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Abstract

The quest continues for cases of interest where the differential equations for the Pólya process are amenable to an asymptotic solution. We introduce a tenable class of urns that generalize the classical Ehrenfest model, and analyze the Ehrenfest process obtained by embedding the discrete evolution in real time. We show that lurking under the Ehrenfest process is a limiting binomial distribution, whose number of trials is an integer invariant property of the process.

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1 Introduction

Associated with a Pólya urn is a process obtained by embedding it in continuous time. It is natural to call this process the Pólya process. Although they did not call it by that

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name, the process was introduced in Athreya and Karlin (1968) to model the growth of an urn in discrete time according to certain rules. These authors pursued strong laws. Balaji and Mahmoud (2005+) looked into the exact and limit distributions in a Pólya process associated with diagonal ball addition matrices. Their formulation started from the general case, where general partial differential equations are obtained.

The quest continues for cases of interest where these differential equations are amenable to an asymptotic solution. We introduce a tenable class of urns that generalize the classical Ehrenfest model, and deal with the process obtained by embedding the discrete evolution in real time. Henceforth, we refer to the embedded process as the *Ehrenfest* process.

The paper is organized as follows. In Section 2 we describe the general Pólya process, its associated ball addition matrix, and state its governing partial differential equation. In Section 3 we specialize the model to the Ehrenfest case. This is done by first motivating the study from the point of view of a ball drawing model in Subsection 3.1, then in Subsection 3.2 we specify the continuous-time embedded Ehrenfest process, the main topic of this paper. We take up the analysis in Section 4. We conclude in Section 5 with some remarks including connections to pseudo-expectation for Markov chains.

2 Overview of the Pólya process

The Pólya process is a renewal process with rewards. It comprises a number of independent processes of various types running in parallel. The process grows out of a certain number of white and blue balls (thought to be contained in an urn). At time t, let the number of white balls be W(t) and the number of blue balls be B(t). Thus, initially we have W(0) white balls, and B(0) blue balls in the urn. Each ball generates a renewal after an independent Exp(1), an exponentially distributed random variable with parameter 1. We call a process evolving from a white ball a *white process*, and a process evolving from a blue ball a *blue process*. When a renewal occurs, a certain number of balls of each color is added. That number depends on which colored process induced the renewal. This induces a natural dependence between W(t) and B(t). It is assumed that ball additions take place instantaneously at the renewals. If a white process causes the renewal we add a white balls and b blue balls to the urn, and if a blue process causes the renewal we add c white balls and d blue balls to the urn. Each new ball comes equipped with its own independent regenerative Poisson process of its color.

The ball addition scheme is often thought of as a 2×2 matrix **A**, the rows of which are indexed by the color of the process inducing the renewal, and the columns of which are labeled by the colors of balls added to the urn:

(2.1)
$$\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

We simply refer to this matrix as the *scheme*. Some of these processes were discussed

on average in Mahmoud (2002, 2004). The full asymptotic distribution was derived for (forward and backward) diagonal schemes in Balaji and Mahmoud (2005+). In the latter reference the following general functional equation was established for any scheme with non-negative entries. Only very minor adaptation of the proof is required to make it valid for a tenable process, where negative entries may be present.

Lemma 2.1 Let **A** be the scheme of a tenable Pólya process. The moment generating function $\phi(t, u, v) := \mathbf{E}[\exp(uW(t) + vB(t))]$ of the joint process satisfies

$$\frac{\partial \phi}{\partial t} + (1 - e^{au + bv})\frac{\partial \phi}{\partial u} + (1 - e^{cu + dv})\frac{\partial \phi}{\partial v} = 0$$

3 The Ehrenfest process

The scheme

$$\mathbf{A} = \begin{pmatrix} -1 & 1\\ 1 & -1 \end{pmatrix}$$

has been known for a long time (see Ehrenfest and Ehrenfest (1907)) and has long been a standard entry in textbooks (see Johnson and Kotz (1977)).

