

Our purpose in the present paper is to develop a general workable framework for the exact distribution theory for Pólya urn models mentioned before and to emphasize the importance of the exact analysis. The approach is to solve a system of equations of conditional probability generating functions (p.g.f.'s). Then, the probability functions and moments are derived from an expansion of the solution regardless of whether or not the constraint is imposed.

In this paper, a Pólya urn model containing balls of m different labels and characterized by a general replacement scheme is considered, which include some important models treated before. We consider the exact joint distribution of the numbers of balls with particular labels which are drawn within n draws. As a special case, a univariate distribution is derived from a Pólya urn model containing balls of 2 different labels.

For the derivation of the main part of the results, we use the method based on the conditional p.g.f.'s. This method was introduced by Ebneshahrashoob and Sobel (1990), and was developed by Aki and Hirano (1993, 1999), Aki et al. (1996). The procedure is very simple and suitable for computation by computer

algebra systems.

Furthermore, we propose two methods for the Pólya urn model. One is a recurrence for obtaining the expected values for all n, which is derived from the system of equations of conditional p.g.f.'s. The other is a useful method for obtaining the p.g.f.'s. Here, a double variable generating function and a notion of truncation parameter are introduced, where, for a sequence of p.g.f.'s  $\{\phi_n(t)\}_{n\geq 0}$ , we define the double variable generating function by  $\Phi(t,z) = \sum_{n=0}^{\infty} \phi_n(t) z^n$ . The p.g.f.'s are derived from the system of equations of the double variable generating functions. The difference between the method of conditional p.g.f.'s and the method based on the double variable generating function is that for a fixed n, the p.g.f.  $\phi_n(t)$  is obtained by the former method, whereas, for a fixed truncation parameter  $u_0$ , all the p.g.f.'s up to  $u_0$ ,  $\phi_0(t)$ ,  $\phi_1(t)$ ,..., $\phi_{u_0}(t)$  are obtained by the latter method. The procedures of two methods presented here are also very simple and suitable for computation by computer algebra systems.

The rest of this paper is organized in the following ways. In Section 2, a Pólya urn model containing balls of m different labels is introduced, which is characterized by the general replacement scheme. As a special case, a univariate distribution is derived from a Pólya urn model containing balls of 2 different labels. Section 3 gives two methods for the Pólya urn models. One is a recurrence for obtaining the expected values for all n. The other is a useful method for obtaining the p.g.f.'s. Here, double variable generating function and a notion of truncation parameter are introduced, which play an important role. Both methods are also very simple and suitable for computation by computer algebra systems. In Section 4, numerical examples are given in order to illustrate the feasibility of our main results.

#### 2. The models

In this section, we consider a Pólya urn model characterized by an  $m \times m$  addition matrix. As a special case, for m = 2, the univariate distribution, the probability generating function and the expected value are derived exactly.

## 2.1. The Pólya urn model containing m different labels

From an urn containing  $\alpha_1$  balls labeled  $1, \alpha_2$  balls labeled  $2, \ldots, \alpha_m$  balls labeled m, a ball is chosen at random, its label is noted and the ball is returned to the urn along with additional balls according to the addition matrix of nonnegative integers,  $A = (a_{ij}) \ i, j = 1, \ldots, m$ , whose rows are indexed by the label of the ball chosen and whose columns are indexed by the label of the ball added. Always starting with the newly constituted urn, this experiment is continued n times. Let  $Z_1, Z_2, \ldots, Z_n$  be a sequence obtained by the above scheme, which take values in a finite set  $B = \{1, 2, \ldots, m\}$ . Let r be a positive integer such that  $1 \le r \le 2^m - 1$  and let  $B_1, B_2, \ldots, B_r$  be subsets of B, where  $B_i \ne \emptyset$  and  $B_i \ne B_j$  for  $i \ne j$ . Then, we define the numbers of balls whose labels belong to the subsets  $B_i$  ( $i = 1, \ldots, r$ ) which are drawn within n draws by  $X_n^{(i)} = \sum_{j=1}^n I_{B_i}(Z_j)$  ( $i = 1, \ldots, r$ ), where  $I_{B_i}(\cdot)$  ( $i = 1, \ldots, r$ ) means the indicator function of the subset  $B_i$ .

In the sequel, we will obtain the p.g.f.  $E[t_1^{X_n^{(1)}}t_2^{X_n^{(2)}}\cdots t_r^{X_n^{(r)}}]$  of the joint distribution of  $(X_n^{(1)},X_n^{(2)},\ldots,X_n^{(r)})$ . Hereafter, we denote the urn composition and the total of the balls in the urn by  $\mathbf{b}=(\alpha_1,\alpha_2,\ldots,\alpha_m)$  and  $|\mathbf{b}|=\alpha_1+\alpha_2+\cdots+\alpha_m$ , respectively. We denote the *i*-th row of the addition matrix A by  $\mathbf{a}_i=(a_{i1},a_{i2},\ldots,a_{im})$ . Needless to say,  $\alpha_i\geq 0$   $(i=1,\ldots,m)$  and  $|\mathbf{b}|\neq 0$  are assumed throughout this paper.

Suppose that we have an urn composition  $\mathbf{b} = (\alpha_1, \alpha_2, \dots, \alpha_m)$  after  $\ell$  ( $\ell = 0, 1, \dots, n$ ) draws. Then, we denote by  $\phi_{n-\ell}(\mathbf{b}; \mathbf{t})$  the p.g.f. of the conditional distribution of the numbers of balls whose labels belong to the subsets  $B_i$  ( $i = 1, \dots, r$ ) which are drawn within  $(n - \ell)$  draws, where  $\mathbf{t} = (t_1, \dots, t_r)$ .

