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THE TIME BACK TO THE MOST RECENT COMMON ANCESTOR IN EXCHANGEABLE POPULATION MODELS

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Abstract

A class of haploid population models with non-overlapping generations and exchangeable offspring distribution is considered. Based on an analysis of the discrete ancestral process, we present solutions, algorithms and strong upper bounds for the expected time back to the most recent common ancestor. New insights into the asymptotical behavior of the expected time back to the most recent common ancestor for large population size are presented relating the results to coalescent theory.

Keywords: Absorption time; Ancestral process; Coalescent; Exchangeability; Moran model; Most recent common ancestor; Wright-Fisher model

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1 Introduction

It is quite natural to ask how long it might take backward in time, in terms of years or generations, until you will find the most recent common ancestor (MRCA) of a sample of n individuals taken from some population. Since the development of coalescent theory going back to Kingman [10, 11, 12] this question was answered for certain haploid populations asymptotically, i.e. for the case when the total population size N is sufficiently large. It will take in average around $2N_e(1-1/n)$ generations, where N_e denotes the effective population size. This result relies on convergence theorems and hence holds only approximately for large N. Recently an immense amount of research in biology, mathematics and other fields focuses on question around the MRCA (see for example Chang [3], Walsh [17]). Unfortunately it is only little known about the accuracy of the approximation by Kingman's coalescent ([14]) in particular when the sample size n is not small in comparison with the total population size N. The time back to the MRCA in a finite population will certainly differ in some way from the limiting result. The aim of this paper is to study the time back to the MRCA in finite haploid population models. The results indicate that the time back to the MRCA in a finite population is in many models smaller than one would expect from coalescent theory. This effect is verified in particular for the most celebrated model, the haploid Wright-Fisher model.
The paper is organized as follows. Section 2 introduces the model and the ancestral process. Furthermore the time back to the MRCA is defined precisely.

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In Section 3 recursive and iterative algorithms are presented which compute or approximate the expected time back to the MRCA in reasonable time. Furthermore, exact solutions are derived which are unfortunately quite time-consuming and hence more of theoretical interest.
In Section 4 upper bounds for the expected time back to the MRCA are presented. A new theorem provides a very strong upper bound under an additional assumption, which is satisfied for many models as pointed out in the examples in Section 5.
The paper proceeds in Section 6 with a discussion of the asymptotic behavior of the expected time back to the MRCA for large population size and puts the results in the context of coalescent theory. The paper finished with a brief discussion of open problems in Section 7. Technical details are deferred to the appendix (Section 8).

2 The model and the ancestral process

Cannings [1, 2] introduced a haploid population model with fixed population size $N \in I\!N := \{1, 2 \ldots\}$ and non-overlapping generations $r \in I\!N_0 := \{0, 1, 2, \ldots\}$. As usual in ancestral population genetics the generations are labelled backward in time. Thus $r = 0$ denotes the current generation, $r = 1$ the parental generation and so on. Each model in this class is characterized by a family of random variables $\{\nu_i^{(r)} \,|\, r \in I\!N, i \in \{1, \ldots, N\}\}$, where $\nu_i^{(r)}$ denotes the number of offspring of the individual i alive in generation r. As the total population size is assumed to be fixed the condition $\sum_{i=1}^N \nu_i^{(r)} = N$ has to be satisfied for each r. It is assumed that for each fixed r the offspring vector $\nu^{(r)} := (\nu_1^{(r)}, \ldots, \nu_N^{(r)})$ is exchangeable, i.e. the distribution of $(\nu_{\pi 1}^{(r)}, \ldots, \nu_{\pi N}^{(r)})$ does not depend on the special permutation π of the indices $1, \ldots, N$. Furthermore it is assumed that the offspring vectors $\nu^{(r)}$, $r \in I\!N$ are independent and identically distributed. This condition ensures that the ancestral process considered later has the Markov property. Write $\nu_i := \nu_i^{(1)}$ and $\nu := \nu^{(1)}$ for convenience. The most celebrated example is the classical Wright-Fisher model where it is assumed that $\nu = (\nu_1, \ldots, \nu_N)$ has a symmetric multinomial distribution.
An important quantity in population genetics is the probability c_N that two individuals, randomly chosen from some generation, have a common ancestor one generation backward in time. Conditioned on $(\nu_1, \ldots, \nu_N)$ two randomly chosen individuals have the parent $i \in \{1, \ldots, N\}$ as their common ancestor with probability $\nu_i(\nu_i - 1)/(N(N-1))$. Thus

$$c_N \;=\; \sum_{i=1}^N \frac{\mathrm{E}(\nu_i(\nu_i - 1))}{N(N-1)} \;=\; \frac{\mathrm{E}(\nu_1(\nu_1 - 1))}{N-1} \;=\; \frac{\mathrm{Var}(\nu_1)}{N-1}. \tag{1}$$

The probability c_N is called the *coalescence probability*. The inverse $N_e := 1/c_N$ of c_N is the *effective population size* (Crow and Kimura [4, p. 347, eqn. 7.6.2.8], Ewens [5]). In order to avoid technical problems it is assumed that $c_N > 0$. This

is the case if and only if $P(\nu_1 = 1) < 1$. In other words we avoid the trivial model where each individual has exactly one offspring.
Let $\mathcal{D} := (\mathcal{D}_r)_{r \in \mathbb{N}_0}$ denote the so called ancestral process which counts by definition the number of ancestors backward in time. It is well known that $\mathcal{D}$ is a Markovian death process with state space $S := \{1, \ldots, N\}$ and transition probabilities $p_{ij} := P(\mathcal{D}_r = j \,|\, \mathcal{D}_{r-1} = i)$, $i, j \in S$ of the form (see [13, p. 766 eqn. (7)])

$$p_{ij} = \frac{\binom{N}{j}}{\binom{N}{i}} \sum_{\substack{i_1, \ldots, i_j \in N \\ i_1 + \cdots + i_j = i}} \mathrm{E}\left(\binom{\nu_1}{i_1} \cdots \binom{\nu_j}{i_j} \right) \tag{2}$$

$$= \frac{\binom{N}{j}}{\binom{N}{i}} \sum_{k=1}^{j} (-1)^{j-k} \binom{j}{k} \mathrm{E}\left(\binom{\nu_1 + \cdots + \nu_k}{i} \right). \tag{3}$$

The formula (2) goes back to Kingman [10, 11, 12] while (3) was derived from (2) by applying the principle of inclusion and exclusion. As the transition matrix $P := (p_{ij})_{i,j \in S}$ is triangular, the corresponding eigenvalues are

$$\lambda_i := p_{ii} \overset{(2)}{=} \mathrm{E}(\nu_1 \cdots \nu_i), \quad i \in \{1, \ldots, N\}, \tag{4}$$

a result which goes back to Cannings [1, 2] and Gladstien [6, 7, 8]. Note that $\lambda_N \leq \cdots \leq \lambda_3 \leq \lambda_2 = \mathrm{E}(\nu_1 \nu_2) = p_{22} = 1 - p_{21} = 1 - c_N < 1$ by assumption.
For $n \in S$ let $T_n := \inf\{r \in \mathbb{N}_0 \,|\, \mathcal{D}_r = 1, \mathcal{D}_0 = n\}$ denote the time back to the most recent common ancestor (MRCA) of a sample of n individuals chosen from the current generation zero. Mathematically, T_n is the time until the process gets absorbed in the absorbing state 1. We are interested in $m_n := \mathrm{E}(T_n)$, the expected time back to the MRCA. If it is helpful for understanding the notation $T_{n,N}$ for T_n and $m_{n,N}$ for m_n is used to indicate the dependence of these quantities on the total population size N.

