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Expansion of error thresholds for the Moran model

Maxime Berger *

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Abstract

We propose new definitions for the error threshold of a population evolving through mutation and selection. We compute the correction term due to the finiteness of the population by estimating the lifetime of master sequences. Our technique consists in bounding from above and below the number of master sequences in the Moran model, by birth and death chains. The expectation of this lifetime is then computed with the help of explicit formulas which are in turn expanded with Laplace method. The first term after $\ln \sigma/\ell$ is computed, it depends on the chosen criterion.

keywords: Markov chain, phase transition, genetics

Mathematics Subject Classification: 60J10, 92D10

1 Introduction

1.1 Context

Evolution is a macroscopic phenomenon that relies on two microscopic forces: mutation and selection. Of course the phenomenon is very complex and other factors (drift, migration, ...) play key roles in evolution, see for example [9]. However, we are going to focus here on mutation and selection only, this paradigm has long been studied in mathematical biology, going back to Haldane, Fisher and Wright in the 20s, see [2] for a review of the subject. In the 70s, Manfred Eigen [7] derived a special case of the mutation-selection model, discussed in [5], choosing a mutation term adapted to the evolution of macromolecules. Under his scheme, individuals are defined by long chains of zeroes and ones coding for their genome, and mutations act independently on each bit during reproduction events. Among them, only one genotype ($0 \cdots 0$ for example) has a fitness different from 1: the master

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sequence. He studied the repartition of the population after a long time and proved the existence of a phase transition. If the parameter governing the mutation rate is above a certain error threshold q^* , the population becomes completely random and all the genetic information is lost, if it is below q^* , a positive concentration of the population retains the fittest genotype. Let ℓ be the length of the genome of the macromolecules, and q the probability for mutation per site, so that the product ℓq represents the average number of mutations for each reproduction event. Eigen computed the error threshold q^* in a model with an infinite number of macromolecules, in an asymptotic regime where

$$\ell \rightarrow \infty, \quad q \rightarrow 0,$$

and he obtained

$$q^* \sim \frac{\ln \sigma}{\ell},$$

where $\sigma > 1$ stands for the fitness of the master sequence, all the other sequences having fitness 1. This fitness landscape is known as the sharp-peak landscape, it is commonly used in population genetics, mainly because computations are easier, but it is also a plausible framework: in real life, most mutations do not modify the fitness, see [2], section 4.2. The present work is also done within this framework.

The error threshold q^* is obtained from looking at a central quantity in the model: the average proportion of master sequences in the population. This proportion r_0 is equivalent in the asymptotic regime to

$$r_0 \sim \frac{\sigma(1-q)^\ell - 1}{\sigma - 1}.$$

This quantity is sufficient to obtain the error threshold of $\ln \sigma / \ell$, indeed, if q is asymptotically greater than q^* , then r_0 goes to zero, otherwise r_0 is strictly positive.

1.2 Motivation and the model

However, real populations are not infinite and it is necessary to study models with a finite population. Of course, for finite parameters of the model, error thresholds are not well defined, and it is only in asymptotic regimes that we can see a critical value. Beside the article of Nowak and Schuster, that we will discuss later, there exists works that tried to describe the correction term in the expansion of the error threshold due to the finite population size [1], [3] but they mainly rely on computer simulations. Our goal in this text is to give theoretical formulas for this correction term. We study the Moran model [13], introduced in the 50s, which has been shown to

converge to Eigen's model by Dalmau [6] with an argument of Kurtz [12]. This model is very classical and referenced in many textbooks such as [10]. This convergence allows us to derive results on the quasispecies model by working within the population genetics framework. As Wilke argued in [19], this is a sensible strategy and it is supported by numerous simulations. Understanding the scaling with the size of the population in the quasispecies model is a key to many applications like optimizing the performance of genetic algorithms [16] or finding ways to eradicate a population of viruses by increasing their mutation rate [18]. Let us first describe the model.

We consider a population of m individuals whose genetic material is coded with a string of ℓ characters chosen in $\{0, \dots, \kappa - 1\}$. All of the κ^ℓ genotypes have fitness equal to 1 except one sequence, say $0 \dots 0$, which has fitness equal to σ , with $\sigma > 1$. The sequence $0 \dots 0$ is called the master sequence. In this model, the time t is discrete, at time $t = 0$, the population starts with one master sequence, the other $m - 1$ individuals are randomly chosen. At time $n + 1$, one individual is chosen from generation n to be a parent, but master sequences have a selective advantage: they are σ times more likely chosen, thus they have better chances to leave more offspring, all the other sequences being equally likely to be chosen. The chosen individual is replicated, yet the replication process is error prone, due to mutations, each bit of its genome is changed independently with probability q into one of the other $\kappa - 1$ letters. The generation $n + 1$ is formed with the new individual and all the individuals from generation n , except one chosen uniformly at random, which is removed. In particular, the size of the population stays constant equal to m . This process is repeated indefinitely.

In a proper asymptotic regime, the Moran model, like the Eigen model, presents a phase transition separating a regime of chaos from a regime where master sequences occupy a non negligible proportion of the population. However, the mathematical definition of the critical parameter is delicate and several choices are possible. Let us look more closely at the dynamics.

