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SIEGMUND DUALITY WITH APPLICATIONS TO THE NEUTRAL MORAN MODEL CONDITIONED ON NEVER BEING ABSORBED

THIERRY HUILLET

ABSTRACT. We shall first consider the classical neutral Moran model with two alleles whose fate is either to become extinct or to reach fixation. We will study an ergodic version of the Moran model obtained by conditioning it to never hit the boundaries, making use of a Doob transform. We shall call it the recurrent Moran model. We will show that the Siegmund dual of the recurrent Moran process exists and is a substochastic birth and death chain. Conditioning this process to exit in its natural absorbing state, we construct a process with a unique absorbing state which is intertwined to the original recurrent Moran process. The time needed for the intertwined process to first hit its absorbing state is related to the time to reach stationarity for the recurrent Moran process. Using spectral information on the intertwined chain, we extract limiting information on this first hitting time that shows that there is no abrupt relaxation to equilibrium for the recurrent Moran chain. This makes use of the relation between duality and intertwining and strong stationarity times. Other related transition times of the recurrent Moran chain are also briefly investigated, namely: the first return time to the ground state and the expected time needed to move from one end to the other end of the state-space.

Running title: Siegmund duality and the recurrent Moran Model

Keywords: Population dynamics, Moran model, Birth and death chains, Fluctuation theory, Relaxation to equilibrium, Siegmund dual, Strong stationarity times.

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1. INTRODUCTION AND OUTLINE OF THE RESULTS

Consider a population constituted of N individuals (alleles) of two types. Suppose at all time n there are Z_n individuals of type 1 and $N - Z_n$ individuals of type 2. Elementary population genetics aims at elucidating the fate of the type 1 allele frequency Z_n , when various driving ‘forces’ are at stake in the gene pool. One major driving source we shall stick to in this manuscript is the genetic drift whose nature is exclusively random. In this context, we shall first consider the classical *neutral* Moran model with two alleles (see [14] or [28]). This process is a well-known birth and death chain on the state-space $\{0, \dots, N\}$. The process Z_n either becomes extinct or it fixes; it has two natural boundaries $\{0, N\}$ which are both absorbing. We will next introduce an ergodic version of Z_n obtained by conditioning Z_n to never hit the boundaries, making use of a Doob transform. We shall call the resulting process, say X_n , the recurrent Moran process. Its state-space is now $\{1, \dots, N - 1\}$.

The recurrent Moran process X_n will be the main concern of this paper. Its main features are first derived in Section 2.

Then we run into the rich duality idea between Markov chains. Dual processes occur in many applications; for typical examples and use of dual processes, we refer the reader to the mathematics and physics literature on interacting particle systems (see for example [7], [32], [27], [31], [18], [4] and [22]). Other examples occur in the population genetics context (see for example [10], [11], [29], [19] and [20]) and essentially go back to Siegmund similar early concerns for stochastically monotone processes (see [30] and [5]).

In this Note, we will focus on the Siegmund duality and on its use in our genetics problem. We will show that the Siegmund dual of the recurrent Moran process X_n exists and is a substochastic birth and death chain. It loses mass at state $\{1\}$ and is absorbed in state $\{N-1\}$. We shall call this process \widehat{X}_n . By adding an extra coffin state, say $\{0\}$, we will consider an enlarged proper Markov chain \widehat{X}_n^+ , now with the two absorbing states $\{0\}$ and $\{N-1\}$. While conditioning the enlarged process \widehat{X}_n^+ to exit in its natural absorbing state $\{N-1\}$, we shall construct another proper stochastic process \widetilde{X}_n , but now with this unique absorbing state. This new process \widetilde{X}_n turns out to be intertwined with the original recurrent Moran process X_n . It is again a birth and death chain.

The intertwining construction shows that the original positive recurrent birth and death chain X_n may also be viewed as the output (through a stochastic link) of a dual hidden Markov chain \widetilde{X}_n which is absorbed in a single state. Its peculiarity is that X_n is a Markov output of \widetilde{X}_n which is itself Markov. As a result of this intertwining construction, the time needed for \widetilde{X}_n to first hit its absorbing state is related to the time to reach stationarity for the recurrent Moran process X_n under study. This is when both intertwined processes X_n and \widetilde{X}_n start in the same state $\{1\}$. Because we deal here with a birth and death chain X_n with known spectral characteristics, the estimation of the hitting time for \widetilde{X}_n is somehow made easier (see [24] and [16]). These constructions are described in Section 3; they are in the spirit of [1] and [7] and actually serve as an additional illustration of the theory.