3 Exact solutions and algorithms for the time back to the most recent common ancestor

We start with presenting a formula for the distribution of T_n for the case when the eigenvalues are distinct.

Lemma 3.1 *Fix $n \in S$ and assume that the eigenvalues $\lambda_1, \ldots, \lambda_n$ are pairwise distinct. Then for all $r \in \mathbb{N}_0$ the distribution of T_n satisfies*

$$P(T_n > r) = \sum_{k=1}^{n-1} \sum_{i_0, \ldots, i_k} \frac{p_{i_k, i_{k-1}}}{1 - \lambda_{i_k}} \cdots \frac{p_{i_1, i_0}}{1 - \lambda_{i_1}} \sum_{m=1}^{k} \lambda_{i_m}^r \prod_{\substack{j=1 \\ j \neq m}}^{k} \frac{1 - \lambda_{i_j}}{\lambda_{i_m} - \lambda_{i_j}}, \tag{5}$$

where the second sum extends over all positive integers $i_0, \ldots, i_k$ satisfying $1 = i_0 < i_1 < \cdots < i_{k-1} < i_k = n$.

Remark. Note that (5) involves all the $\sum_{k=1}^{n-1}\sum_{i_0,\ldots,i_k} 1 = \sum_{k=1}^{n-1}\binom{n-2}{k-1} = 2^{n-2}$ possible paths the process $\mathcal{D}$ might take. Thus for large n numerical calculations using (5) are time-consuming. For practical purposes it is better to use the recursion $P(T_n > 0) = 1 - \delta_{n1}$ and $P(T_n > r) = \sum_{j=1}^{n} p_{nj}\, P(T_j > r-1)$ for $r = 1, 2, \ldots$ in order to compute $P(T_n > r)$ numerically.

Proof. Fix $r \in I\!N_0$. The process $\mathcal{D}$ moves from the initial state n to the absorbing state 1. This will happen due to $k \in \{1, \ldots, n-1\}$ jumps. If $n = i_k > \cdots > i_1 > i_0 = 1$ denote the states of the corresponding path it follows that $P(T_n > r) = \sum_{k=1}^{n-1}\sum_{i_0,\ldots,i_k} a_k$, where $a_k = a_k(i_1, \ldots, i_k)$ is defined via

$$a_k \;:=\; \sum_{\substack{r_1,\ldots,r_k \in N \\ r_1+\cdots+r_k > r}} p_{i_k,i_k}^{r_k-1} p_{i_k,i_{k-1}} \cdots p_{i_1,i_1}^{r_1-1} p_{i_1,i_0} \;=\; (\prod_{j=1}^{k} p_{i_j,i_{j-1}}) b_k$$

with $b_k = b_k(i_1, \ldots, i_k)$ of the form

$$\begin{aligned} b_k \;&:=\; \sum_{\substack{r_1,\ldots,r_k \in N \\ r_1+\cdots+r_k > r}} \lambda_{i_1}^{r_1-1} \cdots \lambda_{i_k}^{r_k-1} \\ &=\; \sum_{m=1}^{k} \frac{\lambda_{i_m}^{r}}{1-\lambda_{i_m}} \prod_{\substack{j=1 \\ j\neq m}}^{k} \frac{1}{\lambda_{i_m} - \lambda_{i_j}} \\ &=\; \sum_{m=1}^{k} \frac{\lambda_{i_m}^{r}}{1-\lambda_{i_m}} \prod_{\substack{j=1 \\ j\neq m}}^{k} \frac{1}{\lambda_{i_m} - \lambda_{i_j}} \\ &=\; \frac{1}{(1-\lambda_{i_1})\cdots(1-\lambda_{i_k})} \sum_{m=1}^{k} \lambda_{i_m}^{r} \prod_{\substack{j=1 \\ j\neq m}}^{k} \frac{1-\lambda_{i_j}}{\lambda_{i_m} - \lambda_{i_j}}, \end{aligned}$$

where the second equality is provided in the appendix (Lemma 8.1). □

We now focus on the expected absorption time m_n. Obviously $m_1 = 0$ and $m_i = 1 + \sum_{j=2}^{i} p_{ij} m_j$ for $i \in \tilde{S} := \{2, \ldots, N\}$. As $\lambda_i < 1$ for $i \in \tilde{S}$ the recursion

$$m_i \;=\; \frac{1}{1-\lambda_i}\left(1 + \sum_{j=2}^{i-1} p_{ij} m_j\right), \quad i = 2, 3, \ldots, N \tag{6}$$

is available. This is quite helpful for numerical calculations of $m_2, \ldots, m_N$ as long as the eigenvalues are not extremely close to one. In matrix notation write $m = Am + a$ with $m := (m_i)_{i\in\tilde{S}}$, $a := (a_i)_{i\in\tilde{S}}$ with $a_i = 1$ for all $i \in \tilde{S}$ and $A := (p_{ij})_{i,j\in\tilde{S}}$. As $\det(I - A) = (1-\lambda_2)\cdots(1-\lambda_N) > 0$ the matrix $I - A$ is non-singular and hence the solution for m is a Neumann series of the form

$$m \;=\; (I - A)^{-1} a \;=\; \sum_{k=0}^{\infty} A^k a. \tag{7}$$

The disadvantage of the algebraic solution (7) is that it involves an infinite series or an inversion of the matrix $I-A$. As $I-A$ is triangular, the inversion of $I-A$ is not difficult, but this is nevertheless not less time-consuming than the above recursion. Thus the interest is to find other solutions or at least bounds for m_n. Explicit solutions for m_n which are simple to calculate are in general not available. Besides the above recursion one can iterate the transformation $Tm := Am+a$ starting with some vector $m^{(0)}$, i.e. to calculate $m^{(1)} := Tm^{(0)}+a$, $m^{(2)} := Tm^{(1)}+a$ and so on. As T^k is contracting for some sufficiently large, but fixed k, i.e. $\|T^k\| := \sup_{x\neq 0} \|T^k x\|/\|x\| < 1$, the Banach fixed point theorem ensures that the sequence $(m^{(n)})_{n\in I\!N_0}$ converges to m. In fact, due to $\|T^k\| < 1$, it can be shown that the convergence is geometrically fast, i.e. there exist $0 < q < 1$ and $C > 0$ such that $\|m^{(n)} - m\| < Cq^n$ for all $n \in I\!N$. This iteration and the above recursion (6) provide algorithms which are useful to calculate or to approximate m numerically in reasonable time. Nevertheless, this is mathematically not very satisfying. The following lemma presents an exact solution for m_n, which is unfortunately quite time-consuming for practical purposes and hence more of theoretical interest. Bounds for m_n will be presented later.

Lemma 3.2 *For all $n \in S$*

$$m_n = \sum_{k=1}^{n-1} \sum_{i_0,\ldots,i_k} \frac{p_{i_k,i_{k-1}}}{1-\lambda_{i_k}} \cdots \frac{p_{i_1,i_0}}{1-\lambda_{i_1}} \left(\frac{1}{1-\lambda_{i_1}} + \cdots + \frac{1}{1-\lambda_{i_k}} \right), \qquad (8)$$

where the second sum extends over all positive integers $i_0, \ldots, i_k$ satisfying $1 = i_0 < i_1 < \cdots < i_{k-1} < i_k = n$.