THEOREM 2.1. From the definitions of  $\phi_{n-\ell}(\mathbf{b}; \mathbf{t})$   $(\ell = 0, 1, ..., n)$ , we have the following system of the equations;

(2.1) 
$$\phi_n(\boldsymbol{b};\boldsymbol{t}) = \sum_{i=1}^m \frac{\alpha_i}{|\boldsymbol{b}|} \boldsymbol{t}^{\mathbf{I_B}(i)} \phi_{n-1}(\boldsymbol{b} + \boldsymbol{a}_i;\boldsymbol{t}),$$

(2.2) 
$$\phi_{n-\ell}(\boldsymbol{b};\boldsymbol{t}) = \sum_{i=1}^{m} \frac{\alpha_i}{|\boldsymbol{b}|} \boldsymbol{t}^{\mathbf{I}_{\mathbf{B}}(i)} \phi_{n-\ell-1}(\boldsymbol{b} + \boldsymbol{a}_i;\boldsymbol{t}), \qquad \ell = 1, 2, \dots, n-1,$$

(2.3) 
$$\phi_0(\mathbf{b}; \mathbf{t}) = 1$$
, where,  $\mathbf{t}^{\mathbf{I}_{\mathbf{B}}(i)} = t_1^{I_{B_1}(i)} t_2^{I_{B_2}(i)} \cdots t_r^{I_{B_r}(i)}$ .

PROOF. It is easy to see that  $\phi_0(\boldsymbol{b};\boldsymbol{t})=1$  by the definition of the p.g.f.. Suppose that the urn composition is  $\boldsymbol{b}=(\alpha_1,\alpha_2,\ldots,\alpha_m)$  after  $\ell$  ( $\ell=0,1,\ldots,n-1$ ) draws. Then, the p.g.f. of the conditional distribution of the numbers of balls whose labels belong to the subsets  $B_j$  ( $j=0,\ldots,r$ ) which are drawn within  $(n-\ell)$  draws is  $\phi_{n-\ell}(\boldsymbol{b};\boldsymbol{t})$  ( $\ell=0,1,\ldots,n-1$ ). We should consider the condition of one-step ahead from every condition. Given the condition we observe the  $(\ell+1)$ -th draw. For every  $i=1,\ldots,m$ , the probability that we draw the ball labeled i is  $\alpha_i/|\boldsymbol{b}|$ . If we have the ball labeled i ( $i=1,\ldots,m$ ), then the p.g.f. of the conditional distribution of the numbers of balls whose labels belong to the subsets  $B_j$  ( $j=0,\ldots,r$ ) which are drawn within  $(n-\ell-1)$  draws is  $\phi_{n-\ell-1}(\boldsymbol{b}+\boldsymbol{a}_i;\boldsymbol{t})$  ( $\ell=0,1,\ldots,n-1$ ). Therefore, we obtain the equations (2.1) and (2.2).  $\square$ 

Example 2.1. Assume that  $B = \{1, 2, 3, 4\}$ ,  $B_1 = \{2, 4\}$ ,  $B_2 = \{3, 4\}$ ,  $t = (t_1, t_2)$  and the addition matrix is equal to the  $4 \times 4$  zero matrix. Suppose that we have an urn composition  $\mathbf{b} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4)$  after  $\ell$  ( $\ell = 0, 1, \ldots, n$ ) draws. Then, we denote by  $\phi_{n-\ell}(\mathbf{b}; \mathbf{t})$  the p.g.f. of the conditional distribution of the numbers of balls whose labels belong to the subsets  $B_1, B_2$  which are drawn within  $(n - \ell)$  draws. Then, we have the following system of the equations;

(2.4) 
$$\phi_{n-\ell}(\mathbf{b}; t_1, t_2) = \left(\frac{\alpha_1}{|\mathbf{b}|} + \frac{\alpha_2}{|\mathbf{b}|} t_1 + \frac{\alpha_3}{|\mathbf{b}|} t_2 + \frac{\alpha_4}{|\mathbf{b}|} t_1 t_2\right) \phi_{n-\ell-1}(\mathbf{b}; t_1, t_2),$$

$$\ell = 0, 1, \dots, n-1,$$

(2.5) 
$$\phi_0(\mathbf{b}; t_1, t_2) = 1.$$

Under an initial urn composition  $\boldsymbol{b}_0 = (\alpha_{01}, \alpha_{02}, \alpha_{03}, \alpha_{04})$ , we get

(2.6) 
$$\phi_n(\mathbf{b}_0; t_1, t_2) = \left(\frac{\alpha_{01}}{|\mathbf{b}_0|} + \frac{\alpha_{02}}{|\mathbf{b}_0|} t_1 + \frac{\alpha_{03}}{|\mathbf{b}_0|} t_2 + \frac{\alpha_{04}}{|\mathbf{b}_0|} t_1 t_2\right)^n.$$

In this example, if the labels 1, 2, 3, 4 are regarded as (0,0), (1,0), (0,1), (1,1), respectively, the equation (2.6) is the p.g.f. of joint distribution of the number of balls with the first label 1 and the number of balls with the second label 1 which are drawn within n draws. The distribution is called the bivariate binomial distribution (see Kocherlakota (1989), Marshall and Olkin (1985)).