We define N_t as the number of master sequences in the population. The population starts with one master sequence, selection plays its part and helps keeping master sequences in the population. This phase is called the **quasispecies phase**, the master sequences occupy a significant proportion of the population, along with a cloud of mutants consisting of individuals that are genetically close to the master sequence. At some point, due to random fluctuations, master sequences disappear, we define this moment as the **persistence time** τ_0 :

$$\tau_0 = \inf \left\{ t \in \mathbb{N} \mid N_t = 0 \right\}.$$

At time $t = \tau_0$, the population enters a new phase: the **neutral phase**. New

genotypes are discovered without changing the global fitness, and selection plays no role. This phase lasts for a certain number of generations that we call the **discovery time**:

$$\tau^* = \inf \left\{ t \geq \tau_0 \mid N_t \neq 0 \right\}.$$

At some point, a random mutation will discover a master sequence and the story will repeat. At time τ^* , we have $N_{\tau^*} = 1$ and we enter a new quasispecies phase, the model is thus $\tau_0 + \tau^*$ -periodic. What will complicate things is that the process (N_t) is not a Markov chain, since the complete repartition of the population is needed in order to compute its transition probabilities. This dynamics admits the same critical point $q^* = \ln \sigma / \ell$, indeed, in the quasispecies phase, the average proportion of master sequences is also equivalent to r_0 , for the same expression of r_0 ,

$$r_0 = \frac{\sigma(1 - q)^\ell - 1}{\sigma - 1}.$$

The parameter for mutation q has a great impact on this dynamics. Increasing the mutation rate reduces the stability of the quasispecies phase because offspring of master sequences are then less likely to be master sequences, however the stability of the neutral phase is barely changed. The comparison between the stability of both phases will yield different criteria for error thresholds.

1.3 Main results

Our main goal here is to estimate the expectation of the time τ_0 . This quantity is interesting in itself as the last sentence of [8] states: estimates on the lifetime of the metastable quasispecies is crucial to understand the Eigen model.

We work with a joint convergence of the parameters in the following asymptotic regime:

$$m \rightarrow \infty, \quad \ell \rightarrow \infty, \quad q \rightarrow 0. \quad (1)$$

We place ourselves in the critical parameter limit

$$\ell q \rightarrow \ln \sigma. \quad (2)$$

We are interested in the critical exponents when $r_0 \rightarrow 0$ with $r_0 > 0$. This quantity is equivalent, in the asymptotic regime, to the average proportion of master sequences in the quasispecies phase. The speed at which r_0 goes to zero is directly related to the term after $\ln \sigma / \ell$ in the asymptotic expansion of q^* .

The estimation on the expectation of the persistence time is stated in Theorem 1, it requires very few hypothesis on the asymptotic behaviour of the parameters ℓ , m and q , contrary to the discussion that follows, which deals with the definition of the error threshold.

Theorem 1. *In the asymptotic regime (1) with condition (2), the persistence time admits the expansion*

$$E(\tau_0) = \exp \left(\frac{\sigma - 1}{2} m r_0^2 + O \left((1 + m q) \ln m + m r_0^3 + \frac{m q^2}{\sigma - 2 + r_0} \right) \right),$$

where

$$r_0 = \frac{\sigma(1 - q)^\ell - 1}{\sigma - 1}.$$

The proof of this theorem will consist in performing the computations for two simpler models: one underestimating the number of master sequences, and another one overestimating it.

In the next section, we will see that the asymptotic expansion of the error threshold depends largely on the choice of the relative sizes of the parameters ℓ and m . However, our upper and lower bounds differ by terms of order $m q$, our results are thus much more precise if we place ourselves in a regime where

$$\frac{m}{\ell} \rightarrow 0,$$

which is what we assume for the following section. We hope to be able to relax this condition in future works. This condition also helps to relate r_0 to q , using the limited development of $\ln(1 - q)$, we obtain

$$(\sigma - 1)r_0 = (\ln \sigma - \ell q) - \frac{\ln \sigma}{2} q + o \left((\ln \sigma - \ell q) + q \right).$$

Therefore,

$$(\sigma - 1)^2 m r_0^2 = m (\ln \sigma - \ell q)^2 + o(1).$$

Under this hypotheses and under the assumption that $\sigma \neq 2$, the expectation of the persistence time expands as

$$E(\tau_0) = P(m) \exp \left(\frac{m(\ell q - \ln \sigma)^2}{2(\sigma - 1)} \right), \quad (3)$$

where $P(m)$ is a polynomial in m .

2 Error thresholds

The problem of defining adequately the error threshold is delicate, as discussed by [2]. We are going to see three ways of defining an error threshold. The first consists in comparing the duration of the two phases. A critical point of the model is reached when both phases last approximatively for the same number of generations. Afterwards, we will consider critical points that take only the quasispecies phase into account. The second one, discussed in section 2.1, consists in controlling the persistence time. The third one is the same that Nowak and Schuster derived in their article [15], it consists in looking at the stationary measure of the proportion of master sequences. It is defined as the point for which the quasispecies phase stops being stable, we discuss it in section 2.3.

2.1 Critical point on the dynamics

The quasispecies phase is quite stable for small q , and the persistence time grows as an exponential in m . However, there exists a critical point q^* for which the growth of the expectation of the persistence time is only polynomial. From the expansion of the persistence time given in formula (3), if q^* admits the asymptotic development

$$q^* = \frac{\ln \sigma}{\ell} - \frac{C}{m^\alpha \ell^\beta},$$

then, the persistence time will be of order

$$E(\tau_0) = P(m) \exp \left(\frac{C^2}{2(\sigma - 1)} m^{1-2\alpha} \ell^{2(1-\beta)} \right).$$

Therefore, this time grows slower than a polynomial as soon as $\alpha \geq 1/2$ and $\beta \geq 1$. This leads to the critical parameter

$$q^* = \frac{\ln \sigma}{\ell} - \frac{C}{\ell \sqrt{m}}.$$

2.2 Critical point on the equilibrium

This criterion will rely upon the ratio of the expectation of the two times. If the ratio $E(\tau^*)/E(\tau_0)$ goes to zero, then the quasispecies phase will last much longer than the neutral phase, thus, if we look at the equilibrium, we will only see the quasispecies phase. On the contrary, if the ratio goes to infinity, we will only see the neutral phase. If the ratio converges to some

constant, we find ourselves in the critical case, we will not discuss it here, it would require the rest of the development of the expectation of both times.