Proof. Define $x_i := 1-\lambda_i$ for convenience. The argument already used in the proof of Lemma 3.1 shows that $m_n = \sum_{k=1}^{n-1} \sum_{i_0,\ldots,i_k} c_k$ with

$$c_k := \sum_{r_1,\ldots,r_k \in I\!N} (r_1 + \cdots + r_k) p_{i_k,i_k}^{r_k-1} p_{i_k,i_{k-1}} \cdots p_{i_1,i_1}^{r_1-1} p_{i_1,i_0} = (\prod_{j=1}^{k} p_{i_j,i_{j-1}}) d_k$$

and $d_k := \sum_{r_1,\ldots,r_k \in I\!N} (r_1 + \cdots + r_k) \lambda_{i_1}^{r_1-1} \cdots \lambda_{i_k}^{r_k-1}$. Due to the recursion

$$\begin{aligned} d_k &= \sum_{r_1,\ldots,r_{k-1} \in I\!N} (r_1 + \cdots + r_{k-1}) (\prod_{j=1}^{k-1} \lambda_{i_j}^{r_j-1}) \sum_{r_k \in I\!N} \lambda_{i_k}^{r_k-1} \\ &\quad + \sum_{r_1,\ldots,r_{k-1} \in I\!N} (\prod_{j=1}^{k-1} \lambda_{i_j}^{r_j-1}) \sum_{r_k \in I\!N} r_k \lambda_{i_k}^{r_k-1} \\ &= d_{k-1} \frac{1}{1-\lambda_{i_k}} + \frac{1}{1-\lambda_{i_1}} \cdots \frac{1}{1-\lambda_{i_{k-1}}} \frac{1}{(1-\lambda_{i_k})^2} \\ &= d_{k-1} \frac{1}{x_{i_k}} + \frac{1}{x_{i_1} \cdots x_{i_{k-1}} x_{i_k}^2} \end{aligned}$$

conclude by induction on k that

$$\begin{aligned} d_k &= \frac{1}{x_{i_1}^2 x_{i_2} \cdots x_{i_k}} + \frac{1}{x_{i_1} x_{i_2}^2 x_{i_3} \cdots x_{i_k}} + \cdots + \frac{1}{x_{i_1} \cdots x_{i_{k-1}} x_{i_k}^2} \\ &= \frac{1}{x_{i_1} \cdots x_{i_k}} \left(\frac{1}{x_{i_1}} + \cdots + \frac{1}{x_{i_k}} \right) \end{aligned}$$

and the lemma is established. □

Example. Assume that $(\mathcal{D}_r)_{r \in \mathbb{N}_0}$ is a pure death process, i.e. $p_{ij} = 0$ for $j < i-1$ and hence $p_{i,i-1} = 1 - p_{ii}$ for all $i \in \{2, \ldots, N\}$. Then only the summand with $k = n-1$ (and hence $i_j = j+1$ for all $i \in \{0, \ldots, k\}$) provides a contribution to the sums in (5) and (8). Therefore

$$P(T_n > r) \;=\; \sum_{i=2}^{n} \lambda_i^r \prod_{\substack{j=2 \\ j \neq i}}^{n} \frac{1-\lambda_j}{\lambda_i - \lambda_j} \qquad \text{and} \qquad m_n \;=\; \sum_{j=2}^{n} \frac{1}{1-\lambda_j}.$$

This corresponds to $T_n = \tau_2 + \cdots + \tau_n$, where τ_j denotes the time the process $\mathcal{D}$ spends in the state j. Note that $\tau_j - 1$ is geometrically distributed with parameter $1 - \lambda_j$ and hence $\mathrm{E}(\tau_j) = 1/(1-\lambda_j)$. For example, for the Moran model, where $(\nu_1, \ldots, \nu_N)$ is by definition a random permutation of $(2, 0, 1, \ldots, 1)$, the eigenvalues are $\lambda_i = 1 - i(i-1)/(N(N-1))$ and therefore

$$m_n \;=\; \sum_{j=2}^{n} \frac{N(N-1)}{j(j-1)} \;=\; N(N-1) \sum_{j=2}^{n} \left(\frac{1}{j-1} - \frac{1}{j}\right) \;=\; N(N-1)\left(1 - \frac{1}{n}\right), \quad (9)$$

a result which is well known from the literature.

Lemma 3.2 indicates that m_n has not a simple structure when the process $\mathcal{D}$ allows for jumps of size larger than one. Thus we focus now on upper bounds for m_n.

4 Upper bounds for the expected time back to the MRCA

Let $\tilde{D}$ be a death process which jumps exactly when $\mathcal{D}$ jumps, but with jumps of size one and let $\tilde{m}_n$ denote the corresponding expected time back to the MRCA. Then $\mathcal{D}_r \leq \tilde{\mathcal{D}}_r$ and hence $m_n \leq \tilde{m}_n = \mathrm{E}(\tau_2 + \cdots + \tau_n) = \sum_{i=2}^{n} 1/(1-\lambda_i)$. Thus we have found the bound

$$m_n \;\leq\; \sum_{i=2}^{n} \frac{1}{1-\lambda_i} \qquad \forall\, n \in S. \quad (10)$$

A better bound (see [16, 4.5.2, pp. 124] is

$$m_n \;\leq\; \sum_{i=2}^{n} \frac{1}{d_i} \qquad \forall\, n \in S, \quad (11)$$

where $d_i := i - \mathrm{E}^i(\mathcal{D}_1) := i - \mathrm{E}(\mathcal{D}_1 \,|\, \mathcal{D}_0 = i) = \sum_{j=1}^{i}(i-j)p_{ij}$. Note that (for a proof see Lemma 8.3 in the appendix) $0 = d_1 < d_2 \leq d_3 \leq \cdots \leq d_N$. Furthermore $d_i = \sum_{j=1}^{i-1}(i-j)p_{ij} \geq \sum_{j=1}^{i-1} p_{ij} = 1-\lambda_i$. Thus the bound in (11) is always smaller than or equal to the bound in (10). Finding upper bounds which are better than (11) is quite complicated and depends on further properties of the transition probabilities p_{ij}. Before such a bound can be derived it is shown in the following lemma that the upper bound (11) is never smaller than $2N_e(1-1/n)$, where $N_e = 1/c_N$ denotes the effective population size.

Lemma 4.1 *The inequality* $\sum_{i=2}^{n} 1/d_i \geq 2N_e(1-1/n)$ *holds for all* $n \in S$.

Proof. Consider a box with N balls, namely $R \in \{0, \ldots, N\}$ black balls and $N-R$ white balls. Take i balls without replacement. For $j \in \{1, \ldots, i\}$ let A_j denote the event that the j-th sampled ball is black. It follows from the inclusion-exclusion bounds that

$$\begin{aligned} 1 - \frac{(N-R)_i}{(N)_i} &= P(\bigcup_{j=1}^{i} A_j) \\ &\geq \sum_{j=1}^{i} P(A_j) - \sum_{1 \leq j < k \leq i} P(A_j \cap A_k) \;=\; i\frac{R}{N} - \binom{i}{2}\frac{(R)_2}{(N)_2}, \end{aligned}$$

where $(x)_k := x(x-1)\cdots(x-k+1)$. Thus with $R := \nu_1$ it follows that

$$\frac{(N-\nu_1)_i}{(N)_i} \;\leq\; 1 - i\frac{\nu_1}{N} + \binom{i}{2}\frac{(\nu_1)_2}{(N)_2}.$$

Now take expectation and use $\mathrm{E}(\nu_1) = 1$ and $\mathrm{E}((\nu_1)_2) = (N-1)c_N$ to conclude together with (14) that

$$\begin{aligned} d_i &= i - \mathrm{E}^i(\mathcal{D}_1) \;=\; i - N + N\frac{\mathrm{E}((N-\nu_1)_i)}{(N)_i} \\ &\leq i - N + N(1 - \tfrac{i}{N} + \tbinom{i}{2}\tfrac{c_N}{N}) \;=\; \tbinom{i}{2}c_N. \end{aligned}$$

Hence

$$\sum_{i=2}^{n}\frac{1}{d_i} \;\geq\; \sum_{i=2}^{n}\frac{2}{i(i-1)c_N} \;=\; \frac{2}{c_N}\sum_{i=2}^{n}(\frac{1}{i-1} - \frac{1}{i}) \;=\; \frac{2(1-\frac{1}{n})}{c_N}.$$

□

The following theorem states that under a certain additional condition on $\mathcal{D}_1$, which is for example satisfied for the Wright-Fisher model as it will be shown later, the inequality

$$m_n \;\leq\; 2N_e(1 - \frac{1}{n}) \tag{12}$$

holds for all $n \in S$. By Lemma 4.1 the bound in (12) is better than or at least as good as the bound in (11). Moreover, (12) is easier to compute than (11) as the

coalescence probability (1) has a simple structure. Note that the term $2(1-1/n)$ on the right hand side in (12) is exactly the time back to the MRCA for the Kingman coalescent (Kingman [10, 11, 12]). This corresponds to the asymptotic behavior of $m_n = m_{n,N}$ for large population size N, which is well known and discussed in more detail in Section 6.

