On a Two-Parameter Yule-Simon Distribution

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Abstract We extend the classical one-parameter Yule-Simon law to a version depending on two parameters, which in part appeared in Bertoin (J Stat Phys 176(3):679–691, 2019) in the context of a preferential attachment algorithm with fading memory. By making the link to a general branching process with age-dependent reproduction rate, we study the tail-asymptotic behavior of the two-parameter Yule-Simon law, as it was already initiated in Bertoin (J Stat Phys 176(3):679–691, 2019). Finally, by superposing mutations to the branching process, we propose a model which leads to the two-parameter range of the Yule-Simon law, generalizing thereby the work of Simon (Biometrika 42(3/4):425–440, 1955) on limiting word frequencies.

Keywords Yule-Simon model · Crump-Mode-Jagers branching process · Population model with neutral mutations · Heavy tail distribution · Preferential attachment with fading memory

1 Introduction

The standard Yule process $Y = (Y(t))_{t \geq 0}$ is a basic population model in continuous time and with values in $\mathbb{N} := \{1, 2, \ldots\}$. It describes the evolution of the size of a population started from a single ancestor, where individuals are immortal and give birth to children at unit rate, independently one from the other. It is well-known that for every $t \geq 0$, $Y(t)$ has the geometric distribution with parameter e^{-t}. As a consequence, if T_ρ denotes an exponentially distributed random time with parameter

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$\rho > 0$ which is independent of the Yule process, then for every $k \in \mathbb{N}$, there is the identity

$$\mathbb{P}\left(Y(T_\rho) = k\right) = \rho \int_0^\infty e^{-\rho t}(1 - e^{-t})^{k-1}e^{-t}dt = \rho B(k, \rho + 1), \qquad (1)$$

where B is the beta function.

The discrete distribution in (1) has been introduced by H.A. Simon [20] in 1955 and is nowadays referred to as the Yule-Simon distribution with parameter ρ. It arises naturally in preferential attachment models and often explains the occurrence of heavy tail variables in stochastic modeling. Indeed, the basic estimate

$$B(k, \rho + 1) \sim \Gamma(\rho + 1)k^{-(\rho+1)} \qquad \text{as } k \to \infty,$$

implies that the Yule-Simon distribution has a fat tail with exponent ρ.

The present work is devoted to a two-parameter generalization of the Yule-Simon distribution, which results from letting the fertility (i.e. the reproduction rate) of individuals in the population model depend on their age. Specifically, imagine that now the rate at which an individual of age $a \geq 0$ begets children is $e^{-\theta a}$ for some fixed $\theta \in \mathbb{R}$. So for $\theta > 0$ the fertility decays with constant rate θ as individuals get older, whereas for $\theta < 0$, the fertility increases with constant rate $-\theta$. Denote the size of the population at time t by $Y_\theta(t)$. In other words, $Y_\theta = (Y_\theta(t))_{t \geq 0}$ is a general (or Crump-Mode-Jagers) branching process, such that the point process on $[0, \infty)$ that describes the ages at which a typical individual begets a child is Poisson with intensity measure $e^{-\theta t}dt$. For $\theta = 0$, $Y_0 = Y$ is the usual Yule process.

Definition 1.1 Let $\theta \in \mathbb{R}$ and $\rho > 0$. Consider Y_θ as above and let T_ρ be an exponential random time with parameter $\rho > 0$, independent of Y_θ. We call the law of the discrete random variable

$$X_{\theta,\rho} := Y_\theta(T_\rho)$$

the Yule-Simon distribution with parameters (θ, ρ).

A key difference with the original Yule-Simon distribution, which corresponds to $\theta = 0$, is that no close expression for the two-parameter distribution is known.[1] Actually, the general branching process Y_θ is not even Markovian for $\theta \neq 0$, and its one-dimensional distributions are not explicit. This generalization of the Yule-Simon distribution has recently appeared in [1] for $\theta > 0$ and $\rho > (1 - \theta)^+$, in connection with a preferential attachment model with fading memory in the vein of Simon's original model. We shall point out in Sect. 5 that the range of parameters $\theta \leq 0$ and $\rho > 0$ arises similarly for a family of related models.

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[1]Although the probability $\mathbb{P}(X_{\theta,\rho} = 1)$ can easily be computed in terms of an incomplete Gamma function, the calculations needed to determine $\mathbb{P}(X_{\theta,\rho} = k)$ for $k \geq 2$ become soon intractable.

One of the purposes of the present contribution is to describe some features of the two-parameter Yule-Simon law, notably by completing [1] and determining the tail-asymptotic behavior of $X_{\theta,\rho}$. It was observed in [1] that the parameter $\theta = 1$ is critical, in the sense that when $\theta < 1$, $X_{\theta,\rho}$ has a fat tail with exponent $\rho/(1-\theta)$, whereas when $\theta > 1$, some exponential moments of positive order of $X_{\theta,\rho}$ are finite. We show here in Sect. 4 that when $\theta > 1$, the tail of $X_{\theta,\rho}$ is actually decaying exponentially fast with exponent $\ln\theta - 1 + 1/\theta$. Further, in the critical case $\theta = 1$, we show that $X_{1,\rho}$ has a stretched exponential tail with stretching exponent $1/3$.

By superposing independent neutral mutations at each birth with fixed probability $1 - p \in (0,1)$ to the classical Yule process, the original Yule-Simon law with parameter $\rho = 1/p$ captures the limit number of species of a genetic type chosen uniformly at random among all types, upon letting time tend to infinity. This fact is essentially a rephrasing of Simon's results in [20]. We give some (historical) background in Sect. 5 and extend Simon's observations to more general branching processes, for which the two-parameter distribution from Definition 1.1 is observed.

In a similar vein, the number of species belonging to a genus chosen uniformly at random has been studied for generalized Yule models in several works by Lansky, Polito, Sacerdote and further co-authors, both at fixed times t and upon letting $t \to \infty$. For instance, in [12], the linear birth process governing the growth of species is replaced by a birth-and-death process, whereas in [13], a fractional nonlinear birth process is considered instead. Both works are formulated in the framework of World Wide Web modeling. Recently, Polito [17] changed also the dynamics of how different genera appear, leading to a considerably different limit behavior.

The rest of this article is organized as follows. In the following Sect. 2, we analyze the branching process Y_θ introduced above and study its large-time behavior. In Sect. 3, we develop an integral representation for the tail distribution of the two-parameter Yule-Simon law, which lies at the heart of our study of the tail asymptotics of $X_{\theta,\rho}$ in the subsequent Sect. 4. This part complements the work [1] and contains our main results. In the last Sect. 5, we relate the generalized Yule-Simon distribution to a population model with mutations, in the spirit of Simon's original work [20].

2 Preliminaries on the General Branching Process Y_θ

The purpose of this section is to gather some basic features about the general branching process Y_θ that has been described in the introduction. We start with a construction of Y_θ in terms of a certain branching random walk.

Specifically, we consider a sequence $\mathbf{Z} = (\mathbf{Z}_n)_{n \geq 0}$ of point processes on $[0, \infty)$ which is constructed recursively as follows. First, $\mathbf{Z}_0 = \delta_0$ is the Dirac point mass at 0, and for any $n \geq 0$, $\mathbf{Z}_{n+1}$ is obtained from $\mathbf{Z}_n$ by replacing each and every atom of $\mathbf{Z}_n$, say located at $z \geq 0$, by a random cloud of atoms $\{z + \omega_i^z\}_{i=1}^{N^z}$, where $\{\omega_i^z\}_{i=1}^{N^z}$ is the family of atoms of a Poisson point measure on $[0, \infty)$ with intensity $e^{-\theta t}dt$ and to different atoms z correspond independent such Poisson point measures. In

particular, each N^z has the Poisson distribution with parameter $1/\theta$ when $\theta > 0$, whereas $N^z = \infty$ a.s. when $\theta \leq 0$. If we now interpret $[0, \infty)$ as a set of times, the locations of atoms as birth-times of individuals, and consider the number of individuals born on the time-interval $[0, t]$,

$$Y_\theta(t) := \sum_{n=0}^{\infty} \mathbf{Z}_n([0, t]), \qquad t \geq 0,$$

then $Y_\theta = (Y_\theta(t))_{t \geq 0}$ is a version of the general branching process generalizing the standard Yule process that was discussed in the introduction.