# 2.2. The Pólya urn model containing 2 different labels

As a special case, for m=2, we study the Pólya urn model containing 2 different labels. Assume that  $B=\{1,2\}$ ,  $B_1=\{2\}$  and  $A=(a_{ij})$  i,j=1,2. Let  $Y_n=\sum_{i=1}^n I_{B_1}(Z_i)$ . Suppose that we have an urn composition  $\boldsymbol{b}=(\alpha_1,\alpha_2)$  after  $\ell$  ( $\ell=0,1,\ldots,n$ ) draws. Then, we denote by  $\psi_{n-\ell}(\boldsymbol{b};t_1)$  the p.g.f. of the conditional distribution of the number of balls labeled 2 which are drawn within  $(n-\ell)$  draws. From Theorem 2.1, we have the following Corollary 2.1.

COROLLARY 2.1. From the definitions of  $\psi_{n-\ell}(\boldsymbol{b};t_1)$   $(\ell=0,1,\ldots,n)$ , we have the following system of the equations;

(2.7) 
$$\psi_{n}(\mathbf{b}; t_{1}) = \frac{\alpha_{1}}{|\mathbf{b}|} \psi_{n-1}(\mathbf{b} + \mathbf{a}_{1}; t_{1}) + \frac{\alpha_{2}}{|\mathbf{b}|} t_{1} \psi_{n-1}(\mathbf{b} + \mathbf{a}_{2}; t_{1}),$$
(2.8) 
$$\psi_{n-\ell}(\mathbf{b}; t_{1}) = \frac{\alpha_{1}}{|\mathbf{b}|} \psi_{n-\ell-1}(\mathbf{b} + \mathbf{a}_{1}; t_{1}) + \frac{\alpha_{2}}{|\mathbf{b}|} t_{1} \psi_{n-\ell-1}(\mathbf{b} + \mathbf{a}_{2}; t_{1}),$$

$$\ell = 1, 2, \dots, n-1,$$

(2.9) 
$$\psi_0(\mathbf{b}; t_1) = 1.$$

We will solve the system of the equations (2.7), (2.8) and (2.9) under an initial urn composition  $b_0 = (\alpha_{01}, \alpha_{02})$ . First, we note that the above equation (2.7) can be written in matrix form as

$$\psi_{n}(\mathbf{b}_{0}; t_{1}) = \frac{\alpha_{01}}{\alpha_{01} + \alpha_{02}} \psi_{n-1}(\mathbf{b}_{0} + \mathbf{a}_{1}; t_{1}) + \frac{\alpha_{02}}{\alpha_{01} + \alpha_{02}} t_{1} \psi_{n-1}(\mathbf{b}_{0} + \mathbf{a}_{2}; t_{1}),$$

$$= \left(\frac{\alpha_{01}}{\alpha_{01} + \alpha_{02}} \frac{\alpha_{02}}{\alpha_{01} + \alpha_{02}} t_{1}\right) \begin{pmatrix} \psi_{n-1}(\mathbf{b}_{0} + \mathbf{a}_{1}; t_{1}) \\ \psi_{n-1}(\mathbf{b}_{0} + \mathbf{a}_{2}; t_{1}) \end{pmatrix},$$

$$= C_{1}(t_{1}) \psi_{n-1}(t_{1}), \quad (\text{say}).$$

Next, for  $\ell = 1$ , we write the equation (2.8) as

$$\psi_{n-1}(\boldsymbol{b}_{0} + \boldsymbol{a}_{1}; t_{1}) = \frac{\alpha_{01} + a_{11}}{\alpha_{01} + \alpha_{02} + a_{11} + a_{12}} \psi_{n-2}(\boldsymbol{b}_{0} + 2\boldsymbol{a}_{1}; t_{1})$$

$$+ \frac{\alpha_{02} + a_{12}}{\alpha_{01} + \alpha_{02} + a_{11} + a_{12}} t_{1} \psi_{n-2}(\boldsymbol{b}_{0} + \boldsymbol{a}_{1} + \boldsymbol{a}_{2}; t_{1}),$$

$$\psi_{n-1}(\boldsymbol{b}_{0} + \boldsymbol{a}_{2}; t_{1}) = \frac{\alpha_{01} + a_{21}}{\alpha_{01} + \alpha_{02} + a_{21} + a_{22}} \psi_{n-2}(\boldsymbol{b}_{0} + \boldsymbol{a}_{1} + \boldsymbol{a}_{2}; t_{1})$$

$$+ \frac{\alpha_{02} + a_{22}}{\alpha_{01} + \alpha_{02} + a_{21} + a_{22}} t_{1} \psi_{n-2}(\boldsymbol{b}_{0} + 2\boldsymbol{a}_{2}; t_{1}),$$

or, equivalently,

$$\begin{pmatrix} \psi_{n-1}(\boldsymbol{b}_{0} + \boldsymbol{a}_{1}; t_{1}) \\ \psi_{n-1}(\boldsymbol{b}_{0} + \boldsymbol{a}_{2}; t_{1}) \end{pmatrix}$$

$$= \begin{pmatrix} \frac{\alpha_{01} + a_{11}}{\alpha_{01} + \alpha_{02} + a_{11} + a_{12}} & \frac{\alpha_{02} + a_{12}}{\alpha_{01} + \alpha_{02} + a_{11} + a_{12}} t_{1} & 0 \\ 0 & \frac{\alpha_{01} + \alpha_{02} + a_{11} + a_{12}}{\alpha_{01} + \alpha_{02} + a_{21} + a_{22}} & \frac{\alpha_{02} + a_{22}}{\alpha_{01} + \alpha_{02} + a_{21} + a_{22}} t_{1} \end{pmatrix}$$

$$\cdot \begin{pmatrix} \psi_{n-2}(\boldsymbol{b}_{0} + 2\boldsymbol{a}_{1}; t_{1}) \\ \psi_{n-2}(\boldsymbol{b}_{0} + a_{1} + \boldsymbol{a}_{2}; t_{1}) \\ \psi_{n-2}(\boldsymbol{b}_{0} + 2\boldsymbol{a}_{2}; t_{1}) \end{pmatrix}.$$