Theorem 4.2 *Assume that* $\mathrm{E}^i(1/\mathcal{D}_1) := \mathrm{E}(1/\mathcal{D}_1 \,|\, \mathcal{D}_0 = i) \geq 1/i + c_N/2$ *for all* $i \in \{2, \ldots, N\}$. *Then (12) holds for all* $n \in S$. *If* $\mathrm{E}^i(1/\mathcal{D}_1) > 1/i + c_N/2$ *for all* $i \in \{3, \ldots, N\}$ *then in (12) the strict inequality holds for all* $n \in \{3, \ldots, N\}$.

Proof. For $i \in S$ define $x_i := 1 - \lambda_i$ for convenience. We prove (12) by induction on $n \in S$. Obviously (12) is satisfied for $n = 1$ as $m_1 = 0$. The step from $n-1$ to n ($n \geq 2$) follows via

$$\begin{aligned}
x_n m_n &= 1 + \sum_{j=2}^{n-1} p_{nj} m_j \overset{\text{ind}}{\leq} 1 + 2N_e \sum_{j=1}^{n-1} p_{nj}(1 - \frac{1}{j}) \\
&= 1 + 2N_e \left(1 - p_{nn} - \sum_{j=1}^{n} \frac{p_{nj}}{j} + \frac{p_{nn}}{n} \right) \\
&= 1 + 2N_e \left(p_n - \mathrm{E}^n(1/\mathcal{D}_1) + \frac{p_{nn}}{n} \right) \\
&\leq 1 + 2N_e \left(p_n - \frac{1}{n} - \frac{c_N}{2} + \frac{p_{nn}}{n} \right) \\
&= 2N_e \left(p_n - \frac{1 - p_{nn}}{n} \right) = 2p_n N_e (1 - \frac{1}{n}),
\end{aligned}$$

i.e. $m_n \leq 2N_e(1 - 1/n)$. The proof of the strict inequality works the same $\square$

Remark. Obviously $\mathrm{E}^2(1/\mathcal{D}_1) = p_{21} + p_{22}/2 = 1/2 + c_N/2$, i.e. the assumption in Theorem 4.2 is always satisfied for $i = 2$. In general

$$\mathrm{E}^i(1/\mathcal{D}_1) = \sum_{j=1}^{i} \frac{p_{ij}}{j} = \frac{p_{ii}}{i} + \sum_{j=1}^{i-1} \frac{p_{ij}}{j} = \frac{1}{i} + \sum_{j=1}^{i-1} \left(\frac{1}{j} - \frac{1}{i} \right) p_{ij},$$

as $p_{ii} = 1 - \sum_{j=1}^{i-1} p_{ij}$. If we assume that there exist g_{ij}, $i, j \in S$, which do not depend on N such that

$$p_{ij} = \delta_{ij} + c_N g_{ij} + o(c_N),$$

then it follows that

$$\begin{aligned}
\mathrm{E}^i(1/\mathcal{D}_1) &= \frac{1}{i} + \sum_{j=1}^{i-1} \left(\frac{1}{j} - \frac{1}{i} \right) (c_N\, g_{ij} + o(c_N)) \\
&= \frac{1}{i} + c_N \sum_{j=1}^{i-1} \left(\frac{1}{j} - \frac{1}{i} \right) g_{ij} + o(c_N).
\end{aligned}$$

If the model is in the domain of the Kingman coalescent, i.e. $\lim_{N\to\infty} p_{31}/c_N = 0$ (see [14, Theorem 4. (b)]), then $g_{i,i-1} = i(i-1)/2$ and $g_{ij} = 0$ for $j < i-1$ and hence

$$\mathrm{E}^i(1/\mathcal{D}_1) \;=\; \frac{1}{i} + c_N\left(\frac{1}{i-1} - \frac{1}{i}\right) g_{i,i-1} + o(c_N) \;=\; \frac{1}{i} + \frac{c_N}{2} + o(c_N).$$

Thus whether or not the condition $\mathrm{E}^i(1/\mathcal{D}_1) \geq 1/i + c_N/2$ holds, depends exactly on the behavior of the $o(c_N)$ term and is hence in general not easy to verify. A formula for $\mathrm{E}^i(1/\mathcal{D}_1)$ is presented in the appendix (see Lemma 8.2) which is in many cases helpful to verify this condition. Important examples satisfying $\mathrm{E}^i(1/\mathcal{D}_1) \geq 1/i + c_N/2$ are presented in the following section.

5 Examples

In this section examples are presented satisfying the inequality $\mathrm{E}^i(1/\mathcal{D}_1) \geq 1/i + c_N/2$ for $i \in \{2, \ldots, N\}$ and hence $m_n \leq 2N_e(1-1/n)$ for all $n \in S$. As a main result of the paper this turns out to be the case for the most important model, the haploid Wright-Fisher model.

1. For the haploid Moran model

$$\begin{aligned}
\mathrm{E}^i(1/\mathcal{D}_1) &= \frac{1}{i}p_{ii} + \frac{1}{i-1}p_{i,i-1} \\
&= \frac{1}{i}\left(1 - \frac{i(i-1)}{N(N-1)}\right) + \frac{1}{i-1}\frac{i(i-1)}{N(N-1)} \\
&= \frac{1}{i} + \frac{1}{N(N-1)} \;=\; \frac{1}{i} + \frac{c_N}{2},
\end{aligned}$$

   as $c_N = 2/(N(N-1))$. Thus in the proof of Theorem 4.2 only equality appear and hence $m_n = 2N_e(1-1/n) = N(N-1)(1-1/n)$ in agreement with (9).

2. For the haploid Wright-Fisher model $C_j := \nu_1 + \cdots + \nu_j$ is binomially distributed with the parameters N and j/N. Hence C_j has factorial moments $\mathrm{E}((C_j)_i) = (N)_i(j/N)^i$ and from Lemma 8.2 conclude that

$$\mathrm{E}^i(1/\mathcal{D}_1) \;=\; \tfrac{1}{N}\sum_{j=1}^{N}(\tfrac{j}{N})^{i-1}.$$

   This is an upper Riemann sum of the the function $f(x) := x^{i-1}$. As f is strictly convex and strictly monotone increasing on $[0,1]$ for $i \geq 3$ it follows that this Riemann sum is larger than the integral $\int_0^1 f(x)\,dx$ plus the sum of the surfaces $V(D_j)$ of all the triangles D_j with edge points $((j-1)/N, f((j-1)/N))$, $((j-1)/N, f(j/N))$ and $(j/N, f(j/N))$,

$j \in \{1, \ldots, N\}$. Thus for the Wright-Fisher model the strict inequality

$$\begin{aligned}
\mathrm{E}^i(1/\mathcal{D}_1) &> \int_0^1 f(x)\,dx + \sum_{j=1}^N V(D_j) \\
&= \int_0^1 x^{i-1}\,dx + \tfrac{1}{2N}\sum_{j=1}^N \big(f(\tfrac{j}{N}) - f(\tfrac{j-1}{N})\big) \\
&= [\tfrac{x^i}{i}]_0^1 + \tfrac{1}{2N}(f(1) - f(0)) \;=\; \tfrac{1}{i} + \tfrac{1}{2N}
\end{aligned}$$

is satisfied for $i \geq 3$ and therefore $m_n < 2N(1-1/n)$ for all $n \in \{3, \ldots, N\}$. For $n \in \{1, 2\}$ always equality $m_n = 2N(1 - 1/n)$ holds.