We readily observe the following formula for the first moments:

Proposition 2.1 *One has for every $t \geq 0$:*

$$\mathbb{E}(Y_\theta(t)) = \begin{cases} (e^{(1-\theta)t} - \theta)/(1 - \theta) & if\ \theta \neq 1, \\ 1 + t & if\ \theta = 1. \end{cases}$$

Proof By definition, the intensity of the point process $\mathbf{Z}_1$ is $e^{-\theta t}\mathrm{d}t$, and by the branching property, the intensity of $\mathbf{Z}_n$ is the nth convolution product of the latter. Considering Laplace transforms, we see that for any $q > 1 - \theta$:

$$q \int_0^\infty \mathbb{E}\left(Y_\theta(t)\right) e^{-qt} \mathrm{d}t = q \int_0^\infty e^{-qt} \left(\sum_{n=0}^\infty \mathbb{E}\left(\mathbf{Z}_n([0, t])\right) \right) \mathrm{d}t$$

$$= \sum_{n=0}^\infty \mathbb{E}\left(\int_0^\infty e^{-qt} \mathbf{Z}_n(\mathrm{d}t) \right)$$

$$= \sum_{n=0}^\infty (\theta + q)^{-n}$$

$$= \frac{\theta + q}{\theta + q - 1}.$$

Inverting this Laplace transform yields our claim.   □

Remark 2.2 The calculation above shows that a two-parameter Yule-Simon variable $X_{\theta,\rho}$, as in Definition 1.1, is integrable if and only if $\theta + \rho > 1$, and in that case we have

$$\mathbb{E}(X_{\theta,\rho}) = \frac{\theta + \rho}{\theta + \rho - 1}.$$

Proposition 2.1 ensures the finiteness of the branching process Y_θ observed at any time. Further, it should be plain that the atoms of the branching random walk $\mathbf{Z}$ (at all generations) occupy different locations. Thus Y_θ is a counting process,

in the sense that its sample paths take values in $\mathbb{N}$, are non-decreasing and all its jumps have unit size. We next discuss its large time asymptotic behavior, and in this direction, we write

$$Y_\theta(\infty) = \lim_{t\to\infty} \uparrow Y_\theta(t) \in \bar{\mathbb{N}} := \mathbb{N} \cup \{\infty\}$$

for its terminal value.

Proposition 2.3

(i) *If $\theta > 0$, then $Y_\theta(\infty)$ has the Borel distribution with parameter $1/\theta$, viz.*

$$\mathbb{P}(Y_\theta(\infty) = n) = \frac{e^{-n/\theta}(n/\theta)^{n-1}}{n!} \qquad \text{for every } n \in \mathbb{N}.$$

In particular $\mathbb{P}(Y_\theta(\infty) < \infty) = 1$ if and only if $\theta \geq 1$.
(ii) *If $\theta < 1$, then*

$$\lim_{t\to\infty} e^{(\theta-1)t} Y_\theta(t) = W_\theta \qquad \text{in probability,}$$

where $W_\theta \geq 0$ is a random variable in $L^k(\mathbb{P})$ for any $k \geq 1$. Moreover, the events $\{W_\theta = 0\}$ and $\{Y_\theta(\infty) < \infty\}$ coincide a.s., and are both negligible (i.e. have probability 0) if $\theta \leq 0$.

Proof

(i) When $\theta > 0$, $(\mathbf{Z}_n([0,\infty)))_{n\geq 0}$ is a Galton-Watson process with reproduction law given by the Poisson distribution with parameter $1/\theta$. In particular, it is critical for $\theta = 1$, sub-critical for $\theta > 1$, and super-critical for $\theta < 1$. In this setting, $Y_\theta(\infty)$ is the total population generated by a single ancestor in this Galton-Watson process; since the reproduction law is Poisson, it is well-known that $Y_\theta(\infty)$ is distributed according to the Borel distribution with parameter $1/\theta$.
(ii) The claims follow by specializing to our setting well-known results on general branching processes. More precisely, the fact that $\int_0^\infty e^{-(1-\theta)t} e^{-\theta t} dt = 1$ shows that the so-called Malthus exponent of the general branching process Y_θ equals $1-\theta$. Then we just combine Theorem A of Doney [4], Theorem 1 of Bingham and Doney [2], and Theorem 3.1 in Nerman [15].   □

Finally, it will be convenient to also introduce

$$F_\theta(t) := \sum_{n=0}^{\infty} \int_0^t e^{-\theta(t-s)} \mathbf{Z}_n(ds), \qquad t \geq 0.$$

We call $F_\theta = (F_\theta(t))_{t\geq 0}$ the fertility process; it can be interpreted as follows. Recall that an atom, say at $s \geq 0$, of the branching random walk (at any generation n) is

viewed as the birth-time of an individual, and $t - s$ is thus its age at time $t \geq s$. The times at which this individual begets children form a Poisson point measure on $[s, \infty)$ with intensity $e^{-\theta(t-s)}dt$. Hence, $F_\theta(t)$ should be viewed as the total rate of birth (therefore the name fertility) at time t for the population model described by Y_θ.

Proposition 2.4 *The fertility process F_θ is a Markov process on $(0, \infty)$ with infinitesimal generator*

$$\mathcal{G}_\theta f(x) = -\theta x f'(x) + x(f(x+1) - f(x)),   \tag{2}$$

say for $f : (0, \infty) \to \mathbb{R}$ a bounded $\mathcal{C}^1$ function with bounded derivative f'.

Remark 2.5 Specialists will have recognized from (2) that the fertility F_θ is a so-called continuous state branching process; see [10] and Chapter 12 in [11] for background.

Proof The fertility process starts from $F_\theta(0) = 1$, takes values in $(0, \infty)$, decays exponentially with constant rate θ (by convention, exponential decay with rate $\theta < 0$ means exponential increase with rate $-\theta > 0$), and makes jumps of unit size corresponding to birth events at time t. That is, there is the identity

$$F_\theta(t) = Y_\theta(t) - \theta \int_0^t F_\theta(s)ds.   \tag{3}$$

The claim should now be intuitively obvious since $F_\theta(t)$ is also the rate at time t at which the counting process Y_θ has a jump of unit size.

To give a rigorous proof, we introduce the filtration $\mathcal{F}_t = \sigma(\mathbf{1}_{[0,t]}\mathbf{Z}_n : n \in \mathbb{N})$ for $t \geq 0$. Since the point measure $\mathbf{Z}_1$ is Poisson with intensity $e^{-\theta s}ds$, the process

$$\mathbf{Z}_1([0, t]) - \int_0^t e^{-\theta s}ds, \qquad t \geq 0$$

is an $(\mathcal{F}_t)$-martingale. By the branching property, we have more generally that for any $n \geq 0$,

$$\mathbf{Z}_{n+1}([0, t]) - \int_0^t \int_0^s e^{-\theta(s-r)}\mathbf{Z}_n(dr)ds, \qquad t \geq 0$$

is also an $(\mathcal{F}_t)$-martingale, and summing over all generations, we conclude that

$$Y_\theta(t) - \int_0^t F_\theta(s)ds \qquad \text{is an } (\mathcal{F}_t)\text{-martingale.}   \tag{4}$$

As Y_θ is a counting process, we deduce from (3) that for any bounded $\mathcal{C}^1$ function $f : (0, \infty) \to \mathbb{R}$ with bounded derivative, there is the identity

$$f(F_\theta(t)) - f(1) = -\theta \int_0^t F_\theta(s) f'(F_\theta(s)) \mathrm{d}s + \int_0^t (f(F_\theta(s-)+1) - f(F_\theta(s-)) \mathrm{d}Y_\theta(s).$$

We now see from (4) that

$$f(F_\theta(t)) - \int_0^t \mathcal{G}_\theta(F_\theta(s)) \mathrm{d}s \qquad \text{is an } (\mathcal{F}_t)\text{-martingale.}$$

It is readily checked that the martingale problem above is well-posed, and the statement follows; see Section 4.4 in [9] for background. □

We point out that for $f(x) = x$, we get $\mathcal{G}_\theta f = (1 - \theta)f$, and it follows that $\mathbb{E}(F_\theta(t)) = \mathrm{e}^{(1-\theta)t}$ for all $t \geq 0$. We then see from (3) that for $\theta \neq 1$,

$$\mathbb{E}(Y_\theta(t)) = \mathrm{e}^{(1-\theta)t} + \theta \int_0^t \mathrm{e}^{(1-\theta)s} \mathrm{d}s = \frac{1}{1-\theta}(\mathrm{e}^{(1-\theta)t} - \theta),$$

and that $\mathbb{E}(Y_1(t)) = 1 + t$ for $\theta = 1$, hence recovering Proposition 2.1.