3.1 A generalized Ehrenfest ball drawing model

We consider first a ball drawing model with the matrix \mathbf{A} . The scheme progresses in discrete time. The matrix stands for an urn scheme in which whenever a ball is picked, it is replaced by a ball of the opposite color. The Ehrenfest urn has applications as a model for the mixing of particles in two connected gas chambers.

We consider the generalization

(3.1)
$$\mathbf{A} = \begin{pmatrix} -\alpha & \beta \\ \alpha & -\beta \end{pmatrix},$$

with positive integers α , and β . We have just added weights to the action of withdrawing a ball.

3.2 The continuous-time embedded model

Our concern in this paper is the underlying Ehrenfest process obtained by embedding a tenable generalized Ehrenfest scheme in real time, and our goal is to push forward the class of urns for which asymptotic solutions of the partial differential equation of Lemma 2.1 can be obtained. The corresponding continuous-time process is the regenerative stochastic process that starts out at time 0 with W(0) balls (multiple of α), and B(0) balls (multiple of β), and progresses in time as follows. (At least one of W(0) and B(0) must be positive.)

The balls are in an urn; every ball carries its own Exp(1) clock, i.e. there is a Poisson process associated with each existing ball. Whenever a white ball (process) generates a renewal, we remove α white balls from the urn (α white processes from the system) and add β blue balls (processes), and whenever a blue ball generates a renewal, we remove β blue balls and add α white processes.

In the presence of negative entries in the urn scheme, the first concern is tenability: Can such a scheme indefinitely sustain ball renewals? Indeed, this general Ehrenfest scheme meets necessary and sufficient tenability conditions which we recall here for reference. A 2×2 deterministic Pólya urn scheme with ball addition matrix **A** as in (2.1) is tenable if and only if:

- (i) W(0) and c are both multiples of |a|.
- (ii) B(0) and b are both multiples of |d|.
- (iii) Both b and c are positive.

These conditions are discussed in Gouet (1997); Balaji and Mahmoud (2003) discuss the tenability conditions of other types of 2×2 schemes.

Thus, in the class of generalized Ehrenfest urn schemes (3.1), if we choose

W(0) a multiple of α and B(0) a multiple of β ,

the necessary and sufficient conditions (i)–(iii) are met. Henceforth, the phrase *tenable Ehrenfest scheme* refers to a scheme with ball addition matrix (3.1) and the suitable set of initial conditions just stated.

The technical definition of the Ehrenfest process is W(t), for $t \ge 0$. The overall structure of the Ehrenfest process is an inhomogeneous stochastic process with rates that are time varying. For instance, the generalized Ehrenfest scheme

$$\begin{pmatrix} -2 & 1 \\ 2 & -1 \end{pmatrix}$$

starting with W(0) = 2 and B(0) = 0 alternates between two states: Either two white balls are in the urn or one blue ball is in the urn. Right after getting in the state with two white balls, the next renewal occurs after $\exp(\frac{1}{2})$ time, whereas right after getting in the state with one blue ball, the next renewal occurs after $\exp(1)$ time. It is a Poisson process with changing rates. It is not hard to see that in the picking (Discrete) model, after *n* draws, the number of white balls in the urn depends on whether *n* is odd or even, with no convergence. The continuous model is more stable in this regard, because the number of renewals by time *t* is random, and we get a good mixing of odd and even cases. There is convergence in the continuous case as we shall study.

4 Distributions in the Ehrenfest process

The following easy lemma is useful throughout. We shall refer to its statement as the *invariant property*.

Lemma 4.1 Let

$$C = \frac{W(0)}{\alpha} + \frac{B(0)}{\beta}.$$

For all $t \geq 0$, we have

$$\frac{W(t)}{\alpha} + \frac{B(t)}{\beta} \stackrel{\text{a.s.}}{=} C.$$

Proof. Suppose the next renewal time after t is t'. There is no change in the scheme between time t and t', i.e.

$$\frac{W(t)}{\alpha} + \frac{B(t)}{\beta} = \frac{W(t'')}{\alpha} + \frac{B(t'')}{\beta}, \quad \text{for all } t \le t'' < t'.$$