This point is hardly seen on the dynamics of the process but rather on the equilibrium, section 2.2 will be dedicated to this critical point. For this value to have a meaning, the population needs to alternate many times from the quasispecies phase to the neutral phase, and conversely. Under conditions 1, it has been proved in [4], chapter 10.5, that the expectation of the time τ^* can be estimated by κ^ℓ , which is the size of the entire sequence space. More precisely, we have the following asymptotic:

$$\lim_{\ell} \frac{1}{\ell} \ln E(\tau^*) = \ln \kappa.$$

Heuristically, the number of possible chain in the population is the time needed by one individual to find the master sequence. Actually, the fact that there are m individuals does not help to significantly reduce it. By comparing this time with the time of theorem 1, we end up with a criterion for a critical parameter, which is the point at which both times are of the same order.

For the two times to be of the same order, it is then necessary that

$$(\ell q - \ln \sigma)^2 = \frac{2(\sigma - 1)\ell \ln \kappa}{m},$$

which leads to the following critical point

$$q^* = \frac{\ln \sigma}{\ell} - \frac{\sqrt{2(\sigma - 1)\ln \kappa}}{\sqrt{\ell m}}. \quad (4)$$

2.3 Critical point on the stationary measure

This critical point appears when we look at the stationary measure of the proportion of master sequences. When there are no mutation, two states are absorbing, a state with no master sequences, and a state with only master sequences. When the parameter for mutation is increased, a maximum is always present at point 0, due to the duration of the neutral phase. The stationary measure looks like the following graph

When q is increased even more, the maximum corresponding to the quasispecies phase gets smaller, it is of order r_0 . Between these two maxima is a minimum, located at point $1/mr_0$, as the next figure shows. This claim is stated in section 3.1.

There exists a value for the parameter q such that the maximum and the minimum coalesce.

The critical point q is such that mr_0^2 tends to 1. Since

$$mr_0^2 \sim \frac{m(\ln \sigma - \ell q)^2}{(\sigma - 1)^2},$$

it leads to the critical development

$$q^* = \frac{\ln \sigma}{\ell} - \frac{\sigma - 1}{\ell \sqrt{m}}.$$

2.4 Comparison of the three criteria

All of the three critical developments have the same power of m in the term after $\ln \sigma / \ell$, namely $1/\sqrt{m}$, however the exponent of ℓ differs. Two of the previous development have the same asymptotic with the term $1/\ell \sqrt{m}$, what these two points have in common is the fact that are defined only through the quasispecies phase. In many applications, as soon as master sequences are lost, the population dies because the time needed to find them back is too long. For example, if a population of viruses loses the master sequence,

the immune system will eradicate the viruses. In genetic algorithm, loosing the master sequence means more computations to get it back. For these kind of applications, a development in

$$q^* = \frac{\ln \sigma}{\ell} - \frac{C}{\ell \sqrt{m}},$$

seems to be relevant.

The other development is smaller, its definition requires that both phases constantly alternate so that the population is close to its equilibrium. This critical parameter seems relevant if the environment is no threat to the population without master sequences.

These asymptotics have been obtained in a regime where the size of the population is much greater than the length of the genome, we hope to be able to generalize this in future work. However, at this point, it is not obvious to decide which criterion is more relevant.

3 The birth and death process

We follow the strategy of [15] to simplify the original process, namely, we classify the individuals in only two types. The first type T_0 gathers all the master sequences, all other sequences are put in the second type T_1 , often called "the error tail". Let us write M_{ij} for the probability for an individual of type T_i to give birth to an individual of type T_j , for $i, j \in \{0, 1\}$. Some of these probabilities can be computed immediately, for example, M_{00} is the probability that a master sequence gives birth to a master sequence, not a single bit must be changed, so $M_{00} = (1 - q)^\ell$, and of course, $M_{01} = 1 - M_{00}$. However, the probability for an individual of type T_1 to give birth to a master sequence depends on the number of bits in its genome that are different from 0. This probability is thus out of reach if we don't assume anything on the repartition of the population in the different Hamming classes. It is for this quantity that Nowak and Schuster assumed a uniform distribution of all genotypes, taking

$$M_{10} = \sum_{k=1}^{\ell} \frac{\binom{\ell}{k}}{\kappa^\ell - 1} q^k (1 - q)^{\ell - k} = \frac{1 - (1 - q)^\ell}{\kappa^\ell - 4}.$$

In the quasispecies phase, master sequences are present in the population, and the other individuals constitute what Eigen called the cloud of mutants. Actually, individuals that are not master sequences are genetically close to master sequences. According to Eigen, mutations from T_1 to T_0 play a minor role in the quasispecies phase, but they still contribute to its stability. In

this phase, the hypothesis of Nowak and Schuster on M_{10} is quite strong because it underestimates largely the probability that a non-master sequence individual gives birth to a master sequence. They make this probability of order $1/\kappa^\ell$, according to our work in progress, it would seem to be of order $r_0 q$.

In this text, we will not make any assumption, we are going to bound the probability M_{10} from below and above. This will give us two processes that will lead to the same estimation for the first terms of the expectation of the persistence time.

- Since we study a regime where there are few mutations ($q \rightarrow 0$), it is easier to get master sequences if individuals of type T_1 need only one mutation to become a master sequence. Under this scheme, the number of master sequences will be greater than in the original process and we will thus obtain a longer persistence time. So we use the inequality

$$M_{10} \leq \frac{q}{\kappa - 1} (1 - q)^{\ell-1} \leq q.$$

- On the contrary, if individuals of type T_1 can never become master sequences, master sequences will extinct faster: $M_{10} > 0$.

