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Long run behaviour of infinite Pólya Urn Models

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Contents

Abstract

Urn schemes and their many generalisations are a key element of study for random processes with reinforcements. We study and analyse a new balanced Pólya urn scheme with countably infinite colour set introduced in [3]. We discuss convergence results with the approach provided by [1], which represents the observed sequence of colors in terms a branching Markov chain on a random recursive tree. Our main goal is to calculate the expectation and variance of the contents of the urn to have a better understanding of the long run behaviour of our model.

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Statement of authorship

The results presented in this report is the work of the author under the supervision of A/Prof Nathan Ross. My supervisor assisted with the work throughout, answered questions, and proofread this report.

1 Introduction

1.1 Background

Pólya urn schemes are a class of fundamental probability models with a long history tracing back to the work of Eggenberger and Pólya [5] and extending to present research. The standard general model begins with balls of different colours in an urn, and at each step a ball is drawn randomly from the urn and returned along with the addition or removal of some prescribed number of balls of each colour. In previous papers, multiple classes of models under different settings have been studied in the literature, such as the classical work by Blackwell and MacQueen where the urn scheme is allowed to have a continuum of colours [4], and the infinite colour generalisation of balanced urn schemes associated with random walks on $\mathbb{Z}^d$ [1, 2].

The popularity of these models stems from the fact that variations of the basic Pólya urn reinforcement mechanism are utilised in a diverse range of fields, including biology, computer science, and statistics. For instance, the Pólya urn model can represent a Dirichlet process, which is commonly employed in statistical Bayesian inference to characterise prior knowledge about the distribution of random variables. Additionally, the Pólya urn scheme has become increasingly relevant in branching phenomena and processes that involve a random tree structure. As a result, it has been applied to epidemics and other spreading phenomena that exhibit branching patterns within a population.; for more details, see Pemantle [9] and Mahmoud [7].

Previous studies have explored Pólya urn models with colours indexed by a finite set. To analyse finite colour urn models, researchers typically use a few standard methods based on martingale techniques, stochastic approximations, and embed-dings into continuous time pure birth processes. These analyses heavily rely on the Perron-Frobenius theory of matrices with positive entries [12] and the Jordan Decomposition of finite dimensional matrices [6]. However, until recently, there has been limited development of the infinite color generalisation of the Pólya urn scheme. The main obstacle in this case is that the techniques applied for finite urn models are not available when the colour set is infinite. To overcome this issue, we adopt an alternative path that leverages the Grand Representation Theorem (Theorem 3.1). The key contribution of this theorem is to establish a correspondence between the observed sequence of colors and the underlying branching Markov chain sequence for general urn schemes. By bypassing standard martingale and matrix theoretic techniques, we can derive asymptotic results. Further discussion on this topic is presented in Section 3. The following section defines the model and presents our primary findings.

1.2 Model

In this report, we use the model introduced in [3] and will focus on the case where the set of colours, denoted by S, is countably infinite. As for the infinite dimension replacement matrix $R := (R(i,j))_{i,j\in S}$, we assume that each row sum is equal and finite. It is conventional to take R to be a stochastic matrix, where, instead of representing the number of balls, each entry $R(i,j) > 0$ is treated as the proportion of balls of colour j to be placed in the the urn when the colour of the selected ball is i (see [2] for details).

We denote the random configuration of the urn at time $n \geq 0$ by $U_n := (U_{n,v})_{v\in S}$, which is an infinite vector with non-negative entries. Without losing generality, we suppose there are t balls in the urn at the beginning and thus we start with a non-random initial configuration U_0 with finite total mass denoted by t. Then we define the random configuration U_n such that, if Z_n represents the randomly chosen colour at the $(n+1)$-th draw, then the conditional distribution of Z_n given **all** past configurations $U_0, U_1, ..., U_n$ **only** depends on U_n. Formally, for all $z \in S$,

$$\mathbb{P}(Z_n = z \mid U_n, U_{n-1}, ..., U_0) = \frac{U_{n,z}}{n+t}, \tag{1}$$

and, starting with a non-random U_0, we define $(U_n)_{n\geq 0} \subset \ell_1$, recursively as

$$U_{n+1} = U_n + R_{Z_n}, \tag{2}$$

where R_{Z_n} denotes the Z_n-th row of the matrix R. Note that for every colour $v \in S$, the corresponding row $R(v,\cdot)$ represents a probability distribution, so in each time step we add a mass 1 vector to the current configuration. Consequently, it can be observed easily that

$$\begin{aligned}\sum_{v\in S} U_{n,v} &= \sum_{v\in S}\Big[U_{0,v} + R(Z_0,v) + R(Z_1,v) + \cdots + R(Z_{n-1},v)\Big]\\ &= \sum_{v\in S} U_{0,v} + \sum_{v\in S} R(Z_0,v) + \sum_{v\in S} R(Z_1,v) + \cdots + \sum_{v\in S} R(Z_{n-1},v) = t+n,\end{aligned}$$

and 1 is a well-defined probability measure. Further, 1 can be interpreted as a draw from urn with the random configuration U_n. So the law for each drawn colour is decided fully by the newest updated configuration. From this viewpoint, it is natural for us to relate the urn model to Markov chain model since they both share the idea of the well-known Markov property which frequently appears in stochastic process analysis. Intuitively, the asymptotic properties of the urn model defined as such are determined by the asymptotic properties of the associated Markov chain. In fact, in [1, 8], the authors have shown in rigorous proof that the drawn colour sequence $(Z_n)_{n\geq 0}$ has same law as that of a branching Markov chain with transition matrix R, initial distribution $\frac{U_0}{t}$ and defined on the random recursive tree. In Section 3.1, we provide the details of this representation.

Before introducing the main result, two assumptions on the replacement matrix R are required.