We write  $\psi_{n-1}(t_1) = C_2(t_1)\psi_{n-2}(t_1)$ . For non-negative integers  $\ell_1$ ,  $\ell_2$  such that  $\ell_1 + \ell_2 = \ell$ , let

$$\psi_{n-\ell}(t_1) = \begin{pmatrix} \psi_{n-\ell}(\mathbf{b}_0 + \ell \mathbf{a}_1; t_1) \\ \psi_{n-\ell}(\mathbf{b}_0 + (\ell - 1)\mathbf{a}_1 + \mathbf{a}_2; t_1) \\ \psi_{n-\ell}(\mathbf{b}_0 + (\ell - 2)\mathbf{a}_1 + 2\mathbf{a}_2; t_1) \\ \vdots \\ \psi_{n-\ell}(\mathbf{b}_0 + \ell_1\mathbf{a}_1 + \ell_2\mathbf{a}_2; t_1) \\ \vdots \\ \psi_{n-\ell}(\mathbf{b}_0 + \ell \mathbf{a}_2; t_1) \end{pmatrix}.$$

Then, the system of the equations (2.7), (2.8) and (2.9) can be written in matrix form as  $\psi_{n-\ell+1}(t_1) = C_{\ell}(t_1)\psi_{n-\ell}(t_1)$  ( $\ell = 1, \ldots, n$ ), and  $\psi_0(t_1) = \mathbf{1}_{(n+1)} = (1, 1, \ldots, 1)'$ , where,  $\mathbf{1}_{(n+1)}$  denotes the  $(n+1) \times 1$  column vector whose components are all unity and  $C_{\ell}(t_1)$  denotes the  $\ell \times (\ell+1)$  matrix whose (i, j)-th component is given by,

$$(2.10) c_{ij}(\ell;t_1) = \begin{cases} \frac{\alpha_{01} + (\ell - i)a_{11} + (i - 1)a_{21}}{\alpha_{01} + \alpha_{02} + (\ell - i)(a_{11} + a_{12}) + (i - 1)(a_{21} + a_{22})}, \\ j = i, i = 1, \dots, \ell, \\ \frac{\alpha_{02} + (\ell - i)a_{12} + (i - 1)a_{22}}{\alpha_{01} + \alpha_{02} + (\ell - i)(a_{11} + a_{12}) + (i - 1)(a_{21} + a_{22})} t_1, \\ j = i + 1, i = 1, \dots, \ell, \\ 0, \\ 0, \\ \text{otherwise.} \end{cases}$$

PROPOSITION 2.1. The probability generating function  $\psi_n(\mathbf{b}_0; t_1)$ , the exact distribution of  $Y_n$  and its expected value are given by

$$\psi_n(\mathbf{b}_0;t_1)=C_1(t_1)C_2(t_1)\cdots C_n(t_1)\mathbf{1}_{(n+1)}=\prod_{i=1}^n C_i(t_1)\mathbf{1}_{(n+1)},$$

$$\begin{split} P(Y_n = y) &= \sum_{1 \leq n_1 < \dots < n_y \leq n} C_1(0) \dots \dot{C}_{n_1}(0) \dots \dot{C}_{n_y}(0) \dots C_n(0) \mathbf{1}_{(n+1)}, \\ E[Y_n; \pmb{b}_0] &= \sum_{i=1}^n C_1(1) \dots \dot{C}_i(1) \dots C_n(1) \mathbf{1}_{(n+1)}, \quad \textit{where}, \\ \dot{C}_k(t_1) &= \frac{dC_k(t_1)}{dt_1} = \left(\frac{dc_{ij}(k; t_1)}{dt_1}\right). \end{split}$$

In a similar way, under an initial urn composition  $b_0 = (\alpha_{01}, \alpha_{02}, \dots, \alpha_{0m})$ , we can solve the system of the equations in Theorem 2.1 by virtue of their linearity and obtain the p.g.f.. However, we do not write it due to lack of space.

Remark 1. In this Pólya urn model, Kotz et al. (2000) derived the exact distribution of  $Y_n$  by another approach, and derived the recurrence relation for the expected value. They also reported that the expected value can be derived from the recurrence relation in a case that the constraint is imposed, whereas the expected value can not be derived from it in a case that the constraint is not imposed. Then, we present a useful recurrence for the expected values, as will be shown later.

## 3. Methods for computation

In this section, we present two methods for the exact analysis, which are very simple and suitable for computation by computer algebra systems. One is a recurrence for obtaining the expected values for all n. The other is a method for obtaining p.g.f.'s.