3   Poissonian Representation for the Tail Distribution

The purpose of this section is to point at the following representation of the tail distribution of the two-parameter Yule-Simon distribution. We first introduce a standard Poisson process $N = (N(t))_{t \geq 0}$. We write

$$\gamma(n) := \inf\{t > 0 : N(t) = n\}$$

for every $n \in \mathbb{N}$ (so that $\gamma(n)$ has the Gamma distribution with parameters $(n, 1)$), and

$$\zeta_\theta := \inf\{t > 0 : N(t) + 1 - \theta t = 0\} \tag{5}$$

for $\theta \in \mathbb{R}$ (in particular $\zeta_\theta = \infty$ a.s. when $\theta \leq 0$).

Proposition 3.1 *Let $\theta \in \mathbb{R}$ and $\rho > 0$. For every $n \in \mathbb{N}$, one has*

$$\mathbb{P}(X_{\theta,\rho} > n) = \mathbb{E}\left(\exp\left(-\rho \int_0^{\gamma(n)} (N(t) + 1 - \theta t)^{-1} \mathrm{d}t\right) \mathbf{1}_{\gamma(n) < \zeta_\theta}\right).$$

This identity could be inferred from [1]; for the sake of completeness, we shall provide here an independent proof based on Proposition 2.4 and the identity (3).

Proof of Proposition 3.1 Observe from Proposition 2.4 that the infinitesimal generator $\mathcal{G}_\theta$ of the fertility process fulfills

$$x^{-1}\mathcal{G}_\theta f(x) = -\theta f'(x) + (f(x+1) - f(x)), \qquad x > 0,$$

and that the right-hand side is the infinitesimal generator of a standard Poisson process with drift $-\theta$ absorbed at 0. If we write

$$\xi_\theta(t) := N(t \wedge \zeta_\theta) + 1 - \theta(t \wedge \zeta_\theta) \qquad \text{for } t \geq 0,$$

so that the process ξ_θ is that described above and started from $\xi_\theta(0) = 1$, then by Volkonskii's formula (see e.g. Formula (21.6) of Section III.21 in [19]), the fertility can be expressed as a time-change of ξ_θ. Specifically, the map $t \mapsto \int_0^t \xi_\theta(s)^{-1}\mathrm{d}s$ is bijective from $[0, \zeta_\theta)$ to $\mathbb{R}_+$, and if we denote its inverse by σ_θ, then the processes F_θ and $\xi_\theta \circ \sigma_\theta$ have the same distribution; we can henceforth assume that they are actually identical.

In this setting, we can further identify $\sigma_\theta(t) = \int_0^t F_\theta(s)\mathrm{d}s$ and then deduce from (3) that $Y_\theta(t) = 1 + N(\sigma_\theta(t))$. As a consequence, if we write

$$\tau_\theta(n) := \inf\{t > 0 : Y_\theta(t) > n\},$$

then we have also

$$\tau_\theta(n) = \inf\{t > 0 : N \circ \sigma_\theta(t) = n\} = \begin{cases} \int_0^{\gamma(n)} \xi_\theta(s)^{-1}\mathrm{d}s & \text{if } \gamma(n) < \zeta_\theta, \\ \infty & \text{otherwise.} \end{cases}$$

Finally, recall from Definition 1.1 that T_ρ has the exponential distribution with parameter $\rho > 0$ and is independent of Y_θ, so

$$\mathbb{P}(X_{\theta,\rho} > n) = \mathbb{P}(Y_\theta(T_\rho) > n) = \mathbb{E}\left(\exp(-\rho\tau_\theta(n))\mathbf{1}_{\tau_\theta(n)<\infty}\right).$$

This completes the proof.   □

Remark 3.2 Following up Remark 2.5, the application of Volkonskii's formula in the proof above amounts to the well-known Lamperti's transformation that relates continuous state branching processes and Lévy processes without negative jumps via a time-change; see [3] for a complete account.

We conclude this section by pointing at a simple inequality between the tail distributions of Yule-Simon processes with different parameters.

Corollary 3.3

(i) *The random variable $X_{\theta,\rho}$ decreases stochastically in the parameters θ and ρ. That is, for every $\theta' \geq \theta$ and $\rho' \geq \rho > 0$, one has*

$$\mathbb{P}(X_{\theta',\rho'} > n) \leq \mathbb{P}(X_{\theta,\rho} > n) \qquad \text{for all } n \in \mathbb{N}.$$

(ii) *For every $\theta \in \mathbb{R}$, $\rho > 0$ and $a > 1$, one has*

$$\mathbb{P}(X_{\theta,\rho} > n)^a \leq \mathbb{P}(X_{\theta,a\rho} > n) \qquad \text{for all } n \in \mathbb{N}.$$

Proof

(i) It should be plain from the construction of the general branching process Y_θ in the preceding section, that for any $\theta \leq \theta'$, one can obtain $Y_{\theta'}$ from Y_θ by thinning (i.e. random killing of individuals and their descent). In particular Y_θ and $Y_{\theta'}$ can be coupled in such a way that $Y_\theta(t) \geq Y_{\theta'}(t)$ for all $t \geq 0$. Obviously, we may also couple T_ρ and $T_{\rho'}$ such that $T_\rho \geq T_{\rho'}$ (for instance by defining $T_{\rho'} = \frac{\rho}{\rho'} T_\rho$), and our claim follows from the fact that individuals are eternal in the population model. Alternatively, we can also deduce the claim by inspecting Proposition 3.1.
(ii) This follows immediately from Hölder's inequality and Proposition 3.1.

$\square$

4 Tail Asymptotic Behaviors

We now state the main results of this work which completes that of [1]. The asymptotic behavior of the tail distribution of a two parameter Yule-Simon distribution exhibits a phase transition between exponential and power decay for the critical parameter $\theta = 1$; here is the precise statement.

Theorem 4.1 *Let $\rho > 0$.*

(i) *If $\theta < 1$, then there exists a constant $C = C(\theta, \rho) \in (0, \infty)$ such that, as $n \to \infty$:*

$$\mathbb{P}(X_{\theta,\rho} > n) \sim Cn^{-\rho/(1-\theta)}.$$

(ii) *If $\theta > 1$, then as $n \to \infty$:*

$$\ln \mathbb{P}(X_{\theta,\rho} > n) \sim -(\ln \theta - 1 + 1/\theta)n.$$

This phase transition can be explained as follows. We rewrite Proposition 3.1 in the form

$$\mathbb{P}(X_{\theta,\rho} > n) = \mathbb{E}\left(\exp\left(-\rho \int_0^{\gamma(n)} (N(t) + 1 - \theta t)^{-1} dt \right) \mid \gamma(n) < \zeta_\theta \right) \times \mathbb{P}(\gamma(n) < \zeta_\theta).$$

On the one hand, the probability that $\gamma(n) < \zeta_\theta$ remains bounded away from 0 when $\theta < 1$ and decays exponentially fast when $\theta > 1$. On the other hand, for $\theta < 1$, the integral $\int_0^{\gamma(n)} (N(t) + 1 - \theta t)^{-1} dt$ is of order $\ln n$ on the event $\{\gamma(n) < \zeta_\theta\}$,

and therefore the first term in the product decays as a power of n when n tends to infinity. Last, when $\theta > 1$, the first term in the product decays sub-exponentially fast.