3. Assume that $(\nu_1, \ldots, \nu_N)$ is uniformly distributed on the discrete simplex, i.e.

$$P(\nu_1 = k_1, \ldots, \nu_N = k_N) \;=\; \frac{1}{\binom{2N-1}{N}}$$

for all $k_1, \ldots, k_N \in I\!N_0$ with $k_1 + \cdots + k_N = N$. We call this model the 'uniform' model. A straightforward but tedious computation shows that the joint distribution of $\nu_1, \ldots, \nu_j$ satisfies

$$P(\nu_1 = k_1, \ldots, \nu_j = k_j) \;=\; \frac{\binom{2N-j-k-1}{N-j-1}}{\binom{2N-1}{N}}$$

whenever $k := k_1 + \cdots + k_j \leq N$. Therefore, the distribution of $C_j = \nu_1 + \cdots + \nu_j$ is

$$P(C_j = k) \;=\; \frac{\binom{2N-j-k-1}{N-j-1}\binom{j+k-1}{j-1}}{\binom{2N-1}{N}}.$$

From this derive the factorial moments

$$\mathrm{E}((C_j)_i) \;=\; \sum_k (k)_i\, P(C_j = k) \;=\; (N)_i \frac{\binom{i+j-1}{i}}{\binom{N+i-1}{i}}$$

and use (8.2) to conclude that

$$\begin{aligned}
\mathrm{E}^i(1/\mathcal{D}_1) &= \frac{1}{(N)_i}\sum_{j=1}^N \frac{\mathrm{E}((C_j)_i)}{j} \;=\; \frac{1}{i\binom{N+i-1}{i}}\sum_{j=1}^N \binom{i+j-1}{i-1} \\
&= \frac{1}{i\binom{N+i-1}{i}}\left(\binom{N+i}{i} - 1\right) \\
&= \frac{N+i}{iN} - \frac{1}{i\binom{N+i-1}{i}} \;=\; \frac{1}{i} + \frac{1}{N} - \frac{1}{N\binom{N+i-1}{N}}.
\end{aligned}$$

As the last fraction is strictly decreasing in i it follows that $\mathrm{E}^i(1/\mathcal{D}_1) > 1/i + 1/N - 1/(N(N+1)) = 1/i + 1/(N+1)$ for $i \in \{3, \ldots, N\}$. As

the coalescence probability is $c_N = \mathrm{E}((C_1)_2)/(N-1) = 2/(N+1)$ this means that $\mathrm{E}^i(1/\mathcal{D}_1) > 1/i + c_N/2$ for all $i \in \{3,\ldots,N\}$. Hence Theorem 4.2 is applicable, i.e. $m_n < 2N_e(1-1/n) = (N+1)(1-1/n)$ for all $n \in \{3,\ldots,N\}$.

4. We provide a Wright-Fisher like model with uniformly bounded offspring sizes: Assume there exists an integer constant $M > 1$ such that

$$P(\nu_1 = k_1, \ldots, \nu_N = k_N) \;=\; \frac{\binom{M}{k_1}\cdots\binom{M}{k_N}}{\binom{NM}{N}}$$

for $k_1 + \cdots + k_N = N$. Note that this is a model with uniformly bounded offspring sizes, as $\sup_{1\le i\le N} \nu_i \le M$ almost surely for all $N \in I\!N$. For $M \to \infty$ this model coincides with the classical Wright-Fisher model discussed in Example 2. In this case C_j is hyper-geometrically distributed with the parameters N, jM, NM and has hence (Johnson and Kotz [9, p. 144] the factorial moments $\mathrm{E}((C_j)_i) = (N)_i(jM)_i/(NM)_i$. The coalescence probability $c_N = \mathrm{E}((C_1)_2)/(N-1) = (M-1)/(NM-1) \le 1/N$ is less than or equal to the coalescence probability $1/N$ in a haploid Wright-Fisher model with population size N. From (15) it follows that

$$\begin{aligned}
\mathrm{E}^i(1/\mathcal{D}_1) \;&=\; \sum_{j=1}^{N} \frac{1}{j}\frac{(jM)_i}{(NM)_i} \;=\; \frac{1}{(NM)_i}\sum_{j=1}^{N} M(jM-1)_{i-1} \\
&=\; \underbrace{\frac{1}{(NM)_i}\sum_{j=1}^{N}\sum_{k=1}^{M}(jM-k)_{i-1}}_{=:\,(I)} \\
&\qquad + \underbrace{\frac{1}{(NM)_i}\sum_{j=1}^{N}\sum_{k=1}^{M}\big((jM-1)_{i-1} - (jM-k)_{i-1}\big)}_{=:\,(II)}.
\end{aligned}$$

The first term (I) is equal to $1/((NM)_i)\sum_{l=0}^{NM-1}(l)_{i-1} = 1/i$. A tedious computation (see Lemma 8.4 in the appendix) shows that the second term (II), considered as a function of $i \in \{2,\ldots,N\}$, takes its minimum at $i = 2$ and is hence larger than or equal to

$$\frac{1}{(NM)_2}\sum_{j=1}^{N}\sum_{k=2}^{M}(k-1) \;=\; \frac{1}{(NM)_2}N\frac{M(M-1)}{2} \;=\; \frac{M-1}{2(NM-1)} \;=\; \frac{c_N}{2}$$

for $i \in \{2,\ldots,N\}$. Thus $\mathrm{E}^i(1/\mathcal{D}_1) \ge 1/i + c_N/2$ for $i \in \{2,\ldots,N\}$ and by Theorem 4.2 $m_n \le 2N_e(1-1/n) = 2(NM-1)(1-1/n)/(M-1)$ for $n \in \{1,\ldots,N\}$.

6 Asymptotical behavior for large population size

The asymptotical behavior of the expected time back to the MRCA for large N is now analyzed. In order to avoid confusion with the limiting quantities write $p_{ij}(N)$ for the transition probabilities (2) of the ancestral process and $m_{n,N} = \mathrm{E}(T_{n,N})$ for the expected time back to the MRCA in order to indicate the dependence on the total population size N.
One of the most important results in coalescent theory ([14, Theorem 4. (b)], [15]) is that for each sample size $n \in I\!N$ the time-scaled ancestral process $(\mathcal{D}^{(n)}_{[t/c_N]})_{t\geq 0}$ converges weakly, i.e. in the Skorohod topology, to a limiting time-continuous pure death process $(D^{(n)}_t)_{t\geq 0}$ with initial value $D^{(n)}_0 = n$ and rates $\gamma_i := i(i-1)/2$, $i \in \{1, \ldots, n\}$ if and only if the condition

$$\lim_{N\to\infty} \frac{p_{31}(N)}{p_{21}(N)} \;=\; 0$$

is satisfied. This fundamental condition states that triple mergers of ancestral lines are asymptotically negligible in comparison with binary collisions of ancestral lines. The following theorem relates this result with the expected time back to the MRCA.

Theorem 6.1 *The following conditions are equivalent:*

(i) $\lim_{N\to\infty} p_{31}(N)/c_N = 0$.