Using spectral information on the intertwined chain \widetilde{X}_n , we will show in Section 4 that there is no abrupt relaxation to equilibrium for X_n (no cutoff phenomenon¹ in the sense of Diaconis, [6]). More precisely, we will show that the expected value of the time $\widetilde{\tau}_{1,N-1}$ for \widetilde{X}_n to first hit its absorbing state $\{N-1\}$, starting from state $\{1\}$, grows like N^2 , just like its standard deviation. We will identify the limit law of $\widetilde{\tau}_{1,N-1}$ (normalized by its mean value) as a quadratically weighted sum of exponentially distributed random variables. The random time $\widetilde{\tau}_{1,N-1}$ being a strong stationarity time, the ergodic chain X_n enters gradually into its invariant measure after about N^2 steps. By the end of this Section 4, we add some considerations on the scaling limit attached to the recurrent Moran model X_n . These follow from the observation that the shifted recurrent Moran model is a Moran model with mutations.

with $\tau_x < \infty$ almost surely. Let

$$\bar{\Pi} = \begin{bmatrix} \rho_1 & \alpha_1 & & & & \\ \beta_2 & \rho_2 & \alpha_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \beta_{N-2} & \rho_{N-2} & \alpha_{N-2} & \\ & & & \beta_{N-1} & \rho_{N-1} & \end{bmatrix}$$

be obtained from Π after removing its first and last rows and columns. This matrix of size $N - 1$ is substochastic in the sense that it loses mass at states $\{1, N - 1\}$.

Let $\bar{\pi}'$ be the transpose row-vector of some column-vector $\bar{\pi}$. Let $\bar{\pi}'$ and $\bar{\psi}$ be defined as the left and right (row and column) eigenvectors associated to the spectral radius (largest eigenvalue) θ_2 of $\bar{\Pi}$, namely:

$$(4) \quad \bar{\pi}'\bar{\Pi} = \theta_2\bar{\pi}' \text{ and } \bar{\Pi}\bar{\psi} = \theta_2\bar{\psi}.$$

We have $\theta_2 = 1 - 2/N^2$ and $\bar{\psi} = (\bar{\psi}_x, x = 1, \dots, N - 1)$, where $\bar{\psi}_x = \frac{x}{N}(1 - \frac{x}{N})$. Note also that $\bar{\pi} = (\bar{\pi}_x, x = 1, \dots, N - 1)$, where $\bar{\pi}_x = \frac{1}{N-1}$. Regardless of the starting point x , we therefore have

$$\mathbb{P}_x(Z_n = z \mid \tau_x > n) \rightarrow \bar{\pi}_z = \frac{1}{N-1} \text{ as } n \rightarrow \infty,$$

and $\bar{\pi}$ has an interpretation in terms of the uniform Yaglom limiting measure of Z_n on $\{1, \dots, N - 1\}$.

Let P be the birth and death stochastic matrix defined from $\bar{\Pi}$ by applying the Doob transform

$$(5) \quad P = \theta_2^{-1} D_{\bar{\psi}}^{-1} \bar{\Pi} D_{\bar{\psi}},$$

where $D_{\bar{\psi}} \equiv \text{diag}(\bar{\psi}_1, \dots, \bar{\psi}_{N-1})$. We have

$$P = \begin{bmatrix} r_1 & p_1 & & & & \\ q_2 & r_2 & p_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & q_{N-2} & r_{N-2} & p_{N-2} & \\ & & & q_{N-1} & r_{N-1} & \end{bmatrix}$$

where

$$(6) \quad p_x = \theta_2^{-1} \alpha_x \frac{\bar{\psi}_{x+1}}{\bar{\psi}_x} = \theta_2^{-1} \frac{x+1}{N} \left(1 - \frac{x+1}{N}\right)$$

$$(7) \quad q_x = \theta_2^{-1} \beta_x \frac{\bar{\psi}_{x+1}}{\bar{\psi}_x} = \theta_2^{-1} \frac{x-1}{N} \left(1 - \frac{x-1}{N}\right)$$

$$(8) \quad r_x = \theta_2^{-1} \rho_x = \theta_2^{-1} \left[\left(\frac{x}{N}\right)^2 + \left(1 - \frac{x}{N}\right)^2 \right]$$

The invariant measure $\boldsymbol{\pi} = (\pi_x, x = 1, \dots, N - 1)$ of the corresponding random walk (say X_n) governed by P is given by $\pi_x = \pi_1 \prod_{y=1}^{x-1} \frac{p_y}{q_{y+1}}$. π_x can also be expressed

in terms of the normalized Hadamard product of $\bar{\pi}$ and $\bar{\psi}$:

$$(9) \quad \pi_x = \frac{\bar{\pi}_x \bar{\psi}_x}{\sum_{x=1}^{N-1} \bar{\pi}_x \bar{\psi}_x} = \frac{6x(N-x)}{N(N-1)(N+1)}.$$

This invariant probability measure is a special incarnation of the bivariate generalized hypergeometric distribution (a discrete version of the beta(2, 2) distribution supported by the unit interval). Note that the recurrent Moran model governed by P is reversible as a result of P obeying detailed balance which is true for all birth and death chains.