In the critical case $\theta = 1$, we observe from the combination of Theorem 4.1 and Corollary 3.3 that the tail of $X_{1,\rho}$ is neither fat nor light, in the sense that

$$\exp(-\alpha n) \ll \mathbb{P}(X_{1,\rho} > n) \ll n^{-\beta}$$

for all $\alpha, \beta > 0$. We obtain a more precise estimate of stretched exponential type. In the following statement, $f \lesssim g$ means $\limsup_{n\to\infty} f(n)/g(n) \leq 1$.

Theorem 4.2 *Consider the critical case $\theta = 1$, and let $\rho > 0$. Then we have as $n \to \infty$:*

$$-20(\rho^2 n)^{1/3} \lesssim \ln \mathbb{P}(X_{1,\rho} > n) \lesssim -(1/2)^{1/3}(\rho^2 n)^{1/3}.$$

Remark 4.3 Note that Theorems 4.1 and 4.2 entail that the series $\sum_{n\geq 0} \mathbb{P}(X_{\theta,\rho} > n)$ converges if and only if $\theta + \rho > 1$, in agreement with Remark 2.2.

The methods we use to prove Theorem 4.2 seem not to be fine enough to obtain the exact asymptotics of $n^{-1/3} \ln \mathbb{P}(X_{1,\rho} > n)$. More specifically, for the lower bound we employ estimates for first exits through moving boundaries proved by Portnoy [18] first for Brownian motion and then transferred via the KMT-embedding to general sums of independent random variables. The constant $c_1 = 20$ is an (rough) outcome of our proof and clearly not optimal.

For obtaining the upper bound, we consider an appropriate exponential martingale and apply optional stopping. The constant $c_2 = (1/2)^{1/3}$ provides the best value given our method, but is very likely not the optimal value neither.

Theorem 4.1(i) has been established in Theorem 1(ii) of [1] in the case $\theta \in (0, 1)$ and $\rho > 1-\theta$. Specifically, the parameters α and $\bar{p}$ there are such that, in the present notation, $\theta = \alpha/\bar{p}(\alpha + 1)$ and $\bar{p}(\alpha + 1) = 1/\rho$. Taking this into account, we see that the claim here extends Theorem 1(ii) in [1] to a larger set of parameters. The argument is essentially the same, relying now on Proposition 2.3(ii) here rather than on the less general Corollary 2 in [1], and we won't repeat it.

We next turn our attention to the proof of Theorem 4.1(ii), which partly relies on the following elementary result on first-passage times of Poisson processes with drift (we refer to [5–7] for related estimates in the setting of general random walks and Lévy processes).

Lemma 4.4 *Let $b > 1$, $x > 0$, and define $\nu(x) := \inf\{t > 0 : bt - N(t) > x\}$. The distribution of the integer-valued variable $b\nu(x) - x$ fulfills*

$$\mathbb{P}(b\nu(x) - x = n) = \frac{1}{n!}e^{-(x+n)/b}x(x + n)^{n-1}b^{-n} \sim \frac{xe^{x(1-1/b)}}{\sqrt{2\pi n^3}}e^{n(1-1/b-\ln b)} \qquad as \ n \to \infty.$$

As a consequence,

$$\lim_{t \to \infty} t^{-1} \ln \mathbb{P}(\nu(x) \geq t) = -(b \ln b - b + 1).$$

Proof The event $b\nu(x) = x$ holds if and only if the Poisson process N stays at 0 up to time x/b at least, which occurs with probability $e^{-x/b}$. The first identity in the statement is thus plain for $n = 0$. Next, note that, since the variable $b\nu(x) - x$ must take integer values whenever it is finite, there is the identity

$$b\nu(x) - x = \inf\{j \geq 0 : N((j + x)/b) = j\}.$$

On the event $N(x/b) = k \in \mathbb{N}$, set $N'(t) = N(t + x/b) - k$, and write

$$b\nu(x) - x = \inf\{j \in \mathbb{N} : N'(j/b) = j - k\}.$$

Since N' is again a standard Poisson process, Kemperman's formula (see, e.g. Equation (6.3) in [16]) applied to the random walk $N'(\cdot/b)$ gives for any $n \geq k$

$$\mathbb{P}(b\nu(x) - x = n \mid N(x/b) = k) = \frac{k}{n} \cdot \frac{e^{-n/b}(n/b)^{n-k}}{(n-k)!}.$$

Since $N(x/b)$ has the Poisson distribution with parameter x/b, this yields for any $n \geq 1$

$$\mathbb{P}(b\nu(x) - x = n) = e^{-(x+n)/b} \sum_{k=1}^{n} \frac{(x/b)^k}{k!} \cdot \frac{k}{n} \cdot \frac{(n/b)^{n-k}}{(n-k)!}$$

$$= \frac{1}{n!} e^{-(x+n)/b} (x/b) \sum_{k=1}^{n} (x/b)^{k-1} (n/b)^{n-k} \cdot \frac{(n-1)!}{(k-1)!(n-k)!}$$

$$= \frac{1}{n!} e^{-(x+n)/b} x(x+n)^{n-1} b^{-n},$$

where we used Newton's binomial formula at the third line. The second assertion in the claim follows from Stirling's formula, and the third one is a much weaker version.   □

We can now proceed to the proof of Theorem 4.1(ii).

Proof of Theorem 4.1(ii) The upper-bound is easy. Indeed on the one hand, Proposition 3.1 yields

$$\mathbb{P}(X_{\theta,\rho} > n) \leq \mathbb{P}(\gamma(n) < \zeta_\theta),$$

and on the other hand, since $N(\zeta_\theta) + 1 = \theta\zeta_\theta$, on the event $\{\gamma(n) < \zeta_\theta\}$, one has obviously $N(\zeta_\theta) \geq n$, and *a fortiori* $\theta\zeta_\theta > n$. Thus $\mathbb{P}(X_{\theta,\rho} > n)$ is bounded from above by $\mathbb{P}(\zeta_\theta > n/\theta)$, and we conclude from Lemma 4.4 specialized for $x = 1$ and $b = \theta$ that

$$\limsup_{n\to\infty} n^{-1} \ln \mathbb{P}(X_{\theta,\rho} > n) \leq -(\ln\theta - 1 + 1/\theta).$$

In order to establish a converse lower bound, let $\varepsilon \in (0, 1)$ be arbitrarily small, and consider the event

$$\Lambda(n, \theta, \varepsilon) := \{N(t) + 1 - \varepsilon - (\theta + \varepsilon)t \geq 0 \text{ for all } 0 \leq t \leq \gamma(n)\}.$$

On that event, one has $N(t) + 1 - \theta t \geq \varepsilon(1 + t)$ for all $0 \leq t \leq \gamma(n)$, and hence

$$\exp\left(-\rho \int_0^{\gamma(n)} (N(t) + 1 - \theta t)^{-1} dt\right) \geq (\gamma(n) + 1)^{-\rho/\varepsilon} \geq (n/(\theta + \varepsilon))^{-\rho/\varepsilon},$$

where for the second inequality, we used that $N(\gamma(n)) + 1 - \varepsilon \geq (\theta + \varepsilon)\gamma(n)$.