Assumption 1.1. The replacement scheme R is a stochastic matrix and is irreducible, aperiodic and positive recurrent, so consequently the associated Markov Chain has a unique stationary distribution π satisfying $\pi R = \pi$ and is ergodic, that is, for any $u, v \in S$,

$$\lim_{n\to\infty} R^n(u,v) = \pi_v.$$

Assumption 1.2. The associated Markov chain is assumed to be *uniformly ergodic*, namely there exists positive constants, $0 < \rho < 1$ and $C > 0$, such that for any time $n \geq 1$ and for any states $u, v \in S$,

$$|R^n(u,v) - \pi_v| \leq C\rho^n.$$

Remark 1.3. Assumption 1.1 means that no matter which state the chain starts from, if we run the Markov chain for long enough time, then the probability of the chain to end up with colour v is going to the stationary distribution π_v.

Remark 1.4. Assumption 1.2 states that, throughout the process, the probability running the chain from colour u and end up with v in n step of time will converge to π_v at a uniformly bounded rate.

1.3 Main Results

As mentioned in the introduction, reflected from the real-world application, there are some frequently asked questions about the infinite urn model. What is the proportion of colour v ball in the urn at time n? What is the number of times the colour v is chosen up to time n? For example, mathematical models of population genetics can be considered equivalent to urn models, as genes in the population correspond to balls in the urn, and genetic type of a gene corresponds to the color of the ball [11]. In particular, geneticists may be interested in what is the proportion for a particular type of gene appearing in the gene sequence asymptotically. This attracts our attention towards the long run behaviour of random variables such as $N_{n,v} := \sum_{i=0}^{n} \mathbb{1}_{\{Z_i=v\}}$ denoting the number of times the colour v is chosen up to time n.

Consider an urn model $(U_n)_{n\geq 0}$ as defined by the Section 1.2 with colours indexed by a countably infinite set S and with assumptions 1.1 and 1.2 both satisfied. In our project we produce some convergence results with the help of the idea from proofs in [3] and derive the long-run behaviour as stated in the form of the following theorem,

Theorem 1.5. *For any $v \in S$, let $N_{n,v} := \sum_{i=0}^{n} \mathbb{1}_{\{Z_i=v\}}$, denote the number of times the colour v is chosen up to time n. Then, as $n \to \infty$,*

$$\mathbb{E}\left(\frac{N_{n,v}}{n+1}\right) \to \pi_v. \tag{3}$$

$$\mathrm{Var}\left(\frac{N_{n,v}}{\sqrt{n+1}}\right) \to \pi_v(1-\pi_v). \tag{4}$$

This complements the Law of Large Number result from [3], and we make the following conjecture:

Conjecture 1.6. For any $v \in S$, let $N_{n,v} := \sum_{i=0}^{n} \mathbb{1}_{\{Z_i=v\}}$, denote the number of times the colour v is chosen up to time n. Define the standardised random variable by

$$X_{n,v} = \frac{N_{n,v} - (n+1)\pi_v}{\sqrt{(n+1)\pi_v(1-\pi_v)}}.$$

Then, as $n \to \infty$,

$$X_{n,v} \xrightarrow{d} \mathcal{N}(0,1)$$

where $\mathcal{N}(0,1)$ is the standard Normal random variable.

The structure of the document is as follows: Section 2 provides an introduction to the fundamental concept of the random recursive tree, which serves as the foundation for our branching Markov process. In Section 3, we present the Grand Representation Theorem, which connects two models and demonstrates how we employ model coupling to convert problems from one model to the other. In Section 4, we present our findings on convergence, supported by expectation and variance calculations. Section 5 proposes two potential approaches for future work in proving the conjecture regarding the Central Limit Theorem result. Lastly, in Section 6, we provide proofs of the key lemmas.

2 Branching Processes

With only the model described in Section 1.2, it is not clear how to analyse $N_{n,v}$ and provide answer to the questions in subsection 1.3. Fortunately, we can define a new model which is highly aligned with the current urn model and consists of two ingredients: the random recursive tree (Section 2.1) and the branching Markov chain (Section 2.2). This model is embellished, keeping track of more information, and thus the related problem can be analysed more easily.

2.1 Random Recursive Trees

We construct random recursive tree sequence of trees $(\mathcal{T}_n)_{n\geq 1}$. $\mathcal{T}_n$ has $n+2$ vertices, where o is the root, and the other vertices are denoted as $\{w_0, w_1, ..., w_n\}$, where the increasing subscripts indicate the order in which they are attached to the tree. The root o is given initial weight $t > 0$, and every other node has weight 1. Initially, we start with $\mathcal{T}_{-1}$ which only consists of the root o. Then, to construct the sequence of trees $(\mathcal{T}_n)_{n\geq -1}$, at time $n+1$ we add one new node w_n to the tree in each step such that

1. $\mathbb{P}$ (the parent of w_n in $\mathcal{T}_{n-1}$ is the root o) $= \frac{t}{n+t+1}$,

2. $\mathbb{P}$ (the parent of w_n in $\mathcal{T}_{n-1}$ is w_j) $= \frac{1}{n+t+1}$, for $j = 0, 1, \ldots, n-1$.