At time t' there is one renewal (almost surely). The renewal is either white, in which case the number of white balls goes down by α , and the number of blue balls goes up by β . In this case

$$\frac{W(t')}{\alpha} + \frac{B(t')}{\beta} = \frac{W(t) - \alpha}{\alpha} + \frac{B(t) + \beta}{\beta} = \frac{W(t)}{\alpha} + \frac{B(t)}{\beta},$$

or the renewal is blue, in which case the number of white balls goes up by α and the number of blue balls goes down by β . In either case we have

$$\frac{W(t')}{\alpha} + \frac{B(t')}{\beta} = \frac{W(t)}{\alpha} + \frac{B(t)}{\beta}$$

At all times $\frac{W(t)}{\alpha} + \frac{B(t)}{\beta}$ remains invariant, and equal to its value at 0. \Box

Remark: Under the tenability conditions (i)-(iii), the invariant quantity C is an integer.

We next study the white process, via its moment generating function

$$\mathbf{E}[e^{W(t)u}] := \psi(t, u) = \phi(t, u, 0)$$

Let us take v = 0 in Lemma 2.1 and write a partial differential equation for ψ . One obtains

$$\frac{\partial \psi}{\partial t} + (1 - e^{-\alpha u})\frac{\partial \psi}{\partial u} + (1 - e^{\alpha u})\frac{\partial \phi}{\partial v}\Big|_{v=0} = 0.$$

Note that

$$\frac{\partial \phi}{\partial v}\Big|_{v=0} = \mathbf{E}[B(t)e^{W(t)u+B(t)v}]\Big|_{v=0} = \mathbf{E}[B(t)e^{W(t)u}].$$

The boundedness of the number of balls ensures that the invariant property carries over to the expectation of bounded functions involving the number of white or blue balls:

$$\frac{\partial \psi}{\partial t} + (1 - e^{-\alpha u})\frac{\partial \psi}{\partial u} + (1 - e^{\alpha u})\mathbf{E}\Big[\beta\Big(C - \frac{W(t)}{\alpha}\Big)e^{W(t)u}\Big] = 0.$$

We can reorganize this equation in the form

(4.1)
$$\frac{\partial\psi}{\partial t} + \left((1 - e^{-\alpha u}) - \frac{\beta}{\alpha}(1 - e^{\alpha u})\right)\frac{\partial\psi}{\partial u} + \beta C(1 - e^{\alpha u})\psi = 0.$$

We shall use the general form of the distribution to guide us to the asymptotic solution of this partial differential equation. We know that, regardless of how we start, the number of white balls can only be a multiple of α lying anywhere between 0 and the maximum value αC (the upper limit follows from the invariance property when B(t) = 0). Thus, $W(t) \in \{0, \alpha, 2\alpha, \dots, C\alpha\}$, and the moment generating function must be of the form

$$\psi(t,u) = P_0(t) + P_1(t)e^{\alpha u} + P_2(t)e^{2\alpha u} + \dots + P_C(t)e^{C\alpha u},$$

with $P_0(t) + \cdots + P_C(t) = 1$. Substituting this form in (4.1), we write

$$\sum_{j=0}^{C} \dot{P}_j(t) e^{j\alpha u} + \left((1 - e^{-\alpha u}) - \frac{\beta}{\alpha} (1 - e^{\alpha u}) \right) \sum_{j=0}^{C} j\alpha P_j(t) e^{j\alpha u}$$
$$+ \beta C (1 - e^{\alpha u}) \sum_{j=0}^{C} P_j(t) e^{j\alpha u} = 0.$$

This equation is valid for every u; the individual coefficient of any of the functions $e^{j\alpha u}$ must vanish. Let us first organize the latter equation in the form

$$\sum_{j=0}^{C} \left(\dot{P}_{j}(t) + (\alpha - \beta) j P_{j}(t) + \beta C P_{j}(t) \right) e^{j\alpha u} + \sum_{j=1}^{C} (j - C - 1) \beta P_{j-1}(t) e^{j\alpha u} - \sum_{j=0}^{C-1} (j+1) \alpha P_{j+1}(t) e^{j\alpha u} = 0.$$