(ii) For each sample size $n \in I\!N$ the time-scaled ancestral process $(\mathcal{D}^{(n)}_{[t/c_N]})_{t\geq 0}$ converges in the Skorohod topology to a pure death process $(D^{(n)}_t)_{t\geq 0}$ with initial state $D^{(n)}_0 = n$ and rates $\gamma_i := i(i-1)/2$. (The parameter n only indicates that the processes start in the initial state n)

(iii) $\lim_{N\to\infty} c_N \,\mathrm{E}(T_{n,N}) = 2(1-1/n)$ *for all* $n \in I\!N$.

(iv) $\lim_{N\to\infty} c_N \,\mathrm{E}(T_{3,N}) = 4/3$.

Proof. The equivalence of (i) and (ii) is known from the literature, as already mentioned at the beginning of this section.
(ii) $\Rightarrow$ (iii): Fix $n \in I\!N$ and define $f_N(t) := P(T_{n,N} > [t/c_N]) = P(\mathcal{D}^{(n)}_{[t/c_N]} > 1)$. From (ii) it follows that $\mathcal{D}^{(n)}_{[t/c_N]}$ converges in distribution to $D^{(n)}_t$ as N tends to infinity, i.e.

$$\lim_{N\to\infty} f_N(t) \;=\; \lim_{N\to\infty} P(\mathcal{D}^{(n)}_{[t/c_N]} > 1) \;=\; P(D^{(n)}_t > 1) \;=:\; f(t)$$

for all $t \geq 0$. Thus the dominated convergence theorem ensures that

$$\begin{aligned} c_N \,\mathrm{E}(T_{n,N}) \;&=\; \sum_{i=0}^{\infty} c_N P(T_{n,N} > i) \;=\; \sum_{i=0}^{\infty} \int_{[ic_N,(i+1)c_N)} P(T_{n,N} > i)\, dt \\ &=\; \int_0^{\infty} P(T_{n,N} > [t/c_N])\, dt \;=\; \int_0^{\infty} f_N(t)\, dt \end{aligned}$$

converges to $\int_0^\infty f(t)\,dt = \int_0^\infty P(D_t^{(n)} > 1)\,dt = \int_0^\infty P(T_n > t)\,dt = \mathrm{E}(T_n) = 2(1-1/n)$. It remains open to clarify that it is allowed to apply the dominated convergence theorem, i.e. a dominating function g for the functions f_N has to be constructed. In order to do this let $\tilde{\mathcal{D}} := (\tilde{\mathcal{D}}_r^{(n)})_{r\in I\!N_0}$ be a discrete time death process with initial state $\tilde{\mathcal{D}}_0^{(n)} = n$ which jumps exactly when $(\mathcal{D}_r^{(n)})_{r\in I\!N_0}$ jumps, but with jumps of size one. Then $\mathcal{D}_r^{(n)} \le \tilde{\mathcal{D}}_r^{(n)}$ and hence

$$f_N(t) \;=\; P(\mathcal{D}_{[t/c_N]}^{(n)} > 1) \;\le\; P(\tilde{\mathcal{D}}_{[t/c_N]}^{(n)} > 1) \;=\; P(\tilde{\tau}_2 + \cdots + \tilde{\tau}_n > [t/c_N]),$$

where $\tilde{\tau}_i$ denotes the time the process $\tilde{\mathcal{D}}$ spends in the state i. As these times are independent and geometrically distributed with parameter $1-\lambda_i$ it follows that

$$f_N(t) \;\le\; \sum_{i=2}^n \lambda_i^{[t/c_N]} \prod_{\substack{j=2\\ j\neq i}}^n \frac{1-\lambda_j}{\lambda_i-\lambda_j}. \tag{13}$$

As the limits $\gamma_i := \lim_{N\to\infty}(1-\lambda_i)/c_N = i(i-1)/2$ exist (these are the rates of the process $(D_t^{(n)})_{t\ge 0}$), it follows that the right hand side in (13) converges as N tends to infinity to

$$h(t) \;:=\; \sum_{i=2}^n \exp(-\gamma_i t) \prod_{\substack{j=2\\ j\neq i}}^n \frac{\gamma_j}{\gamma_j-\gamma_i}.$$

The convergence of $\lambda_i^{[t/c_N]}$ to $\exp(-\gamma_i t)$ is uniformly in $t\in[0,\infty)$ and n is fixed. Hence there exists some $N_0 \in I\!N$ (which does not depend on t) such that for all $t\in[0,\infty)$ the inequality $f_N(t) \le 2h(t)$ holds for all $N > N_0$. Thus $f_N \le g := 2h$ for $N > N_0$. Obviously $\int h(t)\,dt < \infty$ and hence g is a dominating function for f_N, $N > N_0$.
(iii) $\Rightarrow$ (iv): This is trivial.
(iv) $\Rightarrow$ (i): For $j, i_1, \ldots, i_j \in I\!N$ introduce the quantities

$$\Phi_j(i_1,\ldots,i_j) \;:=\; \frac{(N)_j}{(N)_i}\mathrm{E}((\nu_1)_{i_1}\cdots(\nu_j)_{i_j})$$

with $i := i_1 + \cdots + i_j$ and note that the recursion

$$\Phi_{j+1}(i_1,\ldots,i_j,1) \;=\; \Phi_j(i_1,\ldots,i_j) - \sum_{k=1}^j \Phi_j(i_1,\ldots,i_{k-1},i_k+1,i_{k+1},\ldots,i_j)$$

holds (see [14, p. 984]). Now define $x_i := 1-\lambda_i$ and conclude from Lemma 3.2 that

$$\begin{aligned}\mathrm{E}(T_{3,N}) \;&=\; \frac{p_{31}}{x_3^2} + \frac{p_{32}}{x_3}\left(\frac{1}{x_2}+\frac{1}{x_3}\right)\\ &=\; \frac{p_{32}}{x_3} + \frac{x_3-p_{31}}{x_3}\left(\frac{1}{x_2}+\frac{1}{x_3}\right) \;=\; \frac{1}{x_2}+\frac{1}{x_3}-\frac{p_{31}}{x_2x_3}.\end{aligned}$$

As $c_N = x_2 = p_{21}$ this is equivalent to

$$c_N \, \mathrm{E}(T_{3,N}) \;=\; 1 + \frac{x_2 - p_{31}}{x_3} \;=\; 1 + x(1-y)$$

with $x := x_2/x_3$ and $y := p_{31}/p_{21}$. Due to the recursions $\lambda_3 = \Phi_3(1,1,1) = \Phi_2(1,1) - 2\Phi_2(2,1) = \lambda_2 - 2\Phi_2(2,1)$, i.e. $\Phi_2(2,1) = (x_3 - x_2)/2$ and

$$p_{31} = \Phi_1(3) = \Phi_1(2) - \Phi_2(2,1) = x_2 - \frac{x_3 - x_2}{2} = \frac{3x_2 - x_3}{2}$$

the relation

$$y \;=\; \frac{p_{31}}{p_{21}} \;=\; \frac{3x_2 - x_3}{2x_2} \;=\; \frac{3}{2} - \frac{1}{2x}$$

holds between x and y and hence

$$c_N \, \mathrm{E}(T_{3,N}) \;=\; \frac{3-x}{2} \;=\; \frac{4-3y}{3-2y}$$

can be expressed in x or y. In particular, $c_N \, \mathrm{E}(T_{3,N})$ converges to $4/3$ if and only if y converges to zero as N tends to infinity. Thus (i) and (iv) are equivalent and the proof is completed. □

Remark. It is not difficult to generalize Theorem 6.1 for the case when the model is in the domain of a coalescent which allows for simultaneous and multiple collisions (see [15]) of ancestral lines: Assume that $c_N > 0$ for sufficiently large N and that $\lim_{N\to\infty} c_N = 0$. Furthermore assume that all the limits

$$g_{ij} \;:=\; \lim_{N\to\infty} \frac{p_{ij}(N)}{c_N},$$

$i, j \in I\!N$ exist. Then obviously all the limits $\gamma_i := \lim_{N\to\infty}(1-\lambda_i)/c_N$, $i \in I\!N$, exist. Furthermore, for each sample size $n \in I\!N$ the time-scaled ancestral process $(\mathcal{D}^{(n)}_{[t/c_N]})_{t\geq 0}$ converges weakly in the Skorohod topology to a time-continuous death process $D = (D^{(n)}_t)_{t\geq 0}$ with initial state $D^{(n)}_0 = n$ and infinitesimal rates g_{ij}. The argument used in the proof of Theorem 6.1 to derive (iii) from (ii) still works which means that

$$\lim_{N\to\infty} c_N \, \mathrm{E}(T_{n,N}) = \mathrm{E}(T_n)$$

holds for all $n \in I\!N$, where $T_n := \inf\{t > 0 \mid D^{(n)}_t = 1\}$ denotes the time back to the MRCA for the limiting process.