Define the infinite random recursive tree as

$$\mathcal{T} := \bigcup_{n\geq -1} \mathcal{T}_n \tag{5}$$

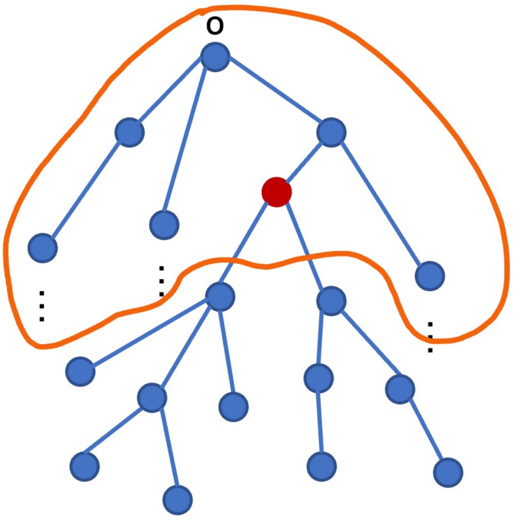

Figure 1: Markov Property

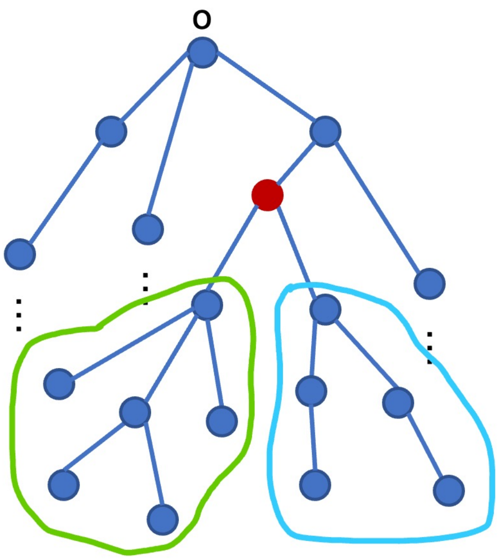

Figure 2: Branching Property

2.2 Branching Markov Processes

Recall that S is the set of colours. Let $\Delta \notin S$ be a symbol (can be considered as dummy variable). Define a stochastic process $(W_n)_{n \geq -1}$ with state space $S \cup \Delta$ starting at the root o and at a position $W_{-1} = \Delta$, and for any $n \geq 0$ and for any $v \in S$,

$$\mathbb{P}(W_n = v \mid W_{n-1}, W_{n-2}, ..., W_{-1}; \mathcal{T}_n) = \begin{cases} \frac{U_0(v)}{t}, & \text{if } \overleftarrow{w_n} = o, \\ R(W_j, v), & \text{if } \overleftarrow{w_n} = w_j, \end{cases} \tag{6}$$

where $\overleftarrow{w_n}$ is the parent of w_n in RRT $\mathcal{T}_n$. Such stochastic process is called a branching Markov chain (also called BMC) on the random recursive tree $\mathcal{T}$. Note that the Markov process has the following two properties inherently embedded in the definition of W_n:

- Markov property: Since the probability distribution of the current W_n only depends on the information about the parent node for the corresponding w_n in the tree, the evolution of the Markov process in next time step depends only on the present state and does not depend on past history with respect to the genealogy of the tree. In other words, given all the past history, the next state is dependent on the past and present only through the present state.
- Branching property: Once the information about the least common ancestor is given, the two child branches develop independently with each other. The W_n's are a population in which each member of the population independently produces offspring.

Remark 2.1. The Markov chain has the replacement matrix R as its transition matrix.

2.3 Bounded Covariance

As mentioned in the introduction, uniform ergodicity of the branching Markov chain gives uniform convergence to its limiting stationary distribution. Combining this with definitions of the RRT and BMC, a nice property of the chain can be obtained, mentioned as Lemma 3.2 in [3]. The lemma bounds the covariance between two random variables in the chain having the same colour given the tree, which helps us interpret how the nodes correlated with each other when the tree expands and grows. Before diving into such result, it is necessary to introduce some graph theory preliminaries.

Definition 2.2. Let $d(x, y)$ denote the graph distance between nodes w_x and w_y in the RRT $\mathcal{T}_n$, representing the number of edges between nodes x and y. In particular, suppose o is the root, then $d(o, x)$ is the depth of w_x, which we also denote by $d(x)$.

Definition 2.3. Let $\mathcal{T}_n$ be a random recursive tree (RRT). Let $\mathcal{L}(x, y)$ denote the least common ancestor for the vertices $w_x, w_y \in \mathcal{T}_n$ in the RRT, which is the nearest parent node shared by w_x and w_y.

Lemma 2.4. *(Lemma 3.1 in [3]) Given the RRT $\mathcal{T}_n$, we have for some suitable constant $C > 0$,*

$$\operatorname{Cov}(W_x = v, W_y = v \mid \mathcal{T}_n) \leq C\rho^{\max(d(x,\mathcal{L}(x,y)),d(y,\mathcal{L}(x,y)))} \leq C\rho^{\frac{d(x,y)}{2}}, \tag{7}$$

where ρ is as in Definition of uniform ergodicity so $0 < \rho < 1$.

Remark 2.5. This implies, once the nodes w_x and w_y in the RRT are far away enough from each other, the covariance for the corresponding random variables W_x and W_y to take the colour v will be bounded by a very small number. So, given the tree, many parts of the random variables W_n are going to behave like pairs of independent Bernoulli random variables.

Remark 2.6. Lemma 2.4 relies totally on the BMC properties and RRT structure and thus has nothing to do with the urn model yet.

3 Model Coupling

3.1 Grand Representation Theorem

Theorem 3.1. *Let $(Z_n)_{n\geq 0}$ denotes the infinite sequence of randomly chosen colours at each draw from the urn. Let $(W_n)_{n\geq 0}$ be the branching Markov chain defined as above. Then,*

$$(Z_n)_{n\geq 0} \overset{d}{=} (W_n)_{n\geq 0}. \tag{8}$$

This representation theorem enables us to transfer the focus and interest on Z_n to the research on W_n, since the two sequences of random variables have the same distributions as processes. This is a fairly strong statement indicating that any limiting distributional statements for W_n will hold the same for the limiting behaviour of the Z_n's, and any collections of subset of indices from these two sequences will have the same distribution not only point-wise but also in terms of the joint distributions.

Remark 3.2. By the Grand representation theorem, we can solve the problems mentioned in Section 1.3 by dealing with random variable W_i instead of Z_i and utilise the graph properties given by the random recursive tree structure to enable further analysis.

Remark 3.3. The indicators $\mathbb{1}_{\{W_i=v\}}$ are not strictly independent with each other, thus, through the process of calculating the quantities and proving the Central Limit Theorem, we need to be careful about the dependency.

4 Convergence Results

Before we state our results, there is a lemma that will be frequently used in the proofs later.