We are left with estimating $\mathbb{P}(\Lambda(n, \theta, \varepsilon))$. Set $b = \theta + \varepsilon$ and use the notation of Lemma 4.4, so that

$$\Lambda(n, \theta, \varepsilon) = \{\gamma(n) < \nu(1 - \varepsilon)\}.$$

On the event $\{b\nu(1 - \varepsilon) \geq n\}$, one has

$$N(\nu(1 - \varepsilon)) = b\nu(1 - \varepsilon) - 1 + \varepsilon \geq n + \varepsilon - 1,$$

so actually $\gamma(n) < \nu(1-\varepsilon)$. Hence $\{b\nu(1-\varepsilon) \geq n\} \subset \Lambda(n, \theta, \varepsilon)$, and we conclude from Lemma 4.4 that

$$\liminf_{n\to\infty} n^{-1} \ln \mathbb{P}(\Lambda(n, \theta, \varepsilon)) \geq 1 - \ln b - 1/b.$$

Putting the pieces together, we have shown that for any $b > \theta$

$$\liminf_{n\to\infty} n^{-1} \ln \mathbb{E}\left(\exp\left(-\rho \int_0^{\gamma(n)} (N(t) + 1 - \theta t)^{-1} dt\right) \mathbf{1}_{\gamma(n)<\zeta_\theta}\right) \geq 1 - \ln b - 1/b.$$

Thanks to Proposition 3.1, this completes the proof. $\square$

We next establish Theorem 4.2.

Proof of Theorem 4.2 We use the abbreviations $\xi(t) := N(t) + 1 - t$ and $\zeta := \zeta_1$, and start with the lower bound. We let $0 < \varepsilon < 1$. First note that there are the inclusions of events

$$\{\gamma(n) < \zeta\} \supset \{\gamma(n) < \min\{\zeta, (1 + \varepsilon)n\}\} \supset \{\xi(t) > 0 \text{ for all } 0 \leq t \leq (1 + \varepsilon)n, \ \gamma(n) < (1 + \varepsilon)n\}$$

$$\supset \{\xi(t) > \rho^{1/3}t^{2/3} \text{ for all } 0 < t \leq (1 + \varepsilon)n, \ \gamma(n) < (1 + \varepsilon)n\}.$$

In particular, with Proposition 3.1 at hand, we obtain for small ε and large n

$$\mathbb{P}(X_{1,\rho} > n) = \mathbb{E}\left(\exp\left(-\rho \int_0^{\gamma(n)} (\xi(t))^{-1}dt\right) \mathbf{1}_{\gamma(n) < \zeta}\right)$$

$$\geq \exp\left(-\rho \int_0^{(1+\varepsilon)n} \frac{1}{\rho^{1/3}t^{2/3}}dt\right) \mathbb{P}\big(\xi(t) > \rho^{1/3}t^{2/3} \text{ for all } 0 < t \leq (1 + \varepsilon)n, \ \gamma(n) < (1 + \varepsilon)n\big)$$

$$\geq \exp\left(-4(\rho^2 n)^{1/3}\right) \mathbb{P}\big(\xi(t) > \rho^{1/3}t^{2/3} \text{ for all } 0 < t \leq (1 + \varepsilon)n\big) - \mathbb{P}\left(\gamma(n) \geq (1 + \varepsilon)n\right),$$

where for the last line, we used that $\exp(-3(\rho^2(1 + \varepsilon)n)^{1/3}) \geq \exp(-4(\rho^2 n)^{1/3})$ for small ε, and that $\mathbb{P}(A \cap B) \geq \mathbb{P}(A) - \mathbb{P}(B^c)$ for arbitrary events A, B. From an elementary large deviation estimate for a sum of n independent standard exponentials, we know that for some $\lambda > 0$

$$\mathbb{P}\left(\gamma(n) \geq (1 + \varepsilon)n\right) = O(\exp(-\lambda \varepsilon^2 n)). \tag{6}$$

Therefore, our claim follows if we show a bound of the form

$$\mathbb{P}\left(\xi(t) > \rho^{1/3}t^{2/3} \text{ for all } 0 < t \leq (1 + \varepsilon)n\right) \geq \exp\left(-16(\rho^2 n)^{1/3}\right) \tag{7}$$

for large n. Essentially, this can be deduced from [18, Theorem 4.1]: In the notation from there, we may consider the random walk $S_j = N(j) - j$, $j \in \mathbb{N}$, and the function

$$g(t) := \frac{3}{2}\rho^{1/3}(t + \max\{\rho, 1\})^{2/3} - 2\max\{\rho, \rho^{1/3}\}, \quad t \geq 0.$$

The function g is monotone increasing with $g(0) < 0$ and regularly varying with index 2/3. Moreover, it is readily checked that

$$\sup_{t \geq 1}\left(g\big((2/3)t\big) - g\big((2/3)(t - 1)\big)\right) \leq 2/3.$$

Therefore, the assumptions of [18, Theorem 4.1] are fulfilled, which ensures after a small calculation that for ε sufficiently small and n large enough,

$$\mathbb{P}\left(S_j > g(j) \text{ for all } j = 1, \ldots, \lfloor(1+\varepsilon)n\rfloor\right) \geq \exp\left(-16(\rho^2 n)^{1/3}\right). \qquad (8)$$

Now let us define for $0 \leq t_0 < t_1$ the event

$$\mathcal{E}(t_0, t_1) := \left\{\xi(t) > \rho^{1/3} t^{2/3} \text{ for all } t_0 < t \leq t_1\right\}.$$

For $j \in \mathbb{N}$ and $t \in \mathbb{R}$ with $j \leq t \leq j + 1$, we have $\xi(t) \geq S_j$ and, provided $j \geq \rho_0 := 8\lceil\rho\rceil$, also

$$g(j) \geq \rho^{1/3}(j+1)^{2/3} \geq \rho^{1/3} t^{2/3}.$$

Therefore, by (8),

$$\mathbb{P}\left(\mathcal{E}(\rho_0, (1+\varepsilon)n)\right) \geq \mathbb{P}\left(S_j > g(j) \text{ for all } j = \rho_0, \ldots, \lfloor(1+\varepsilon)n\rfloor\right) \geq \exp\left(-16(\rho^2 n)^{1/3}\right).$$
$$(9)$$

Writing

$$\mathbb{P}\left(\mathcal{E}(0, (1+\varepsilon)n)\right) = \mathbb{P}\left(\mathcal{E}(\rho_0, (1+\varepsilon)n) \mid \mathcal{E}(0, \rho_0)\right) \cdot \mathbb{P}\left(\mathcal{E}(0, \rho_0)\right),$$

we note that $\mathbb{P}\left(\mathcal{E}(0, \rho_0)\right)$ is bounded from below by a strictly positive constant (depending on ρ). Moreover, since ξ is a spatially homogeneous Markov process, we clearly have

$$\mathbb{P}\left(\mathcal{E}(\rho_0, (1+\varepsilon)n) \mid \mathcal{E}(0, \rho_0)\right) \geq \mathbb{P}\left(\mathcal{E}(\rho_0, (1+\varepsilon)n)\right),$$

so that our claim (7) follows from (9). En passant, let us mention that $n^{1/3}$ is the correct stretch for the exponential in (7). Indeed, this can be seen from Theorem 4.2 in [18], where an analogous upper bound on the probability in (7) is given.

We now turn our attention to the upper bound. We fix a small $0 < \varepsilon < 1$. On the event

$$\left\{\gamma(n) \geq (1-\varepsilon)n \text{ and } \sup_{t \leq (1-\varepsilon)n} \xi(t) \leq (2\rho)^{1/3} n^{2/3}\right\},$$

we have

$$\exp\left(-\rho \int_0^{\gamma(n)} \xi(t)^{-1} dt\right) \leq \exp\left(-(1-\varepsilon)(\rho^2/2)^{1/3} n^{1/3}\right),$$

and from Proposition 3.1, $\mathbb{P}(X_{1,\rho} > n)$ can be bounded from above by

$$\exp\left(-(1-\varepsilon)(\rho^2/2)^{1/3}n^{1/3}\right) + \mathbb{P}(\gamma(n) < (1-\varepsilon)n) + \mathbb{P}(\sup_{t \leq (1-\varepsilon)n} \xi(t) > (2\rho)^{1/3}n^{2/3}).$$

On the one hand, from an elementary large deviation estimate similar to (6), we get that for some $\lambda > 0$:

$$\mathbb{P}(\gamma(n) < (1-\varepsilon)n) = \mathbb{P}(N((1-\varepsilon)n) \geq n) = O(\exp(-\lambda\varepsilon^2 n)).$$