# 3.1. The recurrences for the expected values

THEOREM 3.1. (The Pólya urn model containing m different labels) The expected values of  $X_n^{(i)}$   $(i=0,1,\ldots,r), E[X_n^{(i)}; \boldsymbol{b}]$  say, satisfy the recurrences;

(3.1) 
$$E[X_n^{(i)}; \boldsymbol{b}] = \sum_{j=1}^m \frac{\alpha_j}{|\boldsymbol{b}|} (I_{B_i}(j) + E[X_{n-1}^{(i)}; \boldsymbol{b} + \boldsymbol{a}_j]), \quad n \ge 1, \quad i = 1, \dots, r,$$

(3.2) 
$$E[X_0^{(i)}; \mathbf{b}] = 0, \quad i = 1, \dots, r.$$

PROOF. It is easy to check the equation (3.2). The equation (3.1) is obtained by differentiating both sides of the equation (2.1) with respect to  $t_i$  (i = 1, ..., r) and then setting  $t_1 = \cdots = t_r = 1$ . The proof is completed.  $\square$ 

As a special case, for m=2, we consider the Pólya urn model containing 2 different labels treated in Section 2.2. Then, from Theorem 3.1, we have the following Corollary 3.1.

COROLLARY 3.1. (The Pólya urn model containing 2 different labels) The expected value of  $Y_n$ ,  $E[Y_n; b]$  say, satisfies the recurrence;

(3.3) 
$$E[Y_n; \boldsymbol{b}] = \frac{\alpha_1}{|\boldsymbol{b}|} E[Y_{n-1}; \boldsymbol{b} + \boldsymbol{a}_1] + \frac{\alpha_2}{|\boldsymbol{b}|} E[Y_{n-1}; \boldsymbol{b} + \boldsymbol{a}_2] + \frac{\alpha_2}{|\boldsymbol{b}|}, \quad n \ge 1,$$
  
(3.4)  $E[Y_0; \boldsymbol{b}] = 0.$ 

## 3.2. The double generating functions

Until now, our results are derived from the p.g.f. directly. The most of this section will be devoted to the double variable generating functions. First, we will begin by considering the Pólya urn model containing 2 different labels treated in Section 2.2. We define

$$\Psi(\boldsymbol{b}) = \sum_{n=0}^{\infty} \psi_n(\boldsymbol{b}; t_1) z^n.$$

Then, the equations (2.7) and (2.9) in Corollary 2.1 lead to

(3.5) 
$$\Psi(\boldsymbol{b}) = 1 + \frac{\alpha_1}{|\boldsymbol{b}|} z \Psi(\boldsymbol{b} + \boldsymbol{a}_1) + \frac{\alpha_2}{|\boldsymbol{b}|} z t_1 \Psi(\boldsymbol{b} + \boldsymbol{a}_2).$$

Given an initial urn composition  $\boldsymbol{b}_0 = (\alpha_{01}, \alpha_{02})$ , we have

(3.6) 
$$\Psi(\mathbf{b}_0) = 1 + \frac{\alpha_{01}}{|\mathbf{b}_0|} z \Psi(\mathbf{b}_0 + \mathbf{a}_1) + \frac{\alpha_{02}}{|\mathbf{b}_0|} z t_1 \Psi(\mathbf{b}_0 + \mathbf{a}_2).$$

We will show that the truncated generating function of  $\Psi(\boldsymbol{b}_0)$ , say  $\hat{\Psi}(\boldsymbol{b}_0)$ , can be obtained in a polynomial form of z up to the arbitrary order by using the equation (3.5) for the right-hand side of the equation (3.6) recursively. The idea of truncation is also illustrated. From the equation (3.5), we have

(3.7) 
$$\Psi(\boldsymbol{b}_0 + \boldsymbol{a}_1) = 1 + \frac{\alpha_{01} + a_{11}}{|\boldsymbol{b}_0 + \boldsymbol{a}_1|} z \Psi(\boldsymbol{b}_0 + 2\boldsymbol{a}_1) + \frac{\alpha_{02} + a_{12}}{|\boldsymbol{b}_0 + \boldsymbol{a}_1|} z t_1 \Psi(\boldsymbol{b}_0 + \boldsymbol{a}_1 + \boldsymbol{a}_2),$$

(3.8) 
$$\Psi(\boldsymbol{b}_0 + \boldsymbol{a}_2) = 1 + \frac{\alpha_{01} + a_{21}}{|\boldsymbol{b}_0 + \boldsymbol{a}_2|} z \Psi(\boldsymbol{b}_0 + \boldsymbol{a}_1 + \boldsymbol{a}_2) + \frac{\alpha_{02} + a_{22}}{|\boldsymbol{b}_0 + \boldsymbol{a}_2|} z t_1 \Psi(\boldsymbol{b}_0 + 2\boldsymbol{a}_2).$$

Substituting (3.7) and (3.8) into the right-hand side of (3.6), we have

(3.9) 
$$\Psi(\boldsymbol{b}_{0})$$
  

$$= 1 + \frac{\alpha_{01}}{|\boldsymbol{b}_{0}|} z \left( 1 + \frac{\alpha_{01} + a_{11}}{|\boldsymbol{b}_{0} + \boldsymbol{a}_{1}|} z \Psi(\boldsymbol{b}_{0} + 2\boldsymbol{a}_{1}) + \frac{\alpha_{02} + a_{12}}{|\boldsymbol{b}_{0} + \boldsymbol{a}_{1}|} z t_{1} \Psi(\boldsymbol{b}_{0} + \boldsymbol{a}_{1} + \boldsymbol{a}_{2}) \right) + \frac{\alpha_{02}}{|\boldsymbol{b}_{0}|} z t_{1} \left( 1 + \frac{\alpha_{01} + a_{21}}{|\boldsymbol{b}_{0} + \boldsymbol{a}_{2}|} z \Psi(\boldsymbol{b}_{0} + \boldsymbol{a}_{1} + \boldsymbol{a}_{2}) + \frac{\alpha_{02} + a_{22}}{|\boldsymbol{b}_{0} + \boldsymbol{a}_{2}|} z t_{1} \Psi(\boldsymbol{b}_{0} + 2\boldsymbol{a}_{2}) \right).$$