The two cases will be coded by the function f , in the sequel, replacing f with the identity function will give formulas for the upper bound, taking $f = 0$ will give formulas for the lower bound.

Under the previous assumptions, in the simplified processes, the number N_t , which we defined as the number of master sequences, evolves according to a birth and death process on the state space $\{0, \dots, m\}$. Let us give names to its transition probabilities. For k between 0 and $m - 1$, we denote by δ_k the probability that N_t jumps from k to $k + 1$:

$$\forall t \in \mathbb{N} \quad \forall k \in \{0, \dots, m - 1\} \quad \delta_k = P(N_{t+1} = k + 1 \mid N_t = k).$$

For the number N_t to increase by 1, the offspring must be a master sequence and replace an individual of type T_1 .

$$\delta_k = \left(1 - \frac{k}{m}\right) \left(\frac{\sigma \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}} M_{00} + \frac{1 - \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}} M_{10} \right).$$

Factorizing the expression, we obtain

$$\delta_k = \left(1 - \frac{k}{m}\right) \left(\frac{(1 - \frac{k}{m}) f(q) + \sigma M_{00} \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}} \right).$$

Since the term containing the function f stands for the upper bound, we can replace it with anything greater, formulas will be simpler if we remove

the square. We will continue with

$$\delta_k = \left(1 - \frac{k}{m}\right) \frac{f(q) + \sigma M_{00} \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}}. \quad (5)$$

For k between 1 and m , we denote by γ_k the probability that N_t jumps from k to $k - 1$:

$$\forall t \in \mathbb{N} \quad \forall k \in \{1, \dots, m\} \quad \gamma_k = P(N_{t+1} = k - 1 \mid N_t = k),$$

For the number N_t to decrease by 1, the offspring must not be a master sequence and replace a master sequence, which happens with probability

$$\gamma_k = \frac{k}{m} \left(\frac{\sigma \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}} M_{01} + \frac{1 - \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}} M_{00} \right).$$

For the probability γ_k , we have

$$\gamma_k = \frac{k}{m} \frac{\sigma \frac{k}{m} (1 - M_{00}) + (1 - \frac{k}{m}) (1 - f(q))}{\sigma \frac{k}{m} + 1 - \frac{k}{m}}.$$

For this probability too, we can simplify further formulas by taking a smaller probability

$$\gamma_k = \frac{k}{m} \frac{1 - f(q) + L_q \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}}, \quad (6)$$

where we set L_q to be

$$L_q = \sigma - 1 - \sigma M_{00}. \quad (7)$$

For such birth and death processes, there exists an explicit formula for the invariant measure of the process. We set $\pi_0 = 1$ and

$$\forall i \in \{1, \dots, m\} \quad \pi_i = \frac{\delta_1 \cdots \delta_i}{\gamma_1 \cdots \gamma_i}. \quad (8)$$

In order to derive a criterion for the critical point, Nowak and Schuster considered the invariant measure, let us first discuss their result.

3.1 The variations of the stationary measure

In [15], Nowak and Schuster looked for a critical parameter in some modified version of the Moran model. In their framework, time is continuous and they work with the infinitesimal generator of the transition probabilities, which correspond to

$$\delta_k = \left(1 - \frac{k}{m}\right) \left(f(q) + \sigma M_{00} \frac{k}{m}\right),$$

and

$$\gamma_k = \frac{k}{m} \left(1 - f(q) + L_q \frac{k}{m} \right).$$

They were interested in the variations of the stationary measure of the proportion of master sequences. As we saw in formula (8),

$$\pi_k = \pi_{k-1} \frac{\delta_{k-1}}{\gamma_k}.$$

In order to know if π_k is increasing or decreasing, we need to know which of the two probabilities δ_{k-1} or γ_k is bigger. Nowak and Schuster thus studied the function ζ , with

$$\zeta\left(\frac{k}{m}\right) = \delta_{k-1} - \gamma_k.$$

The zeroes of function ζ lead to the extrema of the stationary measure. If ζ is positive, then the measure increases, and it decreases when ζ is negative. In their continuous time model, the function ζ is a quadratic polynomial in the variable $(1-q)^\ell$, which can be explicitly solved, as we show in section 2.3. It yields two zeroes, one of order $1/mr_0$, the other of order r_0 , therefore the two roots coalesce when mr_0^2 is bounded.

We also conducted the analog computations in our discrete time model, they lead to a third degree polynomial, that we were able to solve following [14]. We found the same asymptotic for the roots of the function ζ , along with a negative one at point $-1/(\sigma - 1)$.

3.2 A formula for the persistence time

For this kind of processes, there also exists explicit formulas for the expectation of the time needed to reach the state 0 starting from 1, which is exactly the persistence time τ_0 . The formula is stated in the next Lemma and can be found in classical textbooks, for example [11].

Lemma 2. *The expectation of the persistence time τ_0 started from $N_0 = 1$ is given by*

$$E(\tau_0) = \sum_{i=1}^{m-1} \frac{1}{\delta_i} \pi_i + \frac{\pi_{m-1}}{\gamma_m}.$$

The last term in this expression will be treated as a remainder term.

To estimate the sum, we will start by working on $\ln(\delta_k/\gamma_k)$, we will then focus on $\ln \pi_i$ that we will estimate by Riemann sums and a clever comparison with an integral. We will finally add up the quantities $\exp(\ln \pi_i)/\delta_i$, and implement Laplace's method to estimate the persistence time.