7 Final remarks, conclusions and open problems

We have seen that the expected time $m_n = m_{n,N}$ back to the MRCA of a sample of size n in a haploid population of total size N is in many cases smaller than (or equal to) the asymptotic value $2N_e(1 - 1/n)$ derived from coalescent

theory. The examples in Section 5 show that it can be quite technical to verify the condition $\mathrm{E}^i(1/\mathcal{D}_1) \geq 1/i + c_N/2$ which is needed in order to derive the bound $2N_e(1-1/n)$ (Theorem 4.2). A general approach would be to rewrite (15) as

$$\mathrm{E}^i(1/\mathcal{D}_1) \;=\; \frac{1}{(N)_i}\sum_{j=1}^{N}\frac{(j)_i}{j} + \frac{1}{(N)_i}\sum_{j=1}^{N}\frac{\mathrm{E}((C_j)_i)-(j)_i}{j} \;=\; \frac{1}{i} + f(i)$$

with $f(i) := ((N)_i)^{-1}\sum_{j=1}^{N}(\mathrm{E}((C_j)_i)-(j)_i)/j$ for $i \in \{2,\ldots,N\}$. Note that

$$\begin{aligned}
\mathrm{E}((C_j)_2) &= \mathrm{E}((\nu_1+\cdots+\nu_j)^2) - j \\
&= j\,\mathrm{E}(\nu_1^2) - j + j(j-1)\,\mathrm{E}(\nu_1\nu_2) \\
&= j\,\mathrm{E}((\nu_1)_2) + j(j-1)(1-c_N) \\
&= j(N-1)c_N + j(j-1)(1-c_N) \\
&= j(N-j)c_N + (j)_2.
\end{aligned}$$

and hence $f(2) = 1/((N)_2)\sum_{j=1}^{N}(N-j)c_N = c_N/2$. Thus, assuming that $f : \{2,\ldots,N\} \to I\!R$ takes its minimum at the left border, i.e. at $i=2$ it follows that

$$\mathrm{E}^i(1/\mathcal{D}_1) \;\geq\; \frac{1}{i} + f(2) \;=\; \frac{1}{i} + \frac{c_N}{2}$$

for $i \in \{2,\ldots,N\}$ and Theorem 4.2 ensures that (12) is satisfied. Unfortunately, a proof of $f(i) \geq f(2)$ for $i \in \{2,\ldots,N\}$ is not known yet. Note that in general f is neither monotone nor unimodal. The author wants to state the conjecture that $f(i) \geq f(2)$ holds and that hence the bound in (12) is always an upper bound for the expected time back to the MRCA.

8 Appendix

Lemma 8.1 *For distinct $x_1,\ldots,x_n \in I\!R$ the equality*

$$\sum_{\substack{i_1,\ldots,i_n \in I\!N \\ i_1+\cdots+i_n=k}} x_1^{i_1}\cdots x_n^{i_n} \;=\; \sum_{i=1}^{n} x_i^k b_{ni}$$

holds for all $k \in I\!N$, where $b_{ni} := \prod_{\substack{j=1\\ j\neq i}}^{n}\frac{x_j}{x_i-x_j}$. If in addition $|x_i|<1$ for all $i \in \{1,\ldots,n\}$ then

$$\sum_{\substack{i_1,\ldots,i_n \in I\!N \\ i_1+\cdots+i_n\geq k}} x_1^{i_1}\cdots x_n^{i_n} \;=\; \sum_{i=1}^{n}\frac{x_i^k}{1-x_i}b_{ni}.$$

Proof. If $x_i = 0$ for some $i \in \{1,\ldots,n\}$ then both sides of the first equation are equal to zero. Assume now that $x_i \neq 0$ for all $i \in \{1,\ldots,n\}$. We verify the

first equation by induction on n. For $n = 1$ the first equation holds as $b_{11} = 1$. Assume now that the first equation holds for $n-1$. Then

$$\begin{aligned}
\sum_{\substack{i_1,\dots,i_n \in N \\ i_1+\cdots+i_n=k}} x_1^{i_1}\cdots x_n^{i_n} &= \sum_{i_n=1}^{k-1} \sum_{\substack{i_1,\dots,i_{n-1}\in N \\ i_1+\cdots+i_{n-1}=k-i_n}} x_1^{i_1}\cdots x_{n-1}^{i_{n-1}} x_n^{i_n} \\
&\overset{\text{ind}}{=} \sum_{i_n=1}^{k-1} \Big(\sum_{i=1}^{n-1} x_i^{k-i_n} b_{n-1,i}\Big) x_n^{i_n} \\
&= \sum_{i=1}^{n-1} b_{n-1,i} x_i^{k-1} x_n \sum_{i_n=1}^{k-1} \Big(\frac{x_n}{x_i}\Big)^{i_n-1} \\
&= \sum_{i=1}^{n-1} b_{n-1,i} x_i^{k-1} x_n \frac{1-(\frac{x_n}{x_i})^{k-1}}{1-\frac{x_n}{x_i}} \\
&= \sum_{i=1}^{n-1} b_{n-1,i} \frac{x_n x_i}{x_i - x_n}(x_i^{k-1} - x_n^{k-1}) \\
&= \sum_{i=1}^{n-1} b_{ni}(x_i^k - x_i x_n^{k-1}) \;=\; \sum_{i=1}^{n} b_{ni}(x_i^k - x_i x_n^{k-1}) \\
&= \sum_{i=1}^{n} b_{ni} x_i^k - x_n^{k-1} \sum_{i=1}^{n} x_i b_{ni}.
\end{aligned}$$

It remains open to verify that $\sum_{i=1}^n x_i b_{ni} = 0$. This follows by choosing $x = 0$ in the exact Lagrange interpolation

$$f(x) \;=\; \sum_{i=1}^{n} f(x_i) \prod_{\substack{j=1 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

of the function $f(x) := x$. Finally, the second equation follows from the first equation via

$$\begin{aligned}
\sum_{\substack{i_1,\dots,i_n \in N \\ i_1+\cdots+i_n \geq k}} x_1^{i_1}\cdots x_n^{i_n} &= \sum_{l=k}^{\infty} \sum_{\substack{i_1,\dots,i_n\in N \\ i_1+\cdots+i_n=l}} x_1^{i_1}\cdots x_n^{i_n} \\
&= \sum_{l=k}^{\infty}\sum_{i=1}^{n} x_i^l b_{ni} \;=\; \sum_{i=1}^{n} \frac{x_i^k}{1-x_i} b_{ni},
\end{aligned}$$

as $\sum_{l=k}^{\infty} x_i^l = x_i^k/(1-x_i)$ for $|x_i| < 1$. □

Lemma 8.2 *Fix $i \in \{1,\dots,N\}$ and assume that the ancestral process starts in the state $\mathcal{D}_0 = i$. Then the mean of $\mathcal{D}_1$ is*

$$\mathrm{E}^i(\mathcal{D}_1) \;=\; N - N\frac{\mathrm{E}((N-\nu_1)_i)}{(N)_i} \tag{14}$$

and the mean of the inverse of $\mathcal{D}_1$ is

$$\mathrm{E}^i(1/\mathcal{D}_1) \;=\; \frac{1}{(N)_i}\sum_{j=1}^{N}\frac{\mathrm{E}((C_j)_i)}{j}, \tag{15}$$

where $C_j := \nu_1 + \cdots + \nu_j$ denotes the number of offspring of the individuals $1,\ldots,j$ and $(x)_i := x(x-1)\cdots(x-i+1)$.