Lemma 4.1. *Let $v \in S$ be some colour. For $n \geq 0$ and $i = 0, 1, 2..., n$, we have*

$$\Big| \mathbb{P}(W_i = v|\mathcal{T}_n) - \pi_v \Big| \leq C\rho^{d(i)} \tag{9}$$

where $C > 0$ is some constant.

Remark 4.2. This implies, once a node w_i in the RRT exists far enough away from the root o, the probability for the corresponding random variables W_i to take the colour v will be very close to π_v. Thus, when the tree grows large in the long run, most of the random variables W_n, except those whose corresponding w_n's are near the root, are expected to have almost identical Bernoulli distribution with the probability of taking colour v to be approximately π_v.

Additionally, in this section, when calculating the expectation and variance for the variable of interest, it often requires us to bound the expectation of the sum for terms $\rho^{d(x)}$ and $\rho^{d(x,y)}$, which basically generated by the upper bound (on the right hand side of the inequality) in Lemma 2.4 and Lemma 4.1. Therefore, it is necessary to introduce another lemma dealing with such asymptotic behaviour, which is stated as follows:

Lemma 4.3. *(Lemma 3.2 in [3]) Let $\mathcal{T}_n' := \mathcal{T}_n \setminus \{o\} = \{w_0, w_1, ..., w_n\}$ be the set of $n+1$ vertices excluding the root. Fix r with $0 < r < 1$ and define*

$$A_n = A_n(r) := \mathbb{E}\left[\sum_{w_x \in \mathcal{T}_n'} r^{d(x)}\right], \tag{10}$$

$$B_n = B_n(r) := \mathbb{E}\left[\sum_{w_x, w_y \in \mathcal{T}_n'} r^{d(x,y)}\right]. \tag{11}$$

Then, for some constant C (possibly depending on r and t) and all $n \geq 1$,

$$A_n \leq Cn^r, \tag{12}$$

$$B_n \leq \begin{cases} Cn^{2r} & \text{if } \frac{1}{2} < r < 1, \\ Cn\log(n+1) & \text{if } r = \frac{1}{2}, \\ Cn & \text{if } 0 < r < \frac{1}{2}. \end{cases} \tag{13}$$

4.1 Expectation

We first prove 3 from Theorem 1.5.

$$\begin{aligned}
\mathbb{E}\Big(\frac{N_{n,v}}{n+1}\Big) &= \frac{1}{n+1}\sum_{i=0}^{n}\mathbb{E}[\mathbb{E}(\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n)] \qquad \text{by double expectation law (a.k.a. the `tower property')}\\
&= \frac{1}{n+1}\sum_{i=0}^{n}\mathbb{E}[\mathbb{P}(\{W_i=v\}|\mathcal{T}_n)-\pi_v+\pi_v]\\
&= \frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n}(\mathbb{P}(\{W_i=v\}|\mathcal{T}_n)-\pi_v)+\frac{1}{n+1}\sum_{i=0}^{n}\pi_v\\
&\le \frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n}(C\rho^{d(i)})+\pi_v \qquad \text{by Lemma 4.1}\\
&= \frac{C}{n+1}A_n(\rho)+\pi_v \le \frac{Cn^{\rho}}{n+1}+\pi_v \qquad \text{by Lemma 4.3}
\end{aligned}$$

Since $0<\rho<1$, then when n goes to ∞, $\frac{Cn^{\rho}}{n+1}$ goes to 0, and thus we obtain $\mathbb{E}(\frac{N_{n,v}}{n+1}) \to \pi_v$ as $n\to\infty$.

4.2 Variance

As mentioned in Remark 2.5 and Remark 4.2, when we run the chain for a time period long enough, it is reasonable to consider that the random variables $\{W_i\}_{i=0,1,2,..,n}$ given the tree $\mathcal{T}_n$ are some almost independent identical Bernoulli trials with 'success probability' approximately π_v. Such inference is also closely related with the uniform ergodicty assumption which is very crucial for our investigation of the long-run behaviour of the urn model. Thus, it is intuitively natural to claim that $\pi_v(1-\pi_v)$ would be a good guess for the variance of $Var(\frac{N_{n,v}}{\sqrt{n+1}})$ as $n\to\infty$. First, we decompose the variance by the conditional variance formula,

$$\begin{aligned}
\mathrm{Var}\left(\frac{N_{n,v}}{\sqrt{n+1}}\right) &= \frac{1}{n+1}\mathbb{E}[\mathrm{Var}(N_{n,v}|\mathcal{T}_n)]+\frac{1}{n+1}\mathrm{Var}[\mathbb{E}(N_{n,v}|\mathcal{T}_n)]\\
&= \frac{1}{n+1}\mathbb{E}\Big[\mathrm{Var}\left(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\right)\Big]+\frac{1}{n+1}\mathrm{Var}\left[\mathbb{E}\Big(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\Big)\right]
\end{aligned}$$

We delegate the tasks to two lemmas explaining how each component of the variance converge in the long run. The detailed proofs can be found in Section 6.

Lemma 4.4. *Given the branching Markov chain W_n defined on the random recursive tree $\mathcal{T}_n$ as in Section 2, as $n\to\infty$,*

$$\frac{1}{n+1}\mathbb{E}\Big[\mathrm{Var}\left(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\right)\Big]\to\pi_v(1-\pi_v). \tag{14}$$

Lemma 4.5. *Given the branching Markov chain W_n defined on the random recursive tree $\mathcal{T}_n$ as in Section 2, as $n\to\infty$,*

$$\frac{1}{n+1}\mathrm{Var}\left[\mathbb{E}\Big(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\Big)\right]\to 0. \tag{15}$$

Combining the results in Lemma 4.4 and 4.5 together, shows that, when $n\to\infty$,

$$\mathrm{Var}(\frac{N_{n,v}}{\sqrt{n+1}}) = \frac{1}{n+1}\mathbb{E}\Big[\mathrm{Var}\left(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\right)\Big]+\frac{1}{n+1}\mathrm{Var}\left[\mathbb{E}\Big(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\Big)\right]\to\pi_v(1-\pi_v)$$