3.3 Computation of $\ln \delta_k / \gamma_k$

In order to compute the ratio $\frac{\delta_k}{\gamma_k}$, let us first factorise the expressions of the two transition probabilities (5) and (6).

$$\delta_k = \left(1 - \frac{k}{m}\right) \frac{f(q) + \sigma M_{11} \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}},$$

and

$$\gamma_k = \frac{k}{m} \frac{1 - f(q) + L_q \frac{k}{m}}{\sigma \frac{k}{m} + 1 - \frac{k}{m}},$$

Notice that

$$L_q = \sigma - 2 - (\sigma M_{00} - 1),$$

since we placed ourselves in a regime where M_{00} tends toward $1/\sigma$, we deduce that

$$-1 + \frac{\sigma}{2} < L_q < \sigma - 2.$$

So that in the case $\sigma \neq 2$, L_q goes to $\sigma - 2$ and is thus not zero if q is small enough. In the case $\sigma = 2$, we always have $L_q < 0$. In both cases, $L_q \neq 0$.

We also define the two affine functions ψ and ϕ by

$$\psi(x) = f(q) + \sigma M_{00} x, \quad (9)$$

and

$$\phi(x) = 1 - f(q) + L_q x. \quad (10)$$

Notice that ψ and ϕ are strictly positive and not constant.

With these notations, the ratio δ_k / γ_k can be rewritten as

$$\frac{\delta_k}{\gamma_k} = \frac{1 - \frac{k}{m}}{\frac{k}{m}} \frac{\psi\left(\frac{k}{m}\right)}{\phi\left(\frac{k}{m}\right)}.$$

Our goal is now to estimate π_i . Sums are easier to work with than products, so we start by looking for an estimate of

$$\ln \frac{\delta_k}{\gamma_k} = \ln \left(\frac{1 - \frac{k}{m}}{\frac{k}{m}} \right) + \ln \psi\left(\frac{k}{m}\right) - \ln \phi\left(\frac{k}{m}\right). \quad (11)$$

Let i be an integer in $\{1, \dots, m-1\}$, summing identity (11) between 1 and i gives

$$\begin{aligned} \ln \pi_i &= \sum_{k=1}^i \ln \frac{\delta_k}{\gamma_k} \\ &= \sum_{k=1}^i \ln \left(\frac{1 - \frac{k}{m}}{\frac{k}{m}} \right) + \sum_{k=1}^i \ln \psi\left(\frac{k}{m}\right) - \sum_{k=1}^i \ln \phi\left(\frac{k}{m}\right). \end{aligned}$$

The first term can be written in a simpler form:

$$\sum_{k=1}^i \ln \left(\frac{1 - \frac{k}{m}}{\frac{k}{m}} \right) = \ln \left(\frac{1}{i!} \prod_{k=1}^i (m - k) \right) = \ln \binom{m}{i} + \ln \left(1 - \frac{i}{m} \right),$$

we thus obtain

$$\ln \pi_i = \ln \binom{m}{i} + \ln \left(1 - \frac{i}{m} \right) + \sum_{k=1}^i \ln \psi \left(\frac{k}{m} \right) - \sum_{k=1}^i \ln \phi \left(\frac{k}{m} \right). \quad (12)$$

Our goal is to estimate these quantities in the asymptotic regime (1). We will use a tricky comparison between a series and an integral to estimate the binomial coefficient and classical Taylor formulas to develop the sums.

3.4 Estimation of the binomial coefficient

We now focus on the estimation of the binomial coefficient $\ln \binom{m}{i}$. Let $\tau(x)$ stand for

$$\tau(x) = -m(1-x) \ln(1-x) - mx \ln x - \frac{1}{2} \ln \left(mx(1-x) \right).$$

This quantity approximates very well our binomial coefficient.

Lemma 3. *For all $i \in \{1, \dots, m-1\}$, we have*

$$\left| \ln \binom{i}{m} - \tau \left(\frac{i}{m} \right) \right| \leq 2.$$

Proof. The proof relies on a tricky comparison between a series and an integral derived by Robbins [17]. It yields the following inequalities,

$$\forall n \geq 1 \quad \frac{1}{12n+1} < \ln n! - n \ln n + n - \frac{1}{2} \ln(2\pi n) < \frac{1}{12n}.$$

We use this inequality three times with i , m and $m-i$ instead of n and we obtain an approximation for $\ln \binom{i}{m}$ along with an error bound. The difference between $\ln \binom{i}{m}$ and $\tau(i)$ can then be bounded by, for every $i \in \{1, \dots, m-1\}$,

$$\begin{aligned} \frac{1}{12m+1} - \frac{1}{12i} - \frac{1}{12(m-i)} \\ \leq \ln \binom{i}{m} - \tau \left(\frac{i}{m} \right) + \frac{1}{2} \ln(2\pi) \leq \\ \frac{1}{12m} - \frac{1}{12i+1} - \frac{1}{12(m-i)+1}. \end{aligned}$$

Therefore, we have the uniform bound:

$$\forall i \in \{1, \dots, m-1\} \quad \left| \ln \binom{i}{m} - \tau \left(\frac{i}{m} \right) \right| \leq \frac{1}{6} + \frac{1}{2} \ln(2\pi) \leq 2.$$

□

3.5 Expansion of the Riemann sums

Let us now consider both the Riemann sum $\sum \ln \psi$ and $\sum \ln \phi$, our first goal is to write them as integrals. Because of the very small value of $\psi(0)$, we will need another formula that stays far from 0.

Lemma 4. *For every $i \in \{1, \dots, m\}$, we have, for the function ϕ*

$$\sum_{k=1}^i \ln \phi \left(\frac{k}{m} \right) = m \int_0^{\frac{i}{m}} \ln \phi(s) \, ds + R,$$

with R uniformly bounded by $4\sigma^2$.