Clearly, the eigenvalues of P are

$$t_k = \theta_2^{-1} \left(1 - \frac{k(k+1)}{N^2} \right), \quad k = 1, \dots, N-1$$

which may be recast as

$$(10) \quad t_k = 1 - \frac{(k-1)(k+2)}{N^2-2}, \quad k = 1, \dots, N-1.$$

Note that $t_1 = 1$, $t_2 = 1 - \frac{4}{N^2-2} < 1$ and the spectral gap of P is $1 - t_2 = \frac{4}{N^2-2}$. We have $t_{N-1} = \frac{N}{N^2-2} > 0$ so that all eigenvalues of P are > 0 .

The random walk X_n , governed by P , corresponds to the random neutral Moran process Z_n conditioned to never become extinct nor fixed in the remote future². See [25] for a continuous-time version of this construction. It is again a birth and death Markov chain but with the modified transition probabilities (6, 8). Because it is a positive recurrent ergodic Markov chain, we shall call the process X_n governed by P the recurrent neutral Moran process (or shortly the *recurrent* Moran model). Note that if $X_0 \stackrel{d}{\sim} \pi$ (meaning that the distribution of X_0 is π), then $X_n \stackrel{d}{\sim} \pi$ for all $n \geq 1$: the distribution of X_n remains unchanged at all times.

We can check from (6, 7) that for all $N \geq 3$ and for all $x \in \{1, \dots, N-2\}$

$$(11) \quad p_x + q_{x+1} \leq 1$$

which means that the random walk X_n is stochastically monotone in the sense that for all $n \geq 0$ and $y \geq 1$, the function $x \rightarrow \mathbb{P}_x(X_n \leq y)$ is a non-increasing function of x . This fact may also be viewed as a direct consequence of P having all its eigenvalues positive. This property will prove essential in the following statement that a Siegmund dual to X_n exists, [30]. See [5] for similar considerations for birth and death chains on the half-line.

Remark²: The original idea of conditioning a Markov chain to never become extinct in the remote future seems to be due to Spitzer (unpublished) in the sixties and then Lamperti-Ney, [26]; see Athreya-Ney [2], p 56–59. It was first introduced in the context of the celebrated Bienyamé-Galton-Watson branching process.

3. THE SIEGMUND DUAL TO THE RECURRENT MORAN MODEL

In this Section, we shall illustrate the power of the duality/intertwining relationship by considering the simplest Siegmund dual of a birth and death chain, with the recurrent neutral Moran birth and death example in mind. This will prove useful to address the question of computing the strong stationary time distribution that

matrix, call it \tilde{P} , of some process \tilde{X}_n on the state-space $\{1, \dots, N-1\}$ which corresponds to \hat{X}_n^+ conditioned to first hit state $\{N-1\}$ before state $\{0\}$. The state $\{1\}$ of this conditioned birth and death process is now partially reflecting whereas its only remaining absorbing state is $\{N-1\}$. See [21] for a similar conditioning in the context of the Ehrenfest urn model.

We now state that \tilde{P} and P (characterized by (6, 8)) are intertwined through a stochastic link Λ .

Proposition 1. (i) *The matrices \tilde{P} and P are similar (with the same eigenvalues), that is*

$$(18) \quad \tilde{P} = \Lambda P \Lambda^{-1}.$$

With π as in (10), the link matrix Λ is given by: $\Lambda(\tilde{x}, x) = \frac{\pi_x}{\pi_{\tilde{x}}} \mathbf{1}(x \leq \tilde{x})$. It corresponds to the entries of a lower-triangular stochastic matrix. Its interpretation is in terms of the conditional probability

$$(19) \quad \Lambda(\tilde{x}, x) = \mathbb{P}(X_n = x \mid \tilde{X}_n = \tilde{x}), \text{ for all } n \geq 1.$$

(ii) *The link matrix Λ satisfies*

$$(20) \quad \Lambda(N-1, x) = \pi_x, \quad x = 0, \dots, N.$$

(iii) $\tilde{\pi}'_0 = \pi'_0 = \mathbf{e}'_0 \equiv (1, 0, \dots, 0)$ are admissible initial distributions for the chains \tilde{X}_n and X_n , satisfying

$$(21) \quad \pi'_0 = \tilde{\pi}'_0 \Lambda.$$

Proof: (i) Using (17) and (13)

$$\tilde{P} = D_{\pi^c}^{-1} \hat{P} D_{\pi^c} = D_{\pi^c}^{-1} H' P' H'^{-1} D_{\pi^c}.$$

The random walk X_n being reversible (detailed balance holds), $P' = D_{\pi} P D_{\pi}^{-1}$. Thus:

$$\tilde{P} = (D_{\pi^c}^{-1} H' D_{\pi}) P (D_{\pi}^{-1} H'^{-1} D_{\pi^c}) = \Lambda P \Lambda^{-1}$$

where $\Lambda = D_{\pi^c}^{-1} H' D_{\pi}$. The entries of Λ are $\Lambda(\tilde{x}, x) = \frac{\pi_x}{\pi_{\tilde{x}}} \mathbf{1}(x \leq \tilde{x})$, satisfying $\sum_{x \leq \tilde{x}} \frac{\pi_x}{\pi_{\tilde{x}}} = 1$. Thus Λ is stochastic as its row sums all sum to 1.