5 Discussion

After we calculate the expectation and variance, it is conventional to take one step forwards to the Central Limit Theorem result, which should explain how fast $\frac{N_{n,v}}{n+1}$ converges to the stationary distribution π_v as stated in 1.5. By standardisation, we define

$$X_{n,v} := \frac{N_{n,v} - (n+1)\pi_v}{\sqrt{(n+1)\pi_v(1-\pi_v)}}.$$

Note that $X_{n,v}$ has expectation converging to 0 and variance (also standard deviation) converging to 1 as $n \to \infty$, this can be derived easily from the results in Section 4.1 and 4.2,

$$\mathbb{E}\left[X_{n,v}\right] = \frac{n+1}{\sqrt{(n+1)\pi_v(1-\pi_v)}}\mathbb{E}\left(\frac{N_{n,v}}{n+1} - \pi_v\right) = \frac{n+1}{\sqrt{(n+1)\pi_v(1-\pi_v)}}\left(\mathbb{E}\left(\frac{N_{n,v}}{n+1}\right) - \pi_v\right) \to 0.$$

$$\mathrm{Var}[X_{n,v}] = Var\left[\frac{N_{n,v} - (n+1)\pi_v}{\sqrt{(n+1)\pi_v(1-\pi_v)}}\right] = \frac{1}{\pi_v(1-\pi_v)}\mathrm{Var}\left(\frac{N_{n,v}}{\sqrt{(n+1)}}\right) \to 1.$$

Our goal is to show that the distribution of $X_{n,v}$ converges to the standard normal distribution as $n \to \infty$. After exploring multiple possible approaches of proving the equivalence of distributions, we reckon the method of moments and the Stein's method are the most suitable to work with in our case. We will introduce how these approaches work in general and how they fit into our model.

5.1 Method of Moments

The method of moments is a technique for proving the distributions of two given random variables are the same, based on matching all of their moments. According to method of moments, we need to show, for all $k \in \mathbb{N}$

$$\lim_{n\to\infty} \mathbb{E}(X_{n,v}^k) = \mathbb{E}(Z^k) \tag{16}$$

where $Z \overset{d}{=} \mathcal{N}(0,1)$ is the standard Normal random variable.

This means, to apply such method, all moments for $X_{n,v}$ are required to be calculated and compared with those of Z. From the calculation by using moment generating function, we know that the odd moments of Z are all zero, and the even moments can be expressed as

$$\mathbb{E}(Z^{2n}) = \frac{(2n)!}{2^n \cdot n!} \qquad \text{where} \quad n \in \mathbb{N}$$

So, one possible solution is to show all sums of products involving odd order terms will eventually vanish, and that only some terms with specific arrangements and order contained in the even moments will be contribute, and turn out to be in the same form as that of the even moments of standard Normal distribution. This process involves in the calculation of not only single variable terms with higher power but also the mixed terms such as $X_{i,v}X_{j,v}X_{k,v}$ where $i \neq j \neq k$, so the work can be quite burdensome.

5.2 Stein's Method

Stein's method is a technique that can quantify the error in the approximation of one distribution by another in a variety of metrics. For the random variables X and Y which have μ and ν as their probability measures respectively, the general metric can be denoted as $d_{\mathcal{H}}(X, Y)$. More specifically,

$$d_{\mathcal{H}}(X, Y) = \sup_{h \in \mathcal{H}} |\mathbb{E}h(X) - \mathbb{E}h(Y)|. \tag{17}$$

where $\mathcal{H}$ is some family of 'test' functions.

There are mainly two components for the method. First, it requires a framework to convert the problem of bounding the error in the approximation of some distribution of interest by another familiar well-known distribution, into a problem of bounding the expectation of a certain functional of the random variable of interest. Second, we need techniques to bound the expectation appearing in the first component, and such step is called 'auxiliary randomisation'.

For example, if we have a bunch of locally dependent random variables such as W_n's in our BMC, then by deciding a proper dependency neighbourhood and restricting a domain for the test functions, then the difference between sum of these random variables and another distribution can be quantified. Section 3.2 of [10] provides a useful theorem which quantifies the heuristic that a sum of many locally dependent random variables will be approximately normal, which states as follows:

Theorem 5.1. *Let $X_1, ..., X_n$ be random variables with $\mathbb{E}[X_i^4] < \infty$, $\mathbb{E}[X_i] = 0$, $\sigma^2 = \mathrm{Var}(\sum_i X_i)$, and define $W = \sum_i X_i/\sigma$. Let the collection $(X_1, ..., X_n)$ have dependency neighbours N_i, $i = 1, ..., n$, with $D := \max_{1 \le i \le n} |N_i|$. Then for Z, a standard normal random variable,*

$$d_W(W, Z) \le \frac{D^2}{\sigma^3} \sum_{i=1}^{n} \mathbb{E}|X_i|^3 + \frac{\sqrt{26} D^{\frac{3}{2}}}{\sqrt{\pi}\sigma^2} \sqrt{\sum_{i=1}^{n} \mathbb{E}[X_i]^4}. \tag{18}$$

where a collection of random variables $(X_1, ..., X_n)$ has dependency neighbourhoods $N_i \subset \{1, ..., n\}, i = 1, ..., n$, if X_i is independent of $\{X_j\}_{j \notin N_i}$, and d_W is the Wasserstein metric.

According to such theorem, if we can bound the sum of third moments, fourth moments and also be careful when dealing with the intermediate terms and matching the terms in Taylor's expansion, then we are able to give an upper bound for the discrepancy between our distribution and the standard normal distribution.