On the other hand, ξ is a Lévy process with no negative jumps started from 1 such that

$$\mathbb{E}(\exp(q(\xi(t) - 1))) = \exp\left(t(e^q - 1 - q)\right), \qquad t \geq 0.$$

It follows classically that the process

$$\exp\left(q\xi(t) - t(e^q - 1 - q)\right), \qquad t \geq 0$$

is a martingale started from e^q. An application of the optional sampling theorem at the first passage time of ξ above $(2\rho)^{1/3}n^{2/3}$ yields the upper-bound

$$\exp\left(q(2\rho)^{1/3}n^{2/3} - (1-\varepsilon)n(e^q - 1 - q)\right)\mathbb{P}(\sup_{t \leq (1-\varepsilon)n} \xi(t) > (2\rho)^{1/3}n^{2/3}) \leq e^q.$$

Specializing this for $q = (2\rho)^{1/3}n^{-1/3}$, we deduce that for n large enough

$$\mathbb{P}(\sup_{t \leq (1-\varepsilon)n} \xi(t) > (2\rho)^{1/3}n^{2/3}) \leq \exp\left(-(1 + (\varepsilon/2))(\rho^2/2)^{1/3}n^{1/3}\right).$$

Since $\varepsilon > 0$ can be taken arbitrarily small, this completes the proof. $\qquad\square$

5 Connection with a Population Model with Neutral Mutations

The Yule-Simon distribution originates from [20], where Simon introduced a simple random algorithm to exemplify the appearance of (1) in various statistical models. More specifically, he proposed a probabilistic model for describing observed linguistic (but also economic and biological) data leading to (1).

We shall now give some details of Simon's model, which he described in terms of word frequencies. Imagine a book that is being written has reached a length of

n words. Write $f(k, n)$ for the number of different words which occurred exactly k times in the first n words. Simon works under the following two assumptions:

A1 The probability that the $(n + 1)$-st word is a word that has already appeared exactly k times is proportional to $kf(k, n)$;
A2 The probability that the $(n + 1)$-st word is a new word is a constant α independent of n.

Setting

$$\rho = \frac{1}{1 - \alpha}, \tag{10}$$

he argues that under these two assumptions, the relative frequencies of words that have occurred exactly k times are in the limit $n \to \infty$ described by a Yule-Simon law (1) with parameter ρ.

Simon's paper initiated a lively dispute between Simon and Mandelbrot (known as the Simon-Mandelbrot debate) on the validity and practical relevance of Simon's model. We mention only Mandelbrot's reply [14] and Simon's response [21], but the discussions includes further (final) notes and post scripta. While Simon's derivation presupposes $\rho > 1$, see (10), the discussion between the two gentlemen evolved in particular around the adequacy and meaning of Simon's model when $0 < \rho < 1$; see pp. 95–96 in [14].

It is one of the purposes of this section to specify a probabilistic population model for which the Yule-Simon law is observed in all cases $\rho > 0$. To that aim, it is convenient to first recast Simon's model in terms of random recursive forests, and then interpret the latter as a population model with neutral mutations. By letting the rate of mutation asymptotically decrease to zero in an appropriate way, we will then obtain the whole family of one-parameter Yule-Simon laws.

However, we will go further: A natural generalization of Simon's algorithm, which we formulate in terms of a more general population model with age-dependent reproduction rate, will finally result in the two-parameter Yule-Simon laws (Proposition 5.1).

5.1 Simon's Model in Terms of Yule Processes with Mutations

Fix $p \in (0, 1)$, take $n \gg 1$ and view $[n] := \{1, \ldots, n\}$ as a set of vertices. We equip every vertex $2 \leq \ell \leq n$ with a pair of variables $(\varepsilon(\ell), u(\ell))$, independently of the other vertices. Specifically, each $\varepsilon(\ell)$ is a Bernoulli variable with parameter p, i.e. $\mathbb{P}(\varepsilon(\ell) = 1) = 1 - \mathbb{P}(\varepsilon(\ell) = 0) = p$, and $u(\ell)$ is independent of $\varepsilon(\ell)$ and has the uniform distribution on $[\ell - 1]$. Simon's algorithm amounts to creating an edge between ℓ and $u(\ell)$ if and only if $\varepsilon(\ell) = 1$. The resulting random graph is a random forest and yields a partition of $[n]$ into random sub-trees. In this setting, Simon showed that for every $k \geq 1$, the proportion of trees of size k, i.e. the ratio

between the number of sub-trees of size k and the total number of sub-trees in the random forest, converges on average as $n \to \infty$ to $\rho B(k, \rho + 1)$, where $\rho = 1/p$.

Let us next enlighten the connection with a standard Yule process $Y = Y_0$. We start by enumerating the individuals of the population model described by the Yule process in the increasing order of their birth dates (so the ancestor is the vertex 1, its first child the vertex 2, ...), and stop the process at time

$$T(n) := \inf\{t \geq 0 : Y(t) = n\}$$

when the population has reached size n. Clearly, the parent $u(\ell)$ of an individual $2 \leq \ell \leq n$ has the uniform distribution on $[\ell-1]$, independently of the other individuals. The genealogical tree obtained by creating edges between parents and their children is known as a random recursive tree of size n; see e.g. [8]. Next imagine that neutral mutations are superposed to the genealogical structure, so that each child is either a clone of its parent or a mutant with a new genetic type, and more precisely, the individual ℓ is a mutant if and only if $\varepsilon(\ell) = 0$, where $(\varepsilon(\ell))_{\ell \geq 2}$ is a sequence of i.i.d. Bernoulli variables with parameter p, independent of the sequence $(u(\ell))_{\ell \geq 2}$. The partition of the population into sub-populations of the same genetic type, often referred to as the allelic partition, corresponds to an independent Bernoulli bond percolation with parameter p on the genealogical tree, that is, it amounts to deleting each edge with probability $1 - p$, independently of the other edges. The resulting forest has the same distribution as that obtained from Simon's algorithm.

Simon's result can then be re-interpreted by stating that the distribution of the size of a typical sub-tree after percolation (i.e. the number of individuals having the same genetic type as a mutant picked uniformly at random amongst all mutants) converges as $n \to \infty$ to the Yule-Simon distribution with parameter $\rho = 1/p$. This can be established as follows. Observe first that a typical mutant is born at time $T(\lfloor Un \rfloor)$, where U is an independent uniform variable on $[0, 1]$. By the branching property, a typical sub-tree can thus be viewed as the genealogical tree of a Yule process with birth rate p per individual (recall that p is the probability for a child to be a clone of its parent), stopped at time $T(n) - T(\lfloor Un \rfloor)$. Then recall that

$$\lim_{t \to \infty} e^{-t} Y(t) = W \qquad \text{a.s.,}$$

where $W > 0$ is some random variable, and hence

$$T(n) - T(\lfloor Un \rfloor) \sim \ln(n/W) - \ln(Un/W) = -\ln U \qquad \text{as } n \to \infty.$$

Since a Yule process with birth rate p per individual and taken at time $t \geq 0$ has the geometric distribution with parameter e^{-pt}, and $-p \ln U$ has the exponential distribution with parameter $\rho = 1/p$, we conclude that the distribution of the size of a typical sub-tree after percolation converges as $n \to \infty$ to (1).

In the following section, we shall generalize Simon's algorithm in two different directions.

5.2   A Generalization of Simon's Model

The random algorithm described above only yields Yule-Simon distributions with parameter $\rho > 1$. A modification dealing with the case $\rho \leq 1$ has already been suggested in Simon's article, see Case II on page 431 in [20]; let us now elaborate on this more specifically.

The Full Range of the One-Parameter Yule-Simon Law

Let us now assume that the $\varepsilon(\ell)$ are independent Bernoulli variables with parameter $p = p(\ell)$ depending possibly on ℓ, again everything independent of the $u(\ell)$'s. As previously, the individuals ℓ such that $\varepsilon(\ell) = 0$ are viewed as mutants, and those with $\varepsilon(\ell) = 1$ as clones.