Suppose $X_0 \stackrel{d}{\sim} \pi_0$, $\tilde{X}_0 \stackrel{d}{\sim} \tilde{\pi}_0$ and assume the initial distributions π_0 and $\tilde{\pi}_0$ are Λ -compatible, that is $\pi'_0 = \tilde{\pi}'_0 \Lambda$. Using (18), $\tilde{P}^n \Lambda = \Lambda P^n$ for all $n \geq 1$. This means $\pi'_n = \tilde{\pi}'_n \Lambda$, for all $n \geq 1$, where $\pi_n(\cdot) = \mathbb{P}_{\pi_0}(X_n = \cdot)$, $\tilde{\pi}_n(\cdot) = \mathbb{P}_{\tilde{\pi}_0}(\tilde{X}_n = \cdot)$ are the laws at time n of X_n and \tilde{X}_n . Thus $\Lambda(\tilde{x}, x) = \mathbb{P}(X_n = x \mid \tilde{X}_n = \tilde{x})$, for all $n \geq 1$.

(ii) The last row of Λ is given by $\Lambda(N-1, x) = \pi_x$ so that once \tilde{X}_n hits state $\{N-1\}$, the law of X_n is π .

(iii) The first row of Λ is $(1, 0, \dots, 0)$ so that $\mathbf{e}'_0 = \mathbf{e}'_0 \Lambda$. Thus both chains X_n and \tilde{X}_n may consistently start in state $\{1\}$. \triangle

So \tilde{P} (as the algebraic composition of the Siegmund dual of P with a Doob-transform) can be obtained from P through a stochastic link Λ .

Intertwining and strong stationary time. The intertwining construction shows that the original positive recurrent birth and death chain X_n with transition matrix P may also be viewed as the output (through the stochastic link Λ) of a dual hidden Markov chain \tilde{X}_n governed by $\tilde{P} = \Lambda P \Lambda^{-1}$ and absorbed in the single state $\{N - 1\}$. This is a setup reminiscent of filtering theory with \tilde{X}_n the hidden process and X_n the observable. The peculiarity of the intertwining construction is that X_n is a Markov output which is itself Markov. We emphasize that there is so far no clear ‘genetical’ interpretation of the process governed by \tilde{P} . Because the starting point process governed by P may be viewed as a Markovian output of the \tilde{P} -process, this suggests that the latter process should have a very basic (still missing) meaning.

What we only get is that once \tilde{X}_n hits its absorbing state $\{N - 1\}$, the random walk X_n is distributed like π , provided both X_n and \tilde{X}_n were both started in $\{1\}$. This suggests that, given $X_0 = \tilde{X}_0 = 1$, the time needed for X_n to enter its invariant probability measure should be related to the entrance time of the hidden process \tilde{X}_n into its absorbing state $\{N - 1\}$.

4. TIME TO REACH STATIONARITY FOR THE RECURRENT MORAN MODEL

We shall let

$$(22) \quad \tilde{\tau}_{1,N-1} = \inf \left(n : \tilde{X}_n = N - 1 \mid \tilde{X}_0 = 1 \right)$$

be the first hitting time of $\{N - 1\}$ of \tilde{X}_n , starting from the state $\{1\}$. The random time $\tilde{\tau}_{1,N-1}$ gives some information on the speed of convergence of the law of the original process X_n to its invariant measure. It is a strong stationary time in the sense of Diaconis and Fill, [7]. The facts (18, 19, 20, 21) indeed guarantee that $\tilde{\tau}_{1,N-1}$ is a strong stationary time of X_n in the sense that $X_{\tilde{\tau}_{1,N-1}} \stackrel{d}{\sim} \pi$ and is independent of $\tilde{\tau}_{1,N-1}$ (see [7] Theorems 2.4 and 2.17 or [16] Theorem 2.1). Equivalently (see [1], Prop. 3.2), it holds that:

$$(23) \quad \text{sep}(\pi_{n,1}, \pi) \leq \mathbb{P}(\tilde{\tau}_{1,N-1} > n) \leq \mathbb{E}(\tilde{\tau}_{1,N-1})/n$$

where $\pi_{n,1}(\cdot) = \mathbb{P}_1(X_n = \cdot)$ is the law of X_n started in $\{1\}$, π its invariant measure. In (23), the separation discrepancy is defined by:

$$\text{sep}(\pi_{n,1}, \pi) \equiv \sup_y [1 - \pi_n(y) / \pi_y].$$

It satisfies $\text{sep}(\pi_{n,1}, \pi) \geq \|\pi_{n,1} - \pi\|_{TV}$ where $\|\pi_{n,1} - \pi\|_{TV} = \frac{1}{2} \sum_y |\pi_{n,1}(y) - \pi_y|$ is the total variation distance between $\pi_{n,1}$ and π .