5.3 Analogous Results of Moments

It is worth noticing that, in both methods, the higher order moments of $X_{n,v}$ are required to be calculated and expressed into an exact formula. This comes down to how we can utilise the formerly defined RRT and BMC model to tackle the problem. Inspired by Lemma 2.4 on bounding the covariance, it is natural to think about establishing some analogues to such results when we proceed the further calculation in moments higher than two. We can first start with case where $k = 3$ and try to show some valid analogues of Lemma 2.4, where one possible lemma can be,

Lemma 5.2. *Suppose nodes w_i, w_j, w_k are in $\mathcal{T}_n$ such that $\mathcal{L}(i, j)$ is the furthest away from the root among all pairwise least common ancestors of the nodes. Then,*

$$\left| \mathbb{P}\left(W_i = v, W_j = v, W_k = v \mid \mathcal{T}_n\right) - \pi_v^3 \right| \le C \left(\rho^{\frac{d(i,j)}{2}} + \rho^{\max\left(\frac{d(i,k)}{2}, \frac{d(j,k)}{2}\right)} \right). \tag{19}$$

Similar to the idea in Lemma 4.3, after producing such an upper bound for the joint probability, we can then investigate the asymptotic behaviour for the sum of expectation of the terms on the right hand side of inequality 19, by first writing down the inductive formula and then solving for the exact mathematical expression of the sum of expectation.

6 Proofs

6.1 Proof for Lemma 4.1

Proof. Given that the branching Markov chain W_n is defined as follows, for any $k \geq 0$ and $v \in S$,

$$\mathbb{P}(W_k = v \mid W_{k-1}, W_{k-2}, ..., W_{-1}; \mathcal{T}_k) = \begin{cases} \frac{U_0(v)}{t} & \text{if } \overleftarrow{w_k} = o \\ R(W_j, z) & \text{if } \overleftarrow{w_j} = w_j \end{cases}$$

Every time we trace back to the parent node of the current node, either multiply with $R(W_j, \cdot)$ if the parent is not root, or multiply simply by U_0/t if the parent is the root. So recursively we get the distribution of W_x for some existing node w_x in the RRT $\mathcal{T}_n$. So by induction, tracing back through the tree with one node each time until hitting the root, we know, for $i = 0, 1, .., n$,

$$\mathbb{E}[\mathbb{1}_{\{W_i = v\}} | \mathcal{T}_n] = \mathbb{P}(W_i = v \mid \mathcal{T}_n) = \frac{U_0}{t} \cdot R^{d(i)}(v) = \sum_{z \in S} \frac{U_0(z)}{t} \cdot R^{d(i)}(z, v) \tag{20}$$

Also, by uniform ergodicity, there exists positive constants, $0 < \rho < 1$ and $C > 0$, such that for any time $n \geq 1$ and for ant states $u, v \in S$,

$$|R^n(u, v) - \pi_v| \leq C\rho^n. \tag{21}$$

And since the initial configuration is defined such that $\sum_{v \in S} U_{0,v} = t$, then

$$\sum_{z \in S} \frac{U_0(z)}{t} = 1. \tag{22}$$

So, having the above facts, combine them together we know

$$\begin{aligned} \Big| \mathbb{P}(W_i = v | \mathcal{T}_n) - \pi_v \Big| &= \Big| \Big(\sum_{z \in S} \frac{U_0(z)}{t} \cdot R^{d(i)}(z, v) \Big) - \pi_v \Big| = \Big| \sum_{z \in S} \frac{U_0(z)}{t} \cdot R^{d(i)}(z, v) - \sum_{z \in S} \frac{U_0(z)}{t} \pi_v \Big| \\ &= \Big| \sum_{z \in S} \frac{U_0(z)}{t} \cdot \Big(R^{d(i)}(z, v) - \pi_v \Big) \Big| \leq \sum_{z \in S} \frac{U_0(z)}{t} \cdot \Big| R^{d(i)}(z, v) - \pi_v \Big| \\ &\leq (\sum_{z \in S} \frac{U_0(z)}{t}) \cdot C\rho^{d(i)} = C\rho^{d(i)} \end{aligned}$$

So, we have

$$\Big| \mathbb{P}(W_i = v | \mathcal{T}_n) - \pi_v \Big| \leq C\rho^{d(i)}.$$

Rewrite it in terms of orders:

$$\mathbb{P}(W_i = v | \mathcal{T}_n) = \pi_v + O(\rho^{d(i)}),$$

where $O(\rho^{d(i)})$ indicates some term which grows no faster than $\rho^{d(i)}$ up to some constants. □

6.2 Proof for Lemma 4.4

Proof. Since the indicator random variables $\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n$ are not independent, the variance of the sum consists of two parts: the sum of variance and the sum of covariance between each pair of distinct random variables,

$$\frac{1}{n+1}\operatorname{Var}\left(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\right)=\frac{1}{n+1}\sum_{i=0}^{n}\operatorname{Var}\left[\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\right]+\frac{1}{n+1}\sum_{i\neq j}\operatorname{Cov}\Big(W_i=v,W_j=v|\mathcal{T}_n\Big). \tag{23}$$

The expectation of the covariance part is easy to deal with by applying Lemma 2.4,

$$\frac{1}{n+1}\mathbb{E}\Big[\sum_{i\neq j}\operatorname{Cov}\Big(W_i=v,W_j=v|\mathcal{T}_n\Big)\Big]\leq\frac{1}{n+1}\mathbb{E}\left[\sum_{i\neq j}C\rho^{d(i,j)/2}\right]<\frac{C}{n+1}\mathbb{E}\left[\sum_{x,y\in\mathcal{T}_n'}\rho^{d(x,y)}\right]=\frac{C}{n+1}B_n(\rho)$$

for some constant C.

By Lemma 4.3, even in the worst case, the highest order of n in $B_n(\rho)$ is no more than 1. Thus, as $n\to\infty$, the term on the right hand side of the inequality will vanish, so the strictly bounded left hand side will go to zero as well.