Setting  $\Psi(\boldsymbol{b}_0 + 2\boldsymbol{a}_1) = \Psi(\boldsymbol{b}_0 + \boldsymbol{a}_1 + \boldsymbol{a}_2) = \Psi(\boldsymbol{b}_0 + 2\boldsymbol{a}_2) = 0$  in the right-hand side of (3.9) (if we need  $\hat{\Psi}(\boldsymbol{b}_0)$  up to the first order), we obtain

$$\hat{\Psi}(\boldsymbol{b}_0) = 1 + \left(\frac{\alpha_{01}}{|\boldsymbol{b}_0|} + \frac{\alpha_{02}}{|\boldsymbol{b}_0|}t_1\right)z.$$

Thus, the above substitution enables us to obtain  $\hat{\Psi}(\boldsymbol{b}_0)$  up to the first order. Hence,  $\psi_0(\boldsymbol{b}_0;t_1)$  and  $\psi_1(\boldsymbol{b}_0;t_1)$  are obtained. If we need  $\hat{\Psi}(\boldsymbol{b}_0)$  up to the second order, we should use the equation (3.5) again. Similarly, by substituting the equation (3.5) into the terms  $\Psi(\boldsymbol{b}_0+2\boldsymbol{a}_1), \Psi(\boldsymbol{b}_0+\boldsymbol{a}_1+\boldsymbol{a}_2), \Psi(\boldsymbol{b}_0+2\boldsymbol{a}_2)$  in the right-hand side of (3.9), respectively, and then setting  $\Psi(\boldsymbol{b}_0+3\boldsymbol{a}_1)=\Psi(\boldsymbol{b}_0+2\boldsymbol{a}_1+\boldsymbol{a}_2)=\Psi(\boldsymbol{b}_0+\boldsymbol{a}_1+2\boldsymbol{a}_2)=\Psi(\boldsymbol{b}_0+3\boldsymbol{a}_2)=0$ , we have  $\hat{\Psi}(\boldsymbol{b}_0)$  up to the second order. Therefore,  $\psi_0(\boldsymbol{b}_0;t_1), \psi_1(\boldsymbol{b}_0;t_1)$  and  $\psi_2(\boldsymbol{b}_0;t_1)$  are obtained. Since we can repeat the above substitution a sufficient number of times, we can obtain the truncated generating function  $\hat{\Psi}(\boldsymbol{b}_0)$  up to the arbitrary order and obtain all the p.g.f.'s  $\psi_n(\boldsymbol{b}_0;t_1)$  ( $n=0,1,\ldots$ ). A parameter of a non-negative integer u is introduced into the generating function  $\Psi(\boldsymbol{b})$ , denoted by  $\Psi(\boldsymbol{b};u)$ . From the equations (3.5) and (3.6), we have

(3.10) 
$$\Psi(\boldsymbol{b}_0;0) = 1 + \frac{\alpha_{01}}{|\boldsymbol{b}_0|} z \Psi(\boldsymbol{b}_0 + \boldsymbol{a}_1;1) + \frac{\alpha_{02}}{|\boldsymbol{b}_0|} z t_1 \Psi(\boldsymbol{b}_0 + \boldsymbol{a}_2;1),$$

(3.11) 
$$\Psi(\mathbf{b}; u) = 1 + \frac{\alpha_1}{|\mathbf{b}|} z \Psi(\mathbf{b} + \mathbf{a}_1; u + 1) + \frac{\alpha_2}{|\mathbf{b}|} z t_1 \Psi(\mathbf{b} + \mathbf{a}_2; u + 1).$$

By using the equation (3.11) for the right-hand side of the equation (3.10) recursively, we can obtain the truncated generating function of  $\Psi(\mathbf{b}_0; 0)$ , say  $\hat{\Psi}(\mathbf{b}_0; 0)$ , in a polynomial form up to the arbitrary order. For the truncation parameter of a non-negative integer  $u_0$ , the following Proposition 3.1 gives the method for obtaining the p.g.f.'s  $\psi_i(\mathbf{b}_0; t_1)$   $(i = 0, \dots, u_0)$ .

Proposition 3.1. (The Pólya urn model containing 2 different labels)

For any non-negative integer  $u_0$ , the following system of the equations leads to the truncated generating function of  $\Psi(\mathbf{b}_0;0)$ ,  $\hat{\Psi}(\mathbf{b}_0;0)$  say, which is in a polynomial form of z up to the  $u_0$ -th order, so that  $\psi_i(\mathbf{b}_0;t_1)$   $(i=0,\ldots,u_0)$  are obtained.

(3.12) 
$$\hat{\Psi}(\boldsymbol{b}_0; 0) = 1 + \frac{\alpha_{01}}{|\boldsymbol{b}_0|} z \hat{\Psi}(\boldsymbol{b}_0 + \boldsymbol{a}_1; 1) + \frac{\alpha_{02}}{|\boldsymbol{b}_0|} z t_1 \hat{\Psi}(\boldsymbol{b}_0 + \boldsymbol{a}_2; 1),$$

(3.13) 
$$\hat{\Psi}(\mathbf{b}; u) = 1 + \frac{\alpha_1}{|\mathbf{b}|} z \hat{\Psi}(\mathbf{b} + \mathbf{a}_1; u + 1) + \frac{\alpha_2}{|\mathbf{b}|} z t_1 \hat{\Psi}(\mathbf{b} + \mathbf{a}_2; u + 1),$$

for 
$$0 \le u \le u_0$$
,

(3.14) 
$$\hat{\Psi}(\mathbf{b}; u) = 0$$
, for  $u > u_0$ .