And for the function ψ ,

$$\sum_{k=1}^i \ln \psi \left(\frac{k}{m} \right) = m \int_{1/m}^{\frac{i}{m}} \ln \psi(s) \, ds + \frac{1}{2} \left(\ln \psi \left(\frac{i}{m} \right) + \ln \psi \left(\frac{1}{m} \right) \right) + R,$$

with R bounded by 1.

The proofs of both these Lemmas consist in the manipulation of Taylor-Lagrange formulas, delayed in section 7.1, we now apply the general Lemmas to our peculiar case.

Proof. We apply Lemma 8 to the function $\ln \phi$. Let us set

$$h(x) = \ln \phi(x) = \ln \left(1 - f(q) + L_q x \right).$$

The second derivative of h is

$$h''(x) = \frac{-L_q^2}{\left(1 - f(q) + L_q x \right)^2}.$$

Since $|h''|$ is either increasing or decreasing according to the sign of L_q , we have

$$|h''(x)| \leq |h''(0)| + |h''(1)| \leq \frac{L_q^2}{1 - f(q)} + \frac{L_q^2}{1 - f(q) + L_q} \leq 4\sigma^2.$$

In the end, Lemma 8 applied to the function $\ln \phi$ gives

$$\sum_{k=1}^i \ln \phi\left(\frac{k}{m}\right) = m \int_0^{\frac{i}{m}} \ln \phi(s) \, ds + R, \quad (13)$$

where the quantity R is uniformly bounded by constants.

We will treat in a similar way the function $\ln \psi$, which we also call h ,

$$h(x) = \ln \psi(x) = \ln \left(f(q) + \sigma M_{00} x \right).$$

However, because of the very small value of $\psi(0)$, the remainder term is more difficult to control here and a uniform bound will not be enough. The second derivative of the function h is

$$h''(x) = \frac{-(\sigma M_{00})^2}{\left(f(q) + \sigma M_{00} x \right)^2}.$$

We will apply Lemma 9 to the function h , for this, we bound the function h'' on each sub-interval $[\frac{k-1}{m}, \frac{k}{m}]$. Since the function $|h''|$ is decreasing, then

$$\sup_{[\frac{k-1}{m}, \frac{k}{m}]} |h''| \leq \frac{(\sigma M_{00})^2}{\left(f(q) + \sigma M_{00} \frac{k-1}{m} \right)^2}.$$

Taking the first term out of the sum of the remainder, shifting the indices, and adding the last term we obtain

$$|R| \leq \frac{(\sigma M_{00})^2}{\left(m f(q) + \sigma M_{00} \right)^2} + \frac{1}{m^2} \sum_{k=2}^m \frac{(\sigma M_{00})^2}{\left(f(q) + \sigma M_{00} \frac{k}{m} \right)^2}. \quad (14)$$

We compare this second sum with an integral, the summed function is positive and decreasing, therefore,

$$\sum_{k=2}^m \frac{(\sigma M_{00})^2}{\left(f(q) + \sigma M_{00} \frac{k}{m} \right)^2} \leq m \int_{\frac{1}{m}}^1 \frac{(\sigma M_{00})^2}{\left(f(q) + \sigma M_{00} s \right)^2} \, ds.$$

A change of variables gives

$$\sum_{k=2}^m \frac{(\sigma M_{00})^2}{\left(f(q) + \sigma M_{00} \frac{k}{m} \right)^2} \leq m \int_{f(q) + \sigma M_{00} \frac{1}{m}}^{f(q) + \sigma M_{00}} \frac{\sigma M_{00}}{u^2} \, du.$$

We calculate the integral and we obtain

$$\begin{aligned} \sum_{k=2}^m \frac{(\sigma M_{00})^2}{\left(f(q) + \sigma M_{00} \frac{k}{m} \right)^2} &\leq \frac{m \sigma M_{00}}{f(q) + \sigma M_{00} \frac{1}{m}} - \frac{m \sigma M_{00}}{f(q) + \sigma M_{00}} \\ &\leq \frac{m^2 \sigma M_{00}}{m f(q) + \sigma M_{00}}, \end{aligned}$$

where we removed the last negative term. We finally get, according to Lemma 9,

$$\sum_{k=1}^i \ln \psi\left(\frac{k}{m}\right) = m \int_{1/m}^{i/m} \ln \psi(s) \, ds + \frac{1}{2} \left(\ln \psi\left(\frac{i}{m}\right) + \ln \psi\left(\frac{1}{m}\right) \right) + R. \quad (15)$$

where

$$|R| \leq \frac{\sigma M_{00}}{m f(q) + \sigma M_{00}} \leq 1.$$

□

3.6 Computation of the sums

We now compute the integrals appearing in the Lemma (8), the functions ψ and ϕ are in fact affine functions, in order to simplify the formulas, let us introduce the following notation, for any affine function f , we will write

$$\Lambda f(x) = \frac{f(x)}{f'} \ln f(x).$$

so that the function $\ln f$ is the derivative of $\Lambda f(x) - x$. Notice that $\Lambda \phi$ always exists because $\phi' = L_q$ is never 0. We have, according to the expressions (9) and (10) of the functions ψ and ϕ ,

$$\int_0^x \ln \phi(s) \, ds = \Lambda \phi(x) - x - \Lambda \phi(0),$$

and

$$\int_{1/m}^x \ln \psi(s) \, ds = \Lambda \psi(x) - x - \Lambda \psi\left(\frac{1}{m}\right) + \frac{1}{m}.$$

Replacing the integral in formula (13) by the previous one gives

$$\sum_{k=1}^i \ln \phi\left(\frac{k}{m}\right) = m \Lambda \phi\left(\frac{i}{m}\right) - i - m \Lambda \phi(0) + R, \quad (16)$$

where R is uniformly bounded by a constant. In a similar way, Formula (15) becomes

$$\begin{aligned} \sum_{k=1}^i \ln \psi\left(\frac{k}{m}\right) &= m \Lambda \psi\left(\frac{i}{m}\right) - i - m \Lambda \psi\left(\frac{1}{m}\right) \\ &\quad + \frac{1}{2} \ln \psi\left(\frac{i}{m}\right) + \frac{1}{2} \ln \psi\left(\frac{1}{m}\right) + R, \end{aligned} \quad (17)$$

where R is uniformly bounded by constant terms.