Then we turn to the sum of variance part and try to solve for its expectation. Note that, conditioned on the RRT $\mathcal{T}_n$, each of the random variable $\mathbb{1}_{\{W_i=v\}}$ is a Bernoulli random variable, so that

$$\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n=\begin{cases}1 & \text{w.p. } \mathbb{P}(W_i=v|\mathcal{T}_n)\\ 0 & \text{w.p. } 1-\mathbb{P}(W_i=v|\mathcal{T}_n)\end{cases}$$

Then, we know

$$\operatorname{Var}\Big(\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\Big)=\mathbb{P}(W_i=v|\mathcal{T}_n)(1-\mathbb{P}(W_i=v|\mathcal{T}_n)).$$

Due to this fact, and since we have shown that the second part in equation 23 contribute nothing, to prove the lemma it is equivalent to show that as $n\to\infty$,

$$\Big|\frac{1}{n+1}\mathbb{E}\left(\sum_{i=0}^{n}\mathbb{P}(W_i=v|\mathcal{T}_n)(1-\mathbb{P}(W_i=v|\mathcal{T}_n))\right)-\pi_v(1-\pi_v)\Big|\to 0. \tag{24}$$

The left hand side of equation 24 can be expanded and simplified as follows

$$\begin{aligned}LHS&=\Big|\frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n}\left[\mathbb{P}(W_i=v|\mathcal{T}_n)-\mathbb{P}(W_i=v|\mathcal{T}_n)^2\right]-\pi_v+\pi_v^2\Big|\\&=\Big|\frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n}\left[\mathbb{P}(W_i=v|\mathcal{T}_n)-\mathbb{P}(W_i=v|\mathcal{T}_n)^2-\pi_v+\pi_v^2\right]\Big|\\&=\Big|\frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n}\left[(\mathbb{P}(W_i=v|\mathcal{T}_n)-\pi_v)-(\mathbb{P}(W_i=v|\mathcal{T}_n)^2-\pi_v^2)\right]\Big|\\&\leq\frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n}\Big|\mathbb{P}(W_i=v|\mathcal{T}_n)-\pi_v\Big|+\frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n}\Big|\mathbb{P}(W_i=v|\mathcal{T}_n)^2-\pi_v^2\Big|\end{aligned}$$

Since from Lemma 4.1 we know, $\mathbb{P}(W_i=v|\mathcal{T}_n)=\pi_v+O(\rho^{d(i)})$ then

$$\mathbb{P}(W_i=v|\mathcal{T}_n)^2=\pi_v^2+O(\rho^{d(i)})+O(\rho^{2d(i)})=\pi_v^2+O(\rho^{d(i)})+O((\rho^2)^{d(i)})=\pi_v^2+O(\rho^{d(i)})$$

the last equation holds because $0 < \rho^2 < 1$ so term $O((\rho^2)^{d(i)})$ can be combined into the term $O(\rho^{d(i)})$. Go back to the inequalities, we have

$$\begin{aligned} LHS &\le \frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n} O(\rho^{d(i)}) + \frac{1}{n+1}\mathbb{E}\sum_{i=0}^{n} O(\rho^{d(i)}) \\ &= \frac{2}{n+1}\sum_{i=0}^{n}\mathbb{E}\left[O(\rho^{d(i)})\right] \\ &= \frac{2}{n+1}A_n(\rho) \le \frac{2}{n+1}Cn^{\rho} \end{aligned}$$

where $0 < \rho < 1$ and C is a constant.

As $n \to \infty$, $\frac{1}{n+1}Cn^{\rho} \to 0$, which implies that the left hand side of equation 24 vanishes to 0 as $n \to \infty$.

Thus, combined with the covariance component, we have finished the proof, which gives

$$\left| \frac{1}{n+1}\mathbb{E}\left[\mathrm{Var}\left(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\right)\right] - \pi_v(1-\pi_v)\right| \to 0$$

as $n \to \infty$. □

6.3 Proof for Lemma 4.5

Proof. Similar to the idea in proof of Lemma 4.4, the variance in Lemma 4.5 can be decomposed into two parts

$$\begin{aligned} \frac{1}{n+1}\mathrm{Var}\left[\mathbb{E}\left(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\right)\right] &= \frac{1}{n+1}\sum_{i=0}^{n}\mathrm{Var}\left[\mathbb{E}\left(\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\right)\right] + \frac{1}{n+1}\sum_{i\neq j}\mathrm{Cov}\left[\mathbb{E}(\mathbb{1}_{\{W_i=v\}}),\mathbb{E}(\mathbb{1}_{\{W_j=v\}})|\mathcal{T}_n\right] \\ &= \frac{1}{n+1}\sum_{i=0}^{n}\mathrm{Var}\left[\mathbb{P}\left(W_i=v|\mathcal{T}_n\right)\right] + \frac{1}{n+1}\sum_{i\neq j}\mathrm{Cov}\left[\mathbb{P}(W_i=v),\mathbb{P}(W_j=v)|\mathcal{T}_n\right] \end{aligned}$$

For the variance part, since adding and subtracting constants does not effect the variance, then

$$\begin{aligned} \frac{1}{n+1}\sum_{i=0}^{n}\mathrm{Var}\left[\mathbb{P}\left(W_i=v|\mathcal{T}_n\right)\right] &= \frac{1}{n+1}\sum_{i=0}^{n}\mathrm{Var}\left[\mathbb{P}\left(W_i=v|\mathcal{T}_n\right)-\pi_v\right] \\ &= \frac{1}{n+1}\sum_{i=0}^{n}\mathrm{Var}\left[O(\rho^{d(i)})\right] \\ &\le \frac{1}{n+1}\sum_{i=0}^{n}\mathbb{E}\left[O((\rho^{d(i)})^2)\right] \\ &= \frac{1}{n+1}\sum_{i=0}^{n}\mathbb{E}\left[O(\rho^{d(i)})\right] \\ &\le \frac{1}{n+1}Cn^{\rho} \qquad \text{where } 0<\rho<1 \text{ and } C \text{ is a constant.} \end{aligned}$$

As $n \to \infty$, $\frac{1}{n+1}Cn^{\rho} \to 0$, which implies that the sum of variance also goes to 0 as $n \to \infty$.