PROOF. We continue to substitute the equation (3.11) into the right-hand side of the equation (3.10) until all the parameters in the generating functions in the right-hand side of the equation (3.10) are equal to  $u_0 + 1$ . Then,  $\Psi(\boldsymbol{b}_0; 0)$  takes the following form;

(3.15) 
$$\Psi(\boldsymbol{b}_0;0) = \sum_{v=0}^{u_0+1} g_v(t_1) z^{u_0+1} \Psi(\boldsymbol{b}_0 + v\boldsymbol{a}_1 + (u_0+1-v)\boldsymbol{a}_2; u_0+1) + f_{u_0}(z),$$

where,  $g_v(t_1)$  is a polynomial of  $t_1$ , and  $f_{u_0}(z)$  is a polynomial of z up to the  $u_0$ -th order. Setting  $\Psi(\boldsymbol{b}_0 + v\boldsymbol{a}_1 + (u_0 + 1 - v)\boldsymbol{a}_2; u_0 + 1) = 0$  for all v such that

 $0 \le v \le u_0 + 1$  in the right-hand side of (3.15), we can obtain the truncated generating function  $\hat{\Psi}(\boldsymbol{b}_0; 0)$  in a polynomial form up to the  $u_0$ -th order. Notice that the order of the vanished terms is greater than  $u_0$ . The proof is completed.  $\square$ 

It is easy to extend this result to the general case. Similarly, the parameter of the non-negative integer u is introduced into the generating function  $\Phi(\mathbf{b})$ , say  $\Phi(\mathbf{b}; u)$ , where,  $\Phi(\mathbf{b}) = \Phi(\mathbf{b}; u) = \sum_{n=0}^{\infty} \phi_n(\mathbf{b}; t) z^n$ . From the following equations,

(3.16) 
$$\Phi(\mathbf{b}_0; 0) = 1 + z \sum_{i=1}^{m} \frac{\alpha_{0i}}{|\mathbf{b}_0|} \mathbf{t}^{\mathbf{I}_{\mathbf{B}}(i)} \Phi(\mathbf{b}_0 + \mathbf{a}_i; 1),$$

(3.17) 
$$\Phi(\boldsymbol{b}; u) = 1 + z \sum_{i=1}^{m} \frac{\alpha_i}{|\boldsymbol{b}|} \boldsymbol{t}^{\mathbf{I}_{\mathbf{B}}(i)} \Phi(\boldsymbol{b} + \boldsymbol{a}_i; u + 1),$$

we can obtain the truncated generating function of  $\Phi(\mathbf{b}_0;0)$ , say  $\hat{\Phi}(\mathbf{b}_0;0)$ .

Theorem 3.2. (The Pólya urn model containing m different labels)

For any non-negative integer  $u_0$ , the following system of the equations leads to the truncated generating function of  $\Phi(\mathbf{b}_0; 0)$ ,  $\hat{\Phi}(\mathbf{b}_0; 0)$  say, which is in a polynomial form of z up to the  $u_0$ -th order, so that  $\phi_i(\mathbf{b}_0; \mathbf{t})$   $(i = 0, ..., u_0)$  are obtained.

(3.18) 
$$\hat{\Phi}(\boldsymbol{b}_0; 0) = 1 + z \sum_{i=1}^{m} \frac{\alpha_{0i}}{|\boldsymbol{b}_0|} \boldsymbol{t}^{\mathbf{I}_{\mathbf{B}}(i)} \hat{\Phi}(\boldsymbol{b}_0 + \boldsymbol{a}_i; 1),$$

(3.19) 
$$\hat{\Phi}(\mathbf{b}; u) = 1 + z \sum_{i=1}^{m} \frac{\alpha_i}{|\mathbf{b}|} \mathbf{t}^{\mathbf{I}_{\mathbf{B}}(i)} \hat{\Phi}(\mathbf{b} + \mathbf{a}_i; u + 1), \quad \text{for } 0 \le u \le u_0,$$

$$(3.20) \quad \hat{\Phi}(\boldsymbol{b}; u) = 0, \quad \text{for} \quad u > u_0, \text{ where, } \boldsymbol{t}^{\mathbf{I_B}(i)} = t_1^{I_{B_1}(i)} t_2^{I_{B_2}(i)} \cdots t_r^{I_{B_r}(i)}. \quad \Box$$

## 4. Numerical examples

In this section, we illustrate how to obtain the distributions and the expected values by using computer algebra systems.