Reading off the coefficient of each $e^{j\alpha u}$, we have the following set of *ordinary* differential equations:

$$\dot{P}_0(t) + \beta C P_0(t) - \alpha P_1(t) = 0,$$

(corresponding to j = 0), and for $j = 1, 2, \ldots, C - 1$,

$$\dot{P}_{j}(t) + ((\alpha - \beta)j + \beta C)P_{j}(t) + (j - C - 1)\beta P_{j-1}(t) - (j + 1)\alpha P_{j+1}(t) = 0,$$

and corresponding to j = C we have the equation

$$\dot{P}_C(t) + \alpha C P_C(t) - \beta P_{C-1}(t) = 0.$$

We can represent this as a system of first order matric differential equations. Let $\mathbf{P}(t) = (P_0(t), \ldots, P_C(t))^T$. Then

$$\dot{\mathbf{P}}(t) = \begin{pmatrix} -\beta C & \alpha & 0 & 0 & 0 & \dots & 0 & 0 \\ \beta C & -\beta C - (\alpha - \beta) & 2\alpha & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \beta & -\alpha C \end{pmatrix} \mathbf{P}(t)$$
$$:= \mathbf{K}_C \mathbf{P}(t).$$

The solution to this system of ordinary differential equations is

$$\mathbf{P}(t) = e^{\mathbf{K}_C t} \mathbf{P}(0),$$

The matrix of coefficients \mathbf{K}_C is a member of a Leonard pair of the Krawtchouk type (see Terwilliger (2005+)). It is known that such a matrix has real eigenvalues $\lambda_0 > \lambda_1 > \dots > \lambda_C$ forming an arithmetic progression. So, for some real positive k we can write the decreasing eigenvalue sequence as $\lambda_0, \lambda_0 - k, \lambda_0 - 2k, \dots, \lambda_0 - Ck$. The matrix \mathbf{K}_C is singular as the sum of all its rows is 0; hence 0 is one eigenvalue. The value k can be computed from the consideration that the sum of all eigenvalues of a matrix must be equal to its trace, namely

$$\lambda_0(C+1) - \frac{kC}{2}(C+1) = -\beta C(C+1) - \frac{1}{2}(\alpha - \beta)C(C+1).$$

This determines k as

$$k = \frac{2\lambda_0}{C} + \alpha + \beta.$$

The eigenvalues λ_i , for $i = 0, \ldots, C$, of K_C are distinct. Hence, the corresponding eigenvectors $\mathbf{v}_0, \mathbf{v}_1, \ldots, \mathbf{v}_C$ are independent. The modal matrix \mathbf{M} formed by lining up the eigenvectors as its columns, i.e. $\mathbf{M} = [\mathbf{v}_1 | \mathbf{v}_2 | \ldots | \mathbf{v}_C]$, is invertible. An exponential like $\exp(\mathbf{K}_C t)$ can be represented in terms of its modal matrix in the form $\mathbf{M} \exp(\mathbf{D}t)\mathbf{M}^{-1}$, where \mathbf{D} is the diagonal matrix $\mathbf{diag}(\lambda_0, \lambda_1 \ldots, \lambda_C)$. In other words,

$$\mathbf{P}(t) = \mathbf{M} \begin{pmatrix} e^{\lambda_0 t} & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & e^{(\lambda_0 - k)t} & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & \ddots & & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & e^{(\lambda_0 - Ck)t} \end{pmatrix} \mathbf{M}^{-1} \mathbf{P}(0).$$

When we multiply out we get

$$\mathbf{P}(t) = \mathbf{p}_0 e^{\lambda_0 t} + \mathbf{p}_1 e^{(\lambda_0 - k)t} + \dots + \mathbf{p}_C e^{(\lambda_0 - Ck)t},$$

for some computable vector coefficients $\mathbf{p}_0, \ldots, \mathbf{p}_C$. However, $\mathbf{P}(t)$ is a vector of probabilities, the largest rate of exponential growth must be 0. Indeed, $\lambda_0 = 0$ is the principle eigenvalue, and the rest of the eigenvalues must be negative, yielding the component-wise convergence

$$\mathbf{P}(t) \to \mathbf{p}_0, \quad \text{as} \quad t \to \infty.$$

We shall call the eigenvector \mathbf{v}_0 that corresponds to the principle eigenvalue the *principle* eigenvector.