Furthermore, from (18, 21), there is a unique ‘witness’ state d for X_n , here with $d = N - 1$, such that either

$$\mathbb{P}_1(\tilde{X}_n = N - 1) \equiv \tilde{\pi}_{n,1}(N - 1) = 0 \Rightarrow \pi_{n,1}(d) = 0$$

or

$$\tilde{\pi}_{n,1}(N - 1) > 0 \Rightarrow \pi_{n,1}(d) = \tilde{\pi}_{n,1}(N - 1) \pi_d > 0,$$

showing that this random time is stochastically the smallest since the first inequality in (23) turns out to be an equality (see Remark 2.39 of [7] and Proposition 13 of [22]).

In our context of the birth and death chain \tilde{X}_n absorbed in $\{N-1\}$, the probability generating function of $\tilde{\tau}_{1,N-1} \geq N-2$ is explicitly given by, [24], [16]:

$$(24) \quad \mathbb{E} \left(z^{\tilde{\tau}_{1,N-1}} \right) = \prod_{k=2}^{N-1} \frac{(1-t_k)z}{1-t_k z}, \quad z \in [0, 1],$$

where $0 < t_k < 1$, $k = 2, \dots, N-1$ are the $N-2$ distinct eigenvalues of both \tilde{P} and P , avoiding $t_1 = 1$ described in (10). Because the eigenvalues t_k are positive, then $\tilde{\tau}_{1,N-1} \stackrel{d}{=} \sum_{k=2}^{N-1} \tau_k$ where the τ_k s are independent with $\tau_k \stackrel{d}{\sim} \text{geom}(1-t_k)$, the geometric distribution with success parameter $1-t_k$ on the half-line $\{1, 2, \dots\}$. The formula (24) also reads

$$\mathbb{E} \left(z^{\tilde{\tau}_{1,N-1}} \right) = \sum_{l=2}^{N-1} A_l \frac{z(1-t_l)}{1-t_l z},$$

where

$$A_l = \prod_{k \neq l} \frac{1-t_k}{t_l - t_k}.$$

Therefore

$$(25) \quad \mathbb{P}(\tilde{\tau}_{1,N-1} > n) = \sum_{l=2}^{N-1} \prod_{k \neq l} \frac{1-t_k}{t_l - t_k} t_l^n, \quad n \geq N-1.$$

Thus, $t_2^{-n} \mathbb{P}(\tilde{\tau}_{1,N-1} > n) \rightarrow_{n \uparrow \infty} \prod_{k=3}^{N-1} \frac{1-t_k}{t_2 - t_k}$ and $\tilde{\tau}_{1,N-1}$ has geometric tails with exponent t_2 . We also have:

$$(26) \quad \mu_N \equiv \mathbb{E}(\tilde{\tau}_{1,N-1}) = \sum_{k=2}^{N-1} (1-t_k)^{-1} \quad \text{and}$$

$$(27) \quad \sigma_N^2 \equiv \sigma^2(\tilde{\tau}_{0,N}) = \sum_{k=2}^{N-1} t_k (1-t_k)^{-2} = \sum_{k=2}^{N-1} (1-t_k)^{-2} - \sum_{k=2}^{N-1} (1-t_k)^{-1}.$$

Note that since t_2 is the dominant eigenvalue

$$(28) \quad \sigma^2(\tilde{\tau}_{1,N-1}) \leq \frac{\mathbb{E}(\tilde{\tau}_{1,N-1})}{1-t_2}.$$

We can summarize these results (in the spirit of [1], [7] and [16]) as follows:

Proposition 2. *The Siegmund dual for the recurrent Moran birth and death chain X_n exists. There exists a Markov chain \tilde{X}_n , intertwined with X_n , with $\{N-1\}$ as an absorbing state and fully described in Proposition 1. The random time $\tilde{\tau}_{1,N-1}$ is a fastest strong stationary time for X_n whose law is characterized either by (24) or (25) involving the spectrum (given in (10)), of either P or \tilde{P} , the transition matrices governing the two processes.*

Conditions for a cutoff phenomenon. Because the eigenvalues t_k of P are known explicitly from (10), it is possible to compute $\mu_N = \mathbb{E}(\tilde{\tau}_{1,N-1})$ and $\sigma_N^2 = \sigma^2(\tilde{\tau}_{1,N-1})$ and decide whether or not

$$(29) \quad \mathbb{E}(\tilde{\tau}_{1,N-1}) \rightarrow \infty \quad \text{and} \quad \sigma^2 \left(\frac{\tilde{\tau}_{1,N-1}}{\mathbb{E}(\tilde{\tau}_{1,N-1})} \right) \rightarrow 0 \quad \text{as } N \rightarrow \infty,$$

meaning $\sigma_N/\mu_N \rightarrow 0$ as $N \rightarrow \infty$.