Next, the covariance part can be expanded by the expectation formula

$$\mathrm{Cov}\left[\mathbb{P}(W_i=v),\mathbb{P}(W_j=v)|\mathcal{T}_n\right] = \mathbb{E}\left[\mathbb{P}(W_i=v|\mathcal{T}_n)\mathbb{P}(W_j=v|\mathcal{T}_n)\right] - \mathbb{E}\left[\mathbb{P}(W_i=v|\mathcal{T}_n)\right]\cdot\mathbb{E}\left[\mathbb{P}(W_j=v|\mathcal{T}_n)\right]$$

where

$$\begin{aligned}
&\mathbb{E}\Big[\mathbb{P}(W_i = v|\mathcal{T}_n)\mathbb{P}(W_j = v|\mathcal{T}_n)\Big] \\
&= \mathbb{E}\Big[\Big(\mathbb{P}(W_i = v|\mathcal{T}_n) - \pi_v\Big)\Big(\mathbb{P}(W_j = v|\mathcal{T}_n) - \pi_v\Big) + \pi_v\Big(\mathbb{P}(W_i = v|\mathcal{T}_n) + \mathbb{P}(W_j = v|\mathcal{T}_n)\Big) - \pi_v^2\Big] \\
&= \mathbb{E}\Big[\Big(O(\rho^{d(i)})\Big)\Big(O(\rho^{d(j)})\Big) + \pi_v\Big(O(\rho^{d(i)}) + O(\rho^{d(j)}) + 2\pi_v\Big) - \pi_v^2\Big] \\
&= \mathbb{E}\Big[O(\rho^{d(i)+d(j)}) + \pi_v\Big(O(\rho^{d(i)}) + O(\rho^{d(j)})\Big) + \pi_v^2\Big] \\
&= \mathbb{E}\Big(O(\rho^{d(i)+d(j)})\Big) + \pi_v\mathbb{E}\Big(O(\rho^{d(i)}) + O(\rho^{d(j)})\Big) + \pi_v^2.
\end{aligned}$$

and we also have

$$\mathbb{E}\Big[\mathbb{P}(W_i = v|\mathcal{T}_n)\Big] = \mathbb{E}\Big[\mathbb{P}(W_i = v|\mathcal{T}_n) - \pi_v\Big] + \pi_v = \mathbb{E}\Big(O(\rho^{d(i)})\Big) + \pi_v$$

so

$$\begin{aligned}
\mathbb{E}\Big[\mathbb{P}(W_i = v|\mathcal{T}_n)\Big] \cdot \mathbb{E}\Big[\mathbb{P}(W_j = v|\mathcal{T}_n)\Big] &= \Big(\mathbb{E}\Big(O(\rho^{d(i)})\Big) + \pi_v\Big)\Big(\mathbb{E}\Big(O(\rho^{d(j)})\Big) + \pi_v\Big) \\
&= \mathbb{E}\Big(O(\rho^{d(i)})\Big)\mathbb{E}\Big(O(\rho^{d(j)})\Big) + \pi_v\mathbb{E}\Big(O(\rho^{d(i)}) + O(\rho^{d(j)})\Big) + \pi_v^2.
\end{aligned}$$

Then we can cancel the shared terms

$$\mathbb{E}\Big[\mathbb{P}(W_i = v|\mathcal{T}_n)\mathbb{P}(W_j = v|\mathcal{T}_n)\Big] - \mathbb{E}\Big[\mathbb{P}(W_i = v|\mathcal{T}_n)\Big] \cdot \mathbb{E}\Big[\mathbb{P}(W_j = v|\mathcal{T}_n)\Big] = \mathbb{E}\Big(O(\rho^{d(i)+d(j)})\Big) - \mathbb{E}\Big(O(\rho^{d(i)})\Big)\mathbb{E}\Big(O(\rho^{d(j)})\Big).$$

Thus, as a result of these,

$$\begin{aligned}
&\frac{1}{n+1}\sum_{i\neq j}\text{Cov}\Big[\mathbb{P}(W_i = v), \mathbb{P}(W_j = v)|\mathcal{T}_n\Big] \\
&= \frac{1}{n+1}\sum_{i\neq j}\mathbb{E}\Big[\mathbb{P}(W_i = v|\mathcal{T}_n)\mathbb{P}(W_j = v|\mathcal{T}_n)\Big] - \mathbb{E}\Big[\mathbb{P}(W_i = v|\mathcal{T}_n)\Big] \cdot \mathbb{E}\Big[\mathbb{P}(W_j = v|\mathcal{T}_n)\Big] \\
&= \frac{1}{n+1}\sum_{i\neq j}\mathbb{E}\Big(O(\rho^{d(i)+d(j)})\Big) - \frac{1}{n+1}\sum_{i\neq j}\mathbb{E}\Big(O(\rho^{d(i)})\Big)\mathbb{E}\Big(O(\rho^{d(j)})\Big) \\
&< \frac{1}{n+1}\mathbb{E}\left[\sum_{i\neq j} C\rho^{d(i,j)/2}\right] \\
&< \frac{C}{n+1}\mathbb{E}\left[\sum_{x,y\in\mathcal{T}_n'}\rho^{d(x,y)}\right] = \frac{C}{n+1}B_n(\rho)
\end{aligned}$$

By Lemma 4.3 again, even in the worst case, the highest order of n in $B_n(\rho)$ is no more than 1. Thus, as $n \to \infty$, the term on the right hand side of the inequality will vanish, so the strictly bounded left hand side will go to zero as well.

So, in conclusion, the proof gives that as $n \to \infty$

$$\frac{1}{n+1}\text{Var}\left[\mathbb{E}\Big(\sum_{i=0}^{n}\mathbb{1}_{\{W_i=v\}}|\mathcal{T}_n\Big)\right] \to 0.$$

□

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