4 First estimation of the persistence time

We can now deal with the expectation of the persistence time, recall that Lemma 2 gave

$$E(\tau_0) = \sum_{i=1}^{m-1} \frac{1}{\delta_i} \exp(\ln \pi_i) + \frac{\pi_{m-1}}{\gamma_m}. \quad (18)$$

Our goal now is to gather the different parts from formulas (12), (16), (17) and Lemma 3 of this expression into new notations. The gathering is quite tricky but it is crucial to discriminating the main terms from remainder terms. First, we gather the constant terms

$$K = \exp \left(m\Lambda\phi(0) - m\Lambda\psi\left(\frac{1}{m}\right) + \frac{1}{2} \ln \psi\left(\frac{1}{m}\right) + \frac{mf(q)}{L_q} \right). \quad (19)$$

Then, we gather the main terms, those that will be prominent in the sum, the following terms will be factors of m .

$$F(x) = -(1-x) \ln(1-x) + x \ln(\sigma M_{00}) - \left(\frac{1}{L_q} + x \right) \ln(1 + L_q x), \quad (20)$$

the first term comes from the binomial coefficient, the second term from $\Lambda\psi(x)$ and the last was extracted from $\Lambda\phi(x)$. Then all the other terms, that we will be able to bound uniformly

$$G(x) = m \left(\Lambda\psi(x) - x \ln(\sigma M_{00}) \right) - mx \ln x - \frac{1}{2} \ln(mx(1-x)) - \frac{1}{2} \ln \psi(x) - m \left(\Lambda\phi(x) - \left(\frac{1}{L_q} + x \right) \ln(1 + L_q x) + \frac{f(q)}{L_q} \right), \quad (21)$$

where the division by δ_i is counted in the $-\frac{1}{2} \ln \psi$.

With these notations, formula (18) reduces to

$$E(\tau_0) = K \sum_{i=1}^{m-1} \exp \left(mF\left(\frac{i}{m}\right) + G\left(\frac{i}{m}\right) + R \right) + T, \quad (22)$$

where R is bounded by some constant and T is a remainder term

$$T = \frac{K}{\gamma_m} \exp \left(mF\left(1 - \frac{1}{m}\right) + G\left(1 - \frac{1}{m}\right) + \ln \psi\left(1 - \frac{1}{m}\right) - \ln m + R \right).$$

The function F in the sum (22) is multiplied by m , which tends towards infinity. If we can bound the function G uniformly over the interval $[\frac{1}{m}, 1 - \frac{1}{m}]$, the indices around the maximum of the function F will govern the asymptotic behavior of the sum.

4.1 The remainder term: Function G

The goal of this section is to prove the following Lemma which uniformly bounds the function G . We will use this upper bound several times in the sequel.

Lemma 5. *In the asymptotic regime (1), with condition (2), we have*

$$\sup_{[\frac{1}{m}, \frac{m-1}{m}]} |G(x)| \leq C \left(1 + mf(q)\right) \ln m + \frac{f(q)^2}{L_q}, \quad (23)$$

for some constant C .

Of course, in the case $\sigma \neq 2$, L_q does not tend to 0 so the last term is smaller than the first, but in the case $\sigma = 2$, where L_q goes to 0, it is not sure yet which one is bigger.

Proof. Let us study the terms that appear in the expression (21) of the function G . Let x belong to the interval $[\frac{1}{m}, 1 - \frac{1}{m}]$. Replacing ψ with its expression leads to

$$\begin{aligned} m \left(\Lambda \psi(x) - x \ln(\sigma M_{00}) \right) - mx \ln x = \\ \frac{mf(q)}{\sigma M_{00}} \ln \left(f(q) + \sigma M_{00} x \right) + mx \ln \left(1 + \frac{f(q)}{\sigma M_{00} x} \right). \end{aligned}$$

Let us then bound these two terms:

- For the first we have, since $\sigma M_{00} > 1$ and $x > 1/m$,

$$\left| \frac{mf(q)}{\sigma M_{00}} \ln \left(f(q) + \sigma M_{00} x \right) \right| \leq mf(q) \ln m.$$

- And for the second,

$$\left| mx \ln \left(1 + \frac{f(q)}{\sigma M_{00} x} \right) \right| \leq mf(q).$$

- Since the function $x \mapsto x(1-x)$ is always smaller than 1/4, then the third term of function G can be controlled by

$$\left| -\frac{1}{2} \ln \left(mx(1-x) \right) \right| \leq \ln m.$$

- Since the function ψ is increasing and smaller than 1,

$$\left| -\frac{1}{2} \ln \psi(x) \right| \leq \left| \frac{1}{2} \ln \psi\left(\frac{1}{m}\right) \right| \leq \ln m.$$

• Finally,

$$\begin{aligned} \Lambda\phi(x) - \left(\frac{1}{L_q} + x\right) \ln(1 + L_q x) = \\ - \frac{f(q)}{L_q} \ln\phi(x) + \left(\frac{1}{L_q} + x\right) \ln\left(1 - \frac{f(q)}{1 + L_q x}\right). \end{aligned} \quad (24)$$