Would these conditions both hold, then $\frac{\tilde{\tau}_{1,N-1}}{\mathbb{E}(\tilde{\tau}_{1,N-1})} \rightarrow 1$ in probability and $\lfloor \mu_N/2 \rfloor$ would be expected to be a cutoff time for X_n started in $\{1\}$ in the sense ([6]) that: With $n_N(x) = \lfloor (\mu_N + x\sigma_N) \rfloor$, then

$$\|\pi_{n_N(x),1} - \pi\|_{TV} \xrightarrow{N \uparrow \infty} c(x)$$

where $c(x) \xrightarrow{x \uparrow \infty} 0$ and $c(x) \xrightarrow{x \uparrow -\infty} 1$. The chain would then exhibit a sharp cutoff: if $n < n_N(x)$, $\|\pi_{n,1} - \pi\|$ would keep close to its maximal value 1, whereas if $n > n_N(x)$ it would suddenly drop to a smaller value.

When there is cutoff, the expected mixing time (measured in terms of $\text{sep}(\pi_{n,1}, \pi)$) is μ_N whereas the spectral gap is $1 - t_2$, the product of the 2 of which tends to ∞ . Recalling $\sigma^2(\tilde{\tau}_{1,N-1}) \leq \frac{\mu_N}{1-t_2}$, then $\sigma^2(\tilde{\tau}_{1,N-1}/\mu_N) = \mu_N^{-2} \sigma^2(\tilde{\tau}_{1,N-1}) \leq 1/((1-t_2)\mu_N)$ and the condition

$$(1-t_2)\mu_N \rightarrow \infty$$

is a sufficient condition for $\sigma^2(\tilde{\tau}_{1,N-1}/\mu_N) \rightarrow 0$. If this condition holds, the contribution of $\sum_{k=3}^{N-1} (1-t_k)^{-1}$ to μ_N dominates the lead term $(1-t_2)^{-1}$ (see [8] for recent developments and precisions).

For some birth and death models, it may happen that $\mu_N \rightarrow \infty$ and $\sigma_N/\mu_N \not\rightarrow 0$ as $N \rightarrow \infty$. In such cases, there is no cutoff and this is precisely what happens for the recurrent Moran model under concern.

Computing the mean and variance of $\tilde{\tau}_{1,N-1}$ for the recurrent Moran model. For the case of the recurrent Moran model, using (10): $1-t_k = \frac{k(k+1)-2}{N^2-2}$ and the large N values of μ_N and σ_N^2 can be estimated. Using indeed the integral approximation

$$\mu_N \sim (N-2)(N^2-2) \int_0^1 \frac{dx}{(2+x(N-2))(3+x(N-2))-2}$$

(where we used the change of variables $\frac{k-2}{N-2} = x$ and $\mu_N \sim \alpha_N \Leftrightarrow \mu_N/\alpha_N \rightarrow 1$ as $N \rightarrow \infty$), with $c_1 \equiv \frac{2 \log 2}{3}$, we easily get

$$\mu_N \sim N \int_0^1 \frac{dx}{(x+1/N)(x+4/N)} = c_1 N^2.$$

In this situation, the contribution of $\sum_{k=3}^{N-1} (1-t_k)^{-1}$ to μ_N contribute equally likely with the lead term $(1-t_2)^{-1}$. Note also that for this model, $(1-t_2)\mu_N \sim 4c_1 \not\rightarrow \infty$ as $N \rightarrow \infty$ suggesting that there is no cutoff.

Using similar techniques indeed, with $c_2 \equiv \frac{5}{36} + \frac{4 \log 2}{27}$, we get

$$\sigma_N^2 \sim N \int_0^1 \frac{dx}{(x+1/N)^2(x+4/N)^2} \sim c_2 N^4$$

showing that $\sigma^2\left(\frac{\tilde{\tau}_{1,N-1}}{\mathbb{E}(\tilde{\tau}_{1,N-1})}\right) \sim \frac{c_2}{c_1^2} \not\rightarrow 0$ as $N \rightarrow \infty$.

Thus $\frac{\tilde{\tau}_{1,N-1}}{\mathbb{E}(\tilde{\tau}_{1,N-1})} \not\rightarrow 1$ in probability and there is no cutoff phenomenon. In fact, in the recurrent Moran case, we have

Proposition 3.

$$\frac{\tilde{\tau}_{1,N-1}}{\mathbb{E}(\tilde{\tau}_{1,N-1})} \xrightarrow{d} T \text{ as } N \rightarrow \infty$$

where the limit T is random with

$$T \stackrel{d}{=} \sum_{l \geq 1} \frac{1}{l(l+3)} E_l(c_1)$$

where the $E_l(c_1)$ are independent and identically distributed (iid) random variables, with common distribution $\mathbb{P}(E_1(c_1) > x) = e^{-c_1 x}$.