We shall consider two mutually exclusive asymptotic regimes:

(a) $\lim_{n \to \infty} p(n) = 1/\rho$ for some $\rho > 1$,
(b) $\lim_{n \to \infty} p(n) = 1$, and $\sum_{\ell=1}^{n} (1 - p(\ell))$ is regularly varying with index $\rho \in (0, 1]$.

Plainly, case (a) holds in particular when the $\varepsilon(\ell)$'s form an i.i.d. sequence of Bernoulli variables with parameter $p = 1/\rho$ as in the preceding section. Regime (b) is a situation where mutations are asymptotically rare. In terms of the number of mutants $m(n) = n - \sum_{\ell=2}^{n} \varepsilon(\ell)$, (b) is implying that, in probability, $m(n) = o(n)$, and $m(n)$ is regularly varying with index ρ.

Just as before, we consider the allelic partition at time $T(n)$, i.e. the partition of the population into sub-population bearing the same genetic type. As we shall see in the following Proposition 5.1, this population model leads under the two different regimes to the full range of the one-parameter Yule-Simon law when studying the limit size of a typical sub-population.

A Two-Parameter Generalization

It remains to appropriately extend the model in order to encompass the two-parameter Yule-Simon distributions. To that aim, we replace the underlying standard Yule process $Y = Y_0$ by a general branching process Y_θ as considered in the introduction. Again, we consider independently a sequence $(\varepsilon(\ell))_{\ell \geq 2}$ of $\{0, 1\}$-valued random variables indicating which individuals are clones or mutants, respectively, and exactly as before, we may study the allelic partition at the time

$$T_\theta(n) = \inf\{t \geq 0 : Y_\theta(t) = n\} \tag{11}$$

when the total population size n is reached. We stress that the case $\theta = 0$ corresponds to the one-parameter model described just above: We have $Y_0 = Y$, and consequently $T_0(n) = T(n)$.

We are now in position to formulate a limit result for the proportion of sub-populations of size k in our extended model, generalizing Simon's result to the two-parameter Yule-Simon distributions. For the sake of simplicity, we focus on the case $\theta \leq 0$ when the total population in the general branching process Y_θ is infinite almost surely.

Proposition 5.1 *Let $\theta \leq 0$ and $\rho > 0$, consider a general branching process Y_θ as in Sect. 2, and define $T_\theta(n)$ as in (11). Let further $(\varepsilon(\ell))_{\ell \geq 2}$ be a sequence of variables in $\{0, 1\}$ which is independent of the branching process and fulfills one of the regimes (a) or (b). Regard every individual ℓ with $\varepsilon(\ell) = 0$ as a mutant, and consider at time $T_\theta(n)$ the (allelic) partition of the whole population into sub-populations of individuals with the same genetic type.*

For every $k \in \mathbb{N}$, write $Q_n(k)$ for the proportion of sub-populations of size k (i.e. the number of such sub-populations divided by the total number of mutants) in the allelic partition at time $T_\theta(n)$. Then

$$\lim_{n \to \infty} Q_n(k) = \mathbb{P}(X_{\vartheta,\varrho} = k) \qquad \text{in probability,}$$

where

$$(\vartheta, \varrho) = \begin{cases} (\theta\rho, (1-\theta)\rho) & \text{in regime (a),} \\ (\theta, (1-\theta)\rho) & \text{in regime (b).} \end{cases}$$

Remark 5.2 We stress that our model leads to the complete range of parameters (ϑ, ϱ) of the Yule-Simon distribution satisfying $\vartheta \leq 0$ and $\varrho > 0$. Indeed, if $\vartheta + \varrho > 1$, then the size of a typical sub-tree converges in law with the choices $\theta := \vartheta/(\vartheta + \varrho)$ and $\rho := \vartheta + \varrho$ under regime (a) to $X_{\vartheta,\varrho}$. If $\vartheta + \varrho \leq 1$, then $\theta := \vartheta$ and $\rho := \varrho/(1 - \vartheta)$ under regime (b) yield the law $X_{\vartheta,\varrho}$.

Remark 5.3 The conditional expectation of the size of a typical sub-tree given that there are $m(n)$ mutants in the population of total size n is clearly $n/m(n)$. Note that $m(n) \sim (1 - 1/\rho)n$ in regime (a), whereas $m(n) = o(n)$ in regime (b). We may thus expect from Proposition 5.1 that

$$\mathbb{E}(X_{\theta\rho,(1-\theta)\rho}) = \rho/(\rho - 1) \qquad \text{when } \theta \leq 0 \text{ and } \rho > 1,$$

and that

$$\mathbb{E}(X_{\theta,(1-\theta)\rho}) = \infty \qquad \text{when } \theta \leq 0 \text{and } \rho \leq 1.$$

That these identities indeed hold has already been observed in Remark 2.2.

We now present the main steps of the proof of Proposition 5.1, leaving some of the technical details to the interested readers. We start with an elementary observation in the case constant mutation rates.

Lemma 5.4 *Suppose that $p(n) \equiv 1/\rho$ for some fixed $\rho > 1$. The process $\tilde{Y}_{\theta,\rho} = (\tilde{Y}_{\theta,\rho}(t))_{t\geq 0}$ of the size of the sub-population bearing the same type as the ancestor has then the same distribution as $(Y_{\theta\rho}(t/\rho))_{t\geq 0}$.*

Proof Since $\tilde{Y}_{\theta,\rho}$ is obtained from Y_θ by killing each of its child (of course, together with its descent) with probability $1 - 1/\rho$ and independently of the others, $\tilde{Y}_{\theta,\rho}$ is also a general branching process. More precisely, thanks to the thinning property of Poisson random measures, typical individuals in $\tilde{Y}_{\theta,\rho}$ reproduce at ages according to a Poisson point measure on $[0, \infty)$ with intensity $\rho^{-1}e^{-\theta t}dt$, and the statement follows from the change of variables $s = t/\rho$. □

We next return to the general situation where mutation rates $p(n)$ may depend on n, and state two technical lemmas involving convergence in distribution in $D([0, \infty), \mathbb{R}) \times D([0, \infty), \mathbb{R})$, where $D([0, \infty), \mathbb{R})$ is the Skorokhod space of càdlàg functions from $[0, \infty)$ to $\mathbb{R}$.

Lemma 5.5 *Suppose $\sum_{n\geq 1} p(n) = \infty$, so there are infinitely many mutants a.s. Let $i, j \geq 1$, and let $Y_\theta^i = (Y_\theta^i(t))_{t\geq 0}$ denote the process of the size of the sub-population (both clones and mutants descents) generated by the ith mutant as a function of its age. Then $Y_\theta^i \overset{(d)}{=} Y_\theta^j \overset{(d)}{=} Y_\theta$, and for $i, j \to \infty, i \neq j$,*

$$\left(Y_\theta^i, Y_\theta^j\right) \overset{(d)}{\Longrightarrow} \left(Y_\theta', Y_\theta''\right),$$

where Y_θ' and Y_θ'' are independent copies of Y_θ.

Proof This is an immediate consequence of the branching property of Y_θ, noting that the probability that the individuals labelled i and j are in the same sub-population tends to zero for $i \neq j \to \infty$. □

Lemma 5.6 *Let $i, j \geq 1$, and let $\tilde{Y}_\theta^i$ denote the process of the size of the clonal sub-population generated by the ith mutant (i.e. $\tilde{Y}_\theta^i(t)$ is the size of the sub-population bearing the same genetic type as the ith mutant when the latter has age t). Then $\tilde{Y}_\theta^i \overset{(d)}{=} \tilde{Y}_\theta^j$, and we have the following convergence for $i, j \to \infty, i \neq j$:*

$$\left(\tilde{Y}_\theta^i, \tilde{Y}_\theta^j\right) \overset{(d)}{\Longrightarrow} \begin{cases} \left(\tilde{Y}_{\theta,\rho}', \tilde{Y}_{\theta,\rho}''\right) & \text{in regime (a)}, \\ (Y_\theta', Y_\theta'') & \text{in regime (b)}, \end{cases}$$

where $\tilde{Y}_{\theta,\rho}', \tilde{Y}_{\theta,\rho}''$ are independent copies of the process $\tilde{Y}_{\theta,\rho}$ in Lemma 5.4, and Y_θ', Y_θ'' are independent copies of Y_θ.