Example 4.1. The Pólya urn model containing 4 different labels Assume that  $\boldsymbol{b}_0 = (1, 2, 1, 2), B = \{1, 2, 3, 4\}, B_1 = \{2, 4\}, B_2 = \{3, 4\}$  and

$$A = \begin{pmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix}. \text{ Let } X_n^{(i)} = \sum_{j=1}^n I_{B_i}(Z_j) \ (i = 1, 2). \text{ For } n = 3, \text{ the p.g.f. is}$$

$$\phi_{3}(\mathbf{b}_{0}; t_{1}, t_{2}) = \frac{1}{108} + \frac{73}{3564}t_{1} + \frac{73}{2376}t_{2} + \frac{269}{7920}t_{1}^{2} + \frac{3209}{35640}t_{1}t_{2} + \frac{269}{7920}t_{2}^{2} + \frac{1}{20}t_{1}^{3} + \frac{3361}{23760}t_{1}^{2}t_{2} + \frac{3191}{35640}t_{1}t_{2}^{2} + \frac{1}{80}t_{2}^{3} + \frac{269}{1980}t_{1}^{3}t_{2} + \frac{4951}{35640}t_{1}^{2}t_{2}^{2} + \frac{269}{11880}t_{1}t_{2}^{3} + \frac{73}{594}t_{1}^{3}t_{2}^{2} + \frac{73}{2376}t_{1}^{2}t_{2}^{3} + \frac{1}{27}t_{1}^{3}t_{2}^{3}.$$

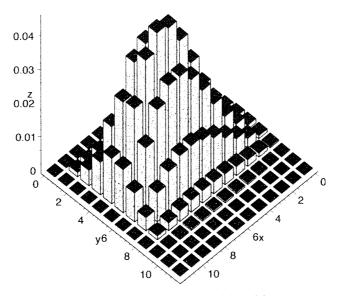


Figure 1. The exact joint probability function of  $(X_{10}^{(1)}, X_{10}^{(2)})$  in the Example 4.1, given  $b_0 = (1, 2, 1, 2)$  and the addition matrix A.

Table 1. The exact joint probability function of  $(X_3^{(1)}, X_3^{(2)})$ , given  $\boldsymbol{b}_0 = (1, 2, 1, 2)$ .

|                 | $X_3^{(1)} = 0$ | $X_3^{(1)} = 1$ | $X_3^{(1)} = 2$ | $X_3^{(1)} = 3$ |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| $X_3^{(2)} = 0$ | 0.009259        | 0.020482        | 0.033965        | 0.05            |
| $X_3^{(2)} = 1$ | 0.030724        | 0.090039        | 0.141456        | 0.135859        |
| $X_3^{(2)} = 2$ | 0.033965        | 0.089534        | 0.138917        | 0.122896        |
| $X_3^{(2)} = 3$ | 0.0125          | 0.022643        | 0.030724        | 0.037037        |

For n = 10, we give Fig. 1, which is the three-dimensional plot of the exact joint probability function of  $(X_{10}^{(1)}, X_{10}^{(2)})$ , given  $\boldsymbol{b}_0 = (1, 2, 1, 2)$  and the addition matrix A.

Marshall and Olkin (1990) discussed this model in case that the addition matrix is the identity matrix. So far as we know, it was first proposed by Kaiser and Stefansky (1972).

Example 4.2. The Pólya urn model containing 2 different labels Assume that  $\mathbf{b}_0 = (2,3)$ ,  $B = \{1,2\}$ ,  $B_1 = \{2\}$  and  $A = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ . Let  $Y_n = \sum_{j=1}^n I_{B_1}(Z_j)$ . For n = 10, the p.g.f. and the expected value are, respectively,

$$\psi_{10}(\mathbf{b}_{0};t_{1}) = \frac{1}{91} + \frac{125291}{3153150}t_{1} + \frac{4404557}{50450400}t_{1}^{2} + \frac{52734593}{367567200}t_{1}^{3} + \frac{8659858873}{46313467200}t_{1}^{4} + \frac{985104707}{5028319296}t_{1}^{5} + \frac{195631373}{1197218880}t_{1}^{6} + \frac{8913571}{84651840}t_{1}^{7} + \frac{16000}{323323}t_{1}^{8} + \frac{10240}{676039}t_{1}^{9} + \frac{1536}{676039}t_{1}^{10},$$

$$E[Y_{10}; \boldsymbol{b}_0] = \dot{\psi}_{10}(\boldsymbol{b}_0; 1) = \frac{11750459755829}{2529873145800} = 4.644683381.$$

We give Fig. 2, which is the two-dimensional plot of the exact expected values of

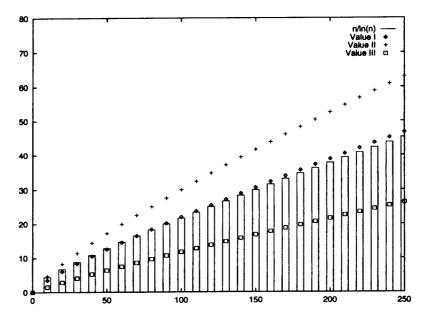


Figure 2. The exact expected values of  $Y_n$ , given three initial urn compositions  $\boldsymbol{b}_0 = (1,1), (2,3), (5,1)$  and the addition matrix A in Example 4.2. Value I, II, III are, respectively, the values given initial urn compositions  $\boldsymbol{b}_0 = (1,1), (2,3), (5,1)$ .

 $Y_n$ , given three initial urn compositions  $\boldsymbol{b}_0 = (1,1), (2,3), (5,1)$  and the addition matrix A.

Remark 2. In this example, Kotz et al. (2000) suggested that the fixed values of the initial condition will be asymptotically negligible with regard to  $Y_n$  for large n and  $E[Y_n] \sim n/\ln n$ , as  $n \to \infty$ . By calculating the exact expected values of  $Y_n$  given three initial conditions, we observe that their values depend on the initial conditions when n is small.

However, when n comes to 250, it seems that the exact expected values of  $Y_n$  still heavily depend on their initial conditions. Therefore, we think that the exact analysis is important.

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