Lemma 4.2 Let \mathbf{v}_0 be the principal eigenvector (normalized so that its component add up to 1). Then,

$$\mathbf{p}_0=\mathbf{v}_0,$$

Proof. Let the *i*th eigenvector be $v_i := (v_{i,0}, \ldots, v_{i,C})$. So,

$$\mathbf{M} = \begin{pmatrix} v_{0,0} & v_{0,1} & \dots & v_{0,C} \\ v_{1,0} & v_{1,1} & \dots & v_{1,C} \\ \vdots & \vdots & \ddots & \vdots \\ v_{C,0} & v_{C,1} & \dots & v_{C,C} \end{pmatrix}.$$

Let the inverse of \mathbf{M} be

$$\mathbf{M}^{-1} := \begin{pmatrix} v'_{0,0} & v'_{0,1} & \dots & v'_{0,C} \\ v'_{1,0} & v'_{1,1} & \dots & v'_{1,C} \\ \vdots & \vdots & \ddots & \vdots \\ v'_{C,0} & v'_{C,1} & \dots & v'_{C,C} \end{pmatrix}.$$

The number of white balls starts in only one state: $W(0) = r\alpha$, for some $0 \le r \le C$, and the initial condition $\mathbf{P}(0)$ must be a vector of the form $(0, 0, \dots, 0, 1, 0, \dots, 0)^T$, with the 1 at the *r*th position.

Multiply out the product

$$\mathbf{M} \begin{pmatrix} e^{\lambda_0 t} & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & e^{(\lambda_0 - k)t} & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & \ddots & & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & e^{(\lambda_0 - Ck)t} \end{pmatrix} \mathbf{M}^{-1} \mathbf{P}(0)$$

to get $v'_{0,r}\mathbf{v}_0$. Note that $v'_{0,r}$ cannot be 0 because the sum of the probabilities must be 1.

A principal eigenvector can be computed to an arbitrary scale. Let us subsume $v'_{0,r}$ in the scale of the principal eigenvector. The lemma follows by the proper scaling of \mathbf{v}_0 that makes its components add up to 1. \Box

Lemma 4.3 For j = 0, ..., C,

$$\operatorname{Prob}(W(t) = j\alpha) \to \frac{\beta^{j} \alpha^{C-j}}{(\alpha + \beta)^{C}} {C \choose j},$$

as $t \to \infty$

Proof. Let us worry about normalization later. We first solve for a principal eigenvector under an arbitrary scale. We wish to solve the matric equation

$$\mathbf{K}_{c}\mathbf{v}_{0} = \begin{pmatrix} -\beta C & \alpha & 0 & 0 & 0 & \dots & 0 & 0 \\ \beta C & -\beta C - (\alpha - \beta) & 2\alpha & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \beta & -\alpha C \end{pmatrix} \mathbf{v}_{0}$$
$$= \lambda_{0}\mathbf{v}_{0}$$
$$= 0,$$

for the vector $\mathbf{v}_0 = (v_{0,0}, \ldots, v_{C,0})^T$. This is a simultaneous system of equations:

$$\begin{aligned} -\beta C v_{0,0} + \alpha v_{1,0} &= 0, \\ \beta (C - i + 1) v_{i-1,0} - (\beta C + (\alpha - \beta)i) v_{i,0} + (i + 1) \alpha v_{i+1,0} &= 0, \quad 1 \le i < C, \\ \beta v_{C-1,0} - \alpha C v_{C,0} &= 0. \end{aligned}$$

Let $p = \beta/(\alpha + \beta)$, and set q = 1 - p. We show by finite induction that the components of any principal eigenvector \mathbf{v}_0 follow the binomial pattern