Proof Recall that $\tilde{Y}_\theta^i$ is obtained from Y_θ^i by superposing neutral mutations to the latter and keeping only the clones of i. Since the nth individual is a mutant with probability $1 - p(n)$, the claim now follows readily from Lemma 5.5 and the fact that $p(n) \to 1/\rho$ in regime (a), whereas $p(n) \to 1$ in regime (b). $\qquad\square$

We now have all the ingredients needed for the proof of Proposition 5.1.

Proof of Proposition 5.1 We will argue that

$$\lim_{n\to\infty} \mathbb{E}\left(Q_n^i(k)\right) = \mathbb{P}(X_{\vartheta,\varrho} = k)^i \quad \text{for } i = 1, 2.$$

The claim then follows via the second moment method.

As before, let us write $m(n)$ for the number of mutants among the first n individuals, i.e. at time $T_\theta(n)$. Writing b_i for the birth-time of the ith mutant (with $b_1 := 0$, interpreting the first individual as a mutant), we have

$$\mathbb{E}\left(Q_n(k)\right) = \mathbb{E}\left(\frac{1}{m(n)} \sum_{i=1}^{m(n)} \mathbb{1}_{\left\{\tilde{Y}_\theta^i(T_\theta(n) - b_i) = k\right\}}\right).$$

We will first prove convergence of the first moment of $Q_n(k)$. From Proposition 2.3 we deduce that the time $T_\theta(n)$ at which the population reaches size n satisfies

$$T_\theta(n) = (1 - \theta)^{-1} \ln(n/W_\theta) + o(1) \tag{12}$$

in probability, where $W_\theta > 0$ denotes the limit in probability of $e^{(\theta-1)t} Y_\theta(t)$ as $t \to \infty$.

Let us first consider regime (a), where $p(n) \to 1/\rho$ as $n \to \infty$. For i tending to infinity, it follows that

$$b_i = (1 - \theta)^{-1} \ln\left(i/((1 - 1/\rho)W_\theta)\right) + o(1)$$

in probability. By the law of large numbers, we have for the number of mutants that $m(n) \sim (1 - 1/\rho)n$ almost surely. Combining the last display with (12) and Lemma 5.6, we deduce by a Riemann-type approximation that

$$\lim_{n\to\infty} \mathbb{E}\left(Q_n(k)\right) = \mathbb{P}\left(\tilde{Y}_{\theta,\rho}\left(-(1 - \theta)^{-1} \ln U\right) = k\right)$$

for $n \to \infty$, where U is an independent uniform variable on $(0, 1)$.

Note that the random variable $-(1 - \theta)^{-1} \ln U$ inside the last probability has the law of an exponentially distributed random variable $T_{1-\theta}$ with parameter $1 - \theta$. Now, thanks to Lemma 5.4,

$$\mathbb{P}\left(\tilde{Y}_{\theta,\rho}\left(T_{1-\theta}\right) = k\right) = \mathbb{P}\left(Y_{\theta\rho}\left(T_{1-\theta}/\rho\right) = k\right) = \mathbb{P}(X_{\theta\rho,(1-\theta)\rho} = k),$$

where for the last equality, we used that $T_{1-\theta}/\rho$ is exponentially distributed with parameter $(1 - \theta)\rho$.

In regime (b), mutations become asymptotically rare, i.e. $p(n) \to 1$ for $n \to \infty$, and the number of mutants $m(n)$ is regularly varying with index $\rho \in (0, 1]$. Now, if $i = i(n) = \lfloor r^\rho m(n) \rfloor$ for some $r \in (0, 1)$, it follows that the ith mutant is born when there are approximately rn individuals in the population system. Therefore, in probability as $n \to \infty$,

$$b_i \sim (1 - \theta)^{-1} \ln (rn/W_\theta) + o(1).$$

A approximation similar to that in regime (a) then allows us to deduce that

$$\lim_{n \to \infty} \mathbb{E}\left(Q_n(k)\right) = \mathbb{P}\left(Y_\theta \left(-(1 - \theta)^{-1}(1/\rho) \ln U\right) = k\right).$$

Since $-(1 - \theta)^{-1}(1/\rho) \ln U$ is exponentially distributed with parameter $(1 - \theta)\rho$, the last expressions is equal to $\mathbb{P}(X_{\rho,(1-\theta)\rho} = k)$.

As far as the second moment is concerned, it is a consequence of the asymptotic independence derived in Lemma 5.6 that

$$\mathbb{E}\left(Q_n^2(k)\right) \sim \mathbb{E}\left(Q_n(k)\right)^2$$

as $n \to \infty$, proving our claim in both regimes (a) and (b).   □

We shall now conclude this work by presenting an alternative proof of Proposition 5.1 in the special (and important) case when $p(n) \equiv 1/\rho$ for some fixed $\rho > 1$, by making the connection with results of Nerman [15]. We thus consider the general branching process Y_θ, where each child is a clone of its parent with fixed probability $1/\rho$, or a mutant bearing a new genetic type with complementary probability $1 - 1/\rho$, independently of the other individuals. We regard this population model as a branching particle system, in which the particles represent the clonal sub-populations. This means that the birth of a mutant child in the population is viewed as the birth of a new particle in the system; the size of the latter then grows as time passes and is given by the size of the sub-population having the same genetic type as this mutant.

The process of the size of a typical particle as a function of the age of the mutant ancestor has the same distribution as the process $\tilde{Y}_{\theta,\rho}$ in Lemma 5.4. Moreover, each particle also gives birth as time passes to daughter particles (i.e. to new mutants) which in turn evolve independently one from the others and according to the same dynamics. In words, the particle system is another general branching process.

Observe that the rate at which a particle with size ℓ gives birth to a daughter particle equals $(1 - 1/\rho)\ell$; hence the reproduction intensity measure $\tilde{\mu}$ of branching particle system is given by

$$\tilde{\mu}(\mathrm{d}t) = (1 - 1/\rho)\mathbb{E}(\tilde{Y}_{\theta,\rho}(t))\mathrm{d}t.$$

So Proposition 2.1 and Lemma 5.4 yield

$$\tilde{\mu}(\mathrm{d}t) = \frac{1 - 1/\rho}{1 - \theta\rho} \left(\mathrm{e}^{(1-\theta\rho)t/\rho} - \theta\rho \right) \mathrm{d}t.$$

It is now readily checked that the so-called Malthusian parameter (see Equation (1.4) in [15]) of the branching particle system equals $1 - \theta$, namely we have

$$\int_0^\infty \mathrm{e}^{-(1-\theta)t} \tilde{\mu}(\mathrm{d}t) = 1.$$

Finally, let us write Z_t for the number of particles (i.e. of genetic types) at time t. For any $k \geq 1$, write Z_t^k for the number of particles with size k at time t, i.e. the number of sub-populations with size exactly k in the allelic partition at time t. According to Theorem 6.3 and Equation (2.7) in [15] (the reader will easily check that the assumptions there are fulfilled in our framework), one has

$$\lim_{t\to\infty} \frac{Z_t^k}{Z_t} = (1 - \theta) \int_0^\infty \mathrm{e}^{-(1-\theta)t} \mathbb{P}(\tilde{Y}_{\theta,\rho}(t) = k)\mathrm{d}t, \qquad \text{almost surely.}$$

Recalling Lemma 5.4, we have thus

$$\lim_{t\to\infty} \frac{Z_t^k}{Z_t} = \mathbb{P}(Y_{\theta\rho}(T_{(1-\theta)\rho}) = k) = \mathbb{P}(X_{\theta\rho,(1-\theta)\rho} = k), \qquad \text{almost surely.}$$

It only remains to observe that for $t = T_\theta(n)$, one has $Z_t^k/Z_t = Q_n(k)$, and we thus have arrived at the claim made in Proposition 5.1.

Finally, we point out that the argument above also applies for $\theta \in (0, 1)$, provided that one works conditionally on the event that the total number of mutants is infinite, which has then a positive probability.

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