Proof: Indeed, from the large N approximation $t_k/(1-t_k) \sim \frac{N^2}{k(k+1)-2}$ and making use of (24), for all $t \in \mathbb{R}$, we get

$$\begin{aligned} \mathbb{E} \left(e^{it \frac{\tilde{\tau}_{1,N-1}}{\mu_N}} \right) &= e^{it \frac{N-2}{\mu_N}} \prod_{k=2}^{N-1} \frac{(1-t_k) e^{\frac{it}{\mu_N}}}{1-t_k e^{\frac{it}{\mu_N}}} \sim e^{\frac{it}{c_1 N}} \prod_{k=2}^{N-1} \frac{1}{1 - \frac{t_k}{1-t_k} \frac{it}{c_1 N^2}} \\ &\sim \prod_{l=1}^{N-2} \frac{1}{1 - \frac{it}{c_1 l(l+3)}} \rightarrow \Phi(t), \end{aligned}$$

where $\Phi(t) = \prod_{l=1}^{\infty} \frac{1}{1 - \frac{it/c_1}{l(l+3)}}$. $\Phi(t)$ is the characteristic function of the random variable

$$T = \sum_{l \geq 1} \frac{1}{l(l+3)} E_l(c_1),$$

where the $E_l(c_1)$ are iid random variables, with common distribution $\mathbb{P}(E_1(c_1) > x) = e^{-c_1 x}$. The limiting T is thus a weighted sum of iid exponentially-distributed random variables with quadratic weights. Such random variables are known to have all their integral moments finite (see [3]). For instance

$$\mathbb{E}(T) = \frac{1}{c_1} \sum_{l \geq 1} \frac{1}{l(l+3)} = \frac{1}{3c_1} \left(\sum_{l \geq 1} \frac{1}{l} - \sum_{l \geq 4} \frac{1}{l} \right) = \frac{11}{18c_1}. \quad \triangle$$

We conclude from (23) that as N is large

$$\text{sep}(\boldsymbol{\pi}_{n,1}, \boldsymbol{\pi}) = \mathbb{P}(\tilde{\tau}_{1,N-1} > n) \sim \bar{F}_T \left(\frac{n}{c_1 N^2} \right)$$

where $\bar{F}_T(x) = \mathbb{P}(T > x)$ is the complementary probability distribution of $T > 0$. This shows that, for the recurrent neutral Moran model, the transition to stationarity occurs gradually after about $c_1 N^2$ steps. There is no abrupt entrance of this particular chain into the invariant measure (no cutoff phenomenon).

A plausible scaling limit. Let $Y_n = X_n - 1$ be a shifted version of the recurrent model with state-space $\{0, \dots, N-2\}$. First, we observe that Y_n is a Moran model with mutations (see [14] p. 107). Indeed, from (6, 8), the transition probabilities of Y_n read: $p_y = \theta_2^{-1} \frac{y+2}{N} \left(1 - \frac{y+2}{N}\right)$, $q_y = \theta_2^{-1} \frac{y}{N} \left(1 - \frac{y}{N}\right)$, $r_y = 1 - (p_y + q_y)$. Recalling $\theta_2 = 1 - \frac{2}{N^2-2}$, these may be recast as

$$p_y = \left(1 - \frac{y}{N-2}\right) \pi \left(\frac{y}{N-2}\right)$$

$$q_y = \frac{y}{N-2} \left(1 - \pi \left(\frac{y}{N-2} \right) \right)$$

$$r_y = \frac{y}{N-2} \pi \left(\frac{y}{N-2} \right) + \left(1 - \frac{y}{N-2} \right) \left(1 - \pi \left(\frac{y}{N-2} \right) \right),$$

where

$$\pi(u) = \mu_1(1-u) + (1-\mu_2)u$$

is an affine mutation mapping from $[0, 1]$ to $[0, 1]$, with mutation probabilities from type 2 to 1 and from type 1 to 2

$$\mu_1 = \frac{2(N-2)}{N^2-2} \sim \frac{2}{N} \quad \text{and} \quad \mu_2 = \frac{2(N-1)}{N^2-2} \sim \frac{2}{N}.$$

Let now $\Delta > 0$ be a small constant. Let $t = n\Delta$ be a discretization of time and consider the scaled process $U_t = Y_{n\Delta}/(N-2) \in [0, 1]$. Given $U_t = u$, assume

$$U_{t+\Delta} = u \pm \frac{1}{N} \text{ with probability } \Delta \cdot p_{(N-2)u} \text{ (respectively } \Delta \cdot q_{(N-2)u})$$

$$= u \text{ with probability } 1 - \Delta \cdot r_{(N-2)u}.$$

Then $\mathbb{E}_u(U_{t+\Delta} - u) = \frac{\Delta}{N-2} (p_{(N-2)u} - q_{(N-2)u}) = \frac{\Delta}{N-2} (\pi(u) - u)$, with $\pi(u) - u \sim \frac{1}{N} (2 - 4u)$ for large N . Thus

$$\frac{1}{\Delta} \mathbb{E}_u(U_{t+\Delta} - u) \sim \frac{1}{N^2} (2 - 4u).$$

Similarly, $\mathbb{E}_u[(U_{t+\Delta} - u)^2] = \frac{\Delta}{(N-2)^2} (1 - r_{(N-2)u})$ leading to the dominant order in N to

$$\frac{1}{\Delta} \mathbb{E}_u[(U_{t+\Delta} - u)^2] \sim \frac{2}{N^2} u(1-u).$$