Proof. Using the representation (2) for the transition probabilities it follows that the probability generating function of $\mathcal{D}_1$ satisfies

$$\begin{aligned}
\mathrm{E}^i(x^{\mathcal{D}_1}) &= \sum_{j=1}^{N} x^j p_{ij} \;=\; \frac{1}{(N)_i}\sum_{j=1}^{N}(N)_j x^j \sum_{k=1}^{j}\frac{(-1)^{j-k}}{k!\,(j-k)!}\mathrm{E}((C_k)_i)\\
&= \frac{1}{(N)_i}\sum_{k=1}^{N}\mathrm{E}((C_k)_i)\frac{1}{k!}\sum_{j=k}^{N}\frac{(N)_j x^j(-1)^{j-k}}{(j-k)!}\\
&= \frac{1}{(N)_i}\sum_{k=1}^{N}\mathrm{E}((C_k)_i)\frac{x^k}{k!}\sum_{r=0}^{N-k}\frac{(N)_{r+k}(-x)^r}{r!}\\
&= \frac{1}{(N)_i}\sum_{k=1}^{N}\mathrm{E}((C_k)_i)x^k\tbinom{N}{k}\sum_{r=0}^{N-k}\tbinom{N-k}{r}(-x)^r\\
&= \frac{1}{(N)_i}\sum_{k=1}^{N}\mathrm{E}((C_k)_i)\tbinom{N}{k}x^k(1-x)^{N-k}
\end{aligned}$$

and (14) follows by differentiating with respect to x and plugging in $x=1$. Dividing both sides of the above equation by x and integrating with respect to $x\in[0,1]$ leads to

$$\begin{aligned}
\mathrm{E}^i(1/\mathcal{D}_1) &= \int_0^1 \mathrm{E}^i(x^{\mathcal{D}_1-1})\,dx\\
&= \frac{1}{(N)_i}\sum_{k=1}^{N}\mathrm{E}((C_k)_i)\tbinom{N}{k}\int_0^1 x^{k-1}(1-x)^{N-k}\,dx\\
&= \frac{1}{(N)_i}\sum_{k=1}^{N}\frac{\mathrm{E}((C_k)_i)}{k},
\end{aligned}$$

where the formula $\int_0^1 x^{k-1}(1-x)^{N-k}\,dx = (k-1)!(N-k)!/N!$ for the beta function has been used. □

Lemma 8.3 *The sequence $d_i := i - \mathrm{E}^i(\mathcal{D}_1)$, $i\in\{1,\ldots,N\}$, is monotone increasing in i. More precisely, $0 = d_1 < d_2 \le d_3 \le \cdots \le d_N$.*

Proof. Obviously $d_1 = 0$ and $d_2 = 2 - \mathrm{E}^2(\mathcal{D}_1) = 2 - p_{21} - 2p_{22} = 2 - p_{21} - 2(1-p_{21}) = p_{21} = c_N > 0$ by assumption. For $i \in \{1, \ldots, N-1\}$ consider

$$\begin{aligned} d_{i+1} - d_i &= 1 - \mathrm{E}^{i+1}(\mathcal{D}_1) + \mathrm{E}^i(\mathcal{D}_1) \\ &\overset{(14)}{=} 1 + N\mathrm{E}\left(\frac{(N-\nu_1)_{i+1}}{(N)_{i+1}} - \frac{(N-\nu_1)_i}{(N)_i}\right) \\ &= 1 - N\frac{\mathrm{E}(\nu_1(N-\nu_1)_i)}{(N)_{i+1}}. \end{aligned}$$

Thus $d_i \le d_{i+1}$ if and only if $N\mathrm{E}(\nu_1(N-\nu_1)_i) \le (N)_{i+1}$. But this is obviously satisfied as $(N-\nu_1)_i \le (N-1)_i$ on $\{\nu_1 \ge 1\}$ and hence

$$N\mathrm{E}(\nu_1(N-\nu_1)_i) \;\le\; N\mathrm{E}(\nu_1(N-1)_i) \;=\; N(N-1)_i\mathrm{E}(\nu_1) \;=\; (N)_{i+1}.$$

□

Lemma 8.4 *Fix $N, M \in \mathbb{N}$. The function $f : \{2, \ldots, N\} \to \mathbb{R}$ defined via*

$$f(i) \;:=\; \frac{1}{NM}\sum_{j=1}^{N}\sum_{k=1}^{M}\frac{\binom{jM-1}{i-1} - \binom{jM-k}{i-1}}{\binom{NM-1}{i-1}}$$

takes its minimum at $i = 2$.

Proof. Obviously

$$f(i) \;=\; \frac{1}{NM}\sum_{j=1}^{N}\frac{1}{2}\sum_{k=1}^{M}\frac{N_{ij}(k)}{\binom{NM-1}{i-1}}.$$

with nominator

$$N_{ij}(k) \;:=\; \binom{jM-1}{i-1} - \binom{jM-k}{i-1} + \binom{jM-1}{i-1} - \binom{jM-(M-k+1)}{i-1}.$$

Note that $N_{ij}(k) = N_{ij}(M-k+1)$ for $k \in \{1, \ldots, M\}$. Due to the convexity of the function $x \mapsto \binom{x}{i-1}$ on $\mathbb{N}_0$ the nominator $N_{ij}(k)$ takes its minimum at the border, i.e. for $k = 1$ (and $k = M$). Thus

$$\begin{aligned} f(i) &\ge \frac{1}{NM}\sum_{j=1}^{N}\frac{1}{2}\sum_{k=1}^{M}\frac{N_{ij}(1)}{\binom{NM-1}{i-1}} \\ &= \frac{1}{2N}\sum_{j=1}^{N}\frac{\binom{jM-1}{i-1} - \binom{jM-M}{i-1}}{\binom{NM-1}{i-1}} \\ &= \frac{1}{2N}\frac{\binom{NM-1}{i-1} + \sum_{j=1}^{N-1}\left(\binom{jM-1}{i-1} - \binom{jM}{i-1}\right)}{\binom{NM-1}{i-1}} \\ &= \frac{1}{2N}\left(1 - \sum_{j=1}^{N-1}\frac{\binom{jM-1}{i-2}}{\binom{NM-1}{i-1}}\right) \end{aligned} \tag{16}$$

For each $j \in \{1, \ldots, N-1\}$ the map $i \mapsto \binom{jM-1}{i-2}/\binom{NM-1}{i-1}$ is decreasing in $i \in \{2, \ldots, N\}$. Thus the last expression (16) takes its minimum at $i = 2$ and this minimum is equal to

$$\frac{1}{2N}\left(1 - \frac{N-1}{NM-1}\right) \;=\; \frac{M-1}{2(NM-1)}.$$

Thus $f(i) \geq (M-1)/(2(NM-1)) = f(2)$ for all $i \in \{2, \ldots, N\}$. □

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