(4.2)
$$v_{i,0} = sp^i q^{C-i} \binom{C}{i},$$

for an arbitrary scale $s \neq 0$. Since we are solving under an arbitrary scale, we can freely take $v_{0,0} = sq^C$. The first of the simultaneous equation yields

$$v_{1,0} = spq^{C-1} \binom{C}{1}.$$

Assume the binomial pattern (4.2) holds up to i - 1. The generic equation for $1 \le i < C$ gives

$$v_{i+1,0} = \frac{s}{\alpha(i+1)} \left[(\beta C + (\alpha - \beta)i)p^i q^{C-i} \binom{C}{i} - \beta(C-i+1)p^{i-1}q^{C-i+1} \binom{C}{i-1} \right]$$
$$= s \frac{\alpha^{C-i-1}\beta^{i-1}}{(\alpha + \beta)^C(i+1)} \left[\beta^2(C-i)\binom{C}{i} + \alpha\beta \left[i\binom{C}{i} - (C-i+1)\binom{C}{i-1} \right] \right].$$

It is straightforward to check the identities

$$\binom{C}{i} - (C-i+1)\binom{C}{i-1} = 0,$$

and

$$\frac{C-i}{i+1}\binom{C}{i} = \binom{C}{i+1},$$

say from the factorial definition of the binomial coefficients. The binomial form (4.2) holds by finite induction, for $1 \leq i < C$. The form of $v_{C-1,0}$ in the last of the simultaneous system of equations extends the validity of the binomial form to $v_{C,0}$. With the scale s = 1, the components of the principal eigenvalue add up to 1, and the statement follows from Lemma 4.2. \Box

The technical development of the previous lemmas proves the main result.

Theorem 4.1 Let W(t) be the number of white balls at time t in the Ehrenfest process with invariant C. As $t \to \infty$, we have convergence in distribution

$$W(t) \xrightarrow{\mathcal{D}} \alpha \operatorname{Bin}\left(C, \frac{\beta}{\alpha + \beta}\right).$$

5 Concluding Remarks

Our interest in generalized Ehrenfest models stemmed from an attempt to assess a general technique for Markov chains. The technique of pseudo-expectation was introduced in Watanabe, Sawai and Takahashi (2003) for analyzing the average speed of randomized algorithms of certain types. It is meant for approximating distributions in Markov chains with large state-space by a composition of simpler one-step conditional expectations. To justify this pseudo-expectation technique, Watanabe (2005+) considered a simple ball drawing urn model that progresses in discrete time, which is our generalized Ehrenfest model with unspecified $\alpha \geq 1$ and $\beta = 1$. In the latter investigation white and blue balls in the urn were considered, but having different "weights." In this model balls are withdrawn with probability proportional to their weights; each white ball has weight α , whereas a blue ball has weight 1. This weighting corresponds to a biased (but still randomized) decision made by a given algorithm. Watanabe, Sawai, and Takahashi (2003), Takahashi and Niikura (2003), Schneider (2004), and Watanabe (2005+) made both experimental and mathematical investigations for justifying the pseudo-expectation. Experimentally, it was shown that the pseudo-expectation is a reasonable shortcut. Some mathematical analysis has been made (Watanabe (2005+)) for the error bound of the pseudo-expectation on the generalized Ehrenfest models. We hope that the investigation of this paper will help us understand the discrete models in the above references on pseudo-expectation and their generalizations.

Recall that in the discrete model, the state depends on the parity of the number of draws, and subsequently no steady state exists. A technical trick to avoid this is to consider average distributions of two consecutive draws. When studying the pseudoexpectation on the generalized Ehrenfest models, Schneider (2004) derived this averaged steady distribution for a generalized Ehrenfest model with a given α and C (where β is fixed to 1).

From several numerical computations, Schneider (2004) found that it is given by

$$\operatorname{Prob}(W_{\infty} = k\alpha) = \frac{\alpha^{C-k}(C+k(\alpha-1))}{2C(1+\alpha)^C} \binom{C}{k}.$$

No systematic way has been developed yet for deriving this distribution. We are hoping the analysis of the embedded processes in this paper may provide good analytic or heuristical approaches for deriving such distributions.

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