Following ([28], Chapter 2), this shows (by passing to the limit in Δ), that $U_t \in [0, 1]$ obeys the Wright-Fisher-like diffusion approximation equation driven by Brownian motion (B_t)

$$dU_t = \frac{2}{N^2} (1 - 2U_t) dt + \frac{1}{N} \sqrt{2U_t(1-U_t)} dB_t.$$

Performing the time substitution $\tau = N^{-2}t$ and defining $V_\tau = U_{N^2\tau}$, V_τ obeys the diffusion equation

$$dV_\tau = 2(1 - 2V_\tau) d\tau + \sqrt{2V_\tau(1 - V_\tau)} dB_\tau$$

with a unit time τ corresponding to N^2 generations in the discrete model. The above considerations on the time to reach stationarity of X_n suggests that V_τ enters gradually into its invariant measure (which is $6v(1-v)dv$) by time $O(1)$.

5. OTHER TRANSITION TIMES FOR THE RECURRENT MORAN MODEL

Consider the ergodic Moran birth and death Markov chain X_n on the state-space $\{1, \dots, N-1\}$. It is well-known that the mean return time to state $\{1\}$ is $\mathbb{E}(\tau_{1,1}) = \frac{1}{\pi_1}$. Thus, using (9)

$$\mathbb{E}(\tau_{1,1}) \sim \frac{N^2}{6} \text{ as } N \rightarrow \infty.$$

We wish now to estimate the time it takes for X_n to move from one end of the state-space to the other, that is from state $\{1\}$ to $\{N-1\}$. Let $\tau_{1,N-1}$ be this random time. We shall prove the following estimation of its mean value:

Proposition 4.

$$\mathbb{E}(\tau_{1,N-1}) \sim \frac{N^3}{6} \text{ as } N \rightarrow \infty.$$

Proof: Let indeed $\tau_{x,x+1}$ be the random time to first hit the state $\{x+1\}$ starting from the state $\{x\}$. Depending on whether the move starting in x is up, down or no move, $\tau_{x,x+1}$ is either 1 or $1 + \tau'_{x,x+1}$ (with $\tau'_{x,x+1}$ a statistical copy of $\tau_{x,x+1}$) or $1 + \tau_{x-1,x} + \tau'_{x,x+1}$. If we let μ_x be the mean value of $\tau_{x,x+1}$, we thus get $\mu_x = p_x + r_x(1 + \mu_x) + q_x(1 + \mu_{x-1} + \mu_x)$, $x \geq 2$. This leads to the recurrence ($\mu_1 = 1/p_1$):

$$\mu_x = \frac{q_x}{p_x} \mu_{x-1} + \frac{1}{p_x}, \quad x \geq 2.$$

This recurrence can be solved to give

$$\mu_x = \frac{1}{p_x \pi_x} \sum_{y=1}^x \pi_y.$$

Thus

$$\mathbb{E}(\tau_{1,N-1}) = \sum_{x=1}^{N-2} \mu_x = \sum_{x=1}^{N-2} \frac{1}{p_x \pi_x} \sum_{y=1}^x \pi_y.$$

Looking at this sum formula, one expects that its leading term is $\frac{1}{p_{N-2} \pi_{N-2}} \sum_{y=1}^{N-2} \pi_y$ because this is where $\sum_{y=1}^x \pi_y$ is the largest and π_x the smallest. Looking at the expressions of p_x and π_x at $x = N-2$ in (6, 9), this crude estimation would lead to $\mathbb{E}(\tau_{1,N-1}) \sim N^3/12$ but this is not quite true because the other terms contribute equally likely.

In fact, the computations can be done explicitly. From (9), we have

$$\sum_{y=1}^x \pi_y = \frac{x(x+1)(3N-(2x+1))}{N(N-1)(N+1)}$$

and so

$$\begin{aligned} \mathbb{E}(\tau_{1,N-1}) &= \frac{\theta_2 N^2}{6} \sum_{x=1}^{N-2} \frac{3N-(2x+1)}{(N-x)(N-x-1)} \\ &= \frac{\theta_2 N^2}{6} \sum_{y=1}^{N-2} \frac{N+1+2y}{y(y+1)} = \frac{\theta_2 N^2}{6} \left(\sum_{y=1}^{N-2} \frac{N+1}{y} - \sum_{y=1}^{N-2} \frac{N-1}{y+1} \right) \\ &= \frac{\theta_2 N^2}{6} [(N+1)H_{N-2} - (N-1)(H_{N-1}-1)] \end{aligned}$$

where H_N is the N -harmonic number. Thus

$$\begin{aligned} \mathbb{E}(\tau_{1,N-1}) &= \frac{\theta_2 N^2}{6} \left[2H_{N-1} - \frac{N+1}{N-1} + N-1 \right] \\ &\sim \frac{N^3}{6} \text{ as } N \rightarrow \infty. \quad \Delta \end{aligned}$$

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