For the first of these two terms,

$$|\ln\phi| \leq |\ln\phi(0)| + |\ln\phi(1)| \leq \frac{f(q)}{2} + \left|\ln\left(1 - f(q) + L_q\right)\right|.$$

In order to bound the second term, we consider two cases,

If L_q is positive, then L_q does not tend towards 0, so we have

$$\left|\ln\left(1 - f(q) + L_q\right)\right| \leq L_q - f(q).$$

If L_q is negative, we use the inequality $-\ln(1 - u) \leq u/2$ which holds if u is positive, it yields

$$\left|\ln\left(1 - f(q) + L_q\right)\right| \leq \frac{f(q) - L_q}{2}.$$

In both cases, we have that

$$\left| - \frac{f(q)}{L_q} \ln\phi(x) \right| \leq \frac{f(q)^2}{|L_q|} + f(q).$$

The second term of expression (24), added to $f(q)/L_q$ has negative numerator

$$\left(1 + L_q x\right) \ln\left(1 - \frac{f(q)}{1 + L_q x}\right) + f(q) \leq 0.$$

The inequality $-\ln(1 - x) \leq x + x^2$ holds if $x \leq 1/2$, it yields

$$\left| \left(\frac{1}{L_q} + x\right) \ln\left(1 - \frac{f(q)}{1 + L_q x}\right) + \frac{f(q)}{L_q} \right| \leq \frac{\sigma f(q)^2}{|L_q|}.$$

Therefore,

$$\left| \Lambda\phi(x) - \left(\frac{1}{L_q} + x\right) \ln(1 + L_q x) + \frac{f(q)}{L_q} \right| \leq \frac{\sigma f(q)^2}{|L_q|} + f(q).$$

Putting together the previous upper bounds, we get for every x in the interval $[\frac{1}{m}, 1 - \frac{1}{m}]$,

$$|G(x)| \leq C(1 + mf(q)) \ln m + C \frac{mf(q)^2}{|L_q|},$$

for some constant C . □

4.2 The main term: Function F

We are now looking for the maximum of F on $[0, 1]$.

Lemma 6. *The function F reaches a unique maximum at point*

$$r_0 = \frac{\sigma M_{00} - 1}{\sigma - 1}.$$

Besides, the quantity $F(r_0)$ is equal to

$$F(r_0) = \varphi(M_{00}).$$

where the function φ is defined as

$$\varphi(x) = \frac{\sigma(1-x) \ln \frac{\sigma(1-x)}{\sigma-1} + \ln(\sigma x)}{1 - \sigma(1-x)}. \quad (25)$$

Proof. The function F defined in expression (20) admits for first derivative

$$F'(x) = \ln(1-x) + \ln(\sigma(1-q)^\ell) - \ln(1 + L_q x),$$

and for second derivative

$$F''(x) = -\frac{1}{1-x} - \frac{L_q}{1 + L_q x}.$$

We have, since $1-x < 1 + L_q x$

$$F''(x) = -\frac{1}{1-x} - \frac{L_q}{1 + L_q x} \leq -\frac{1 + L_q}{1 + L_q x}. \quad (26)$$

If $L_q > 0$, F'' increases so $F'' \leq F''(1) \leq -1$.

If $L_q < 0$, F'' decreases so

$$F'' \leq F''(0) \leq -(1 + L_q) \leq -\frac{\sigma}{2}.$$

In both cases, F'' is strictly smaller than $-1/2$, the function F is therefore concave, its critical point satisfies the following equation:

$$\ln(1-x) + \ln(\sigma M_{00}) - \ln(1 + L_q x) = 0. \quad (27)$$

Therefore, we find r_0 as the critical point for the function F .

$$r_0 = \frac{\sigma M_{00} - 1}{\sigma - 1}.$$

The quantity $1 + L_q r_0$ will appear often in the sequel, the equation (27) provides the following expression for this quantity:

$$1 + L_q r_0 = \sigma M_{00}(1 - r_0). \quad (28)$$

We will replace the term $F(i/m)$ in the sum (22) by its Taylor development around r_0 , so we need to compute $F(r_0)$.

$$F(r_0) = -(1 - r_0) \ln(1 - r_0) + r_0 \ln(\sigma M_{00}) - \left(\frac{1}{L_q} + r_0\right) \ln(1 + L_q r_0).$$

Equation (28) gives

$$\left(\frac{1}{L_q} + r_0\right) \ln(1 + L_q r_0) = \left(\frac{1}{L_q} + r_0\right) \ln(\sigma M_{00}(1 - r_0)).$$

Splitting the logarithmic term, we obtain

$$F(r_0) = -\frac{1 + L_q}{L_q} \ln(1 - r_0) - \frac{1}{L_q} \ln(\sigma M_{00}).$$

Replacing L_q with its expression (7) finally gives

$$F(r_0) = \frac{\sigma(1 - M_{00}) \ln \frac{\sigma(1 - M_{00})}{\sigma - 1} + \ln(\sigma M_{00})}{1 - \sigma(1 - M_{00})}.$$

□

5 Implementation of Laplace's method

We now introduce a notation for the sum (22): we set

$$S_m = \sum_{i=1}^{m-1} \exp\left(mF\left(\frac{i}{m}\right) + G\left(\frac{i}{m}\right)\right). \quad (29)$$

This section is dedicated to the proof of the following Lemma

Lemma 7. *The sum S_m is equivalent to*

$$S_m = e^{mF(r_0)} e^{O\left(\sup_{[\frac{1}{m}, \frac{m-1}{m}] |G|}\right)}.$$

Proof. The main contributions in the sum will arise from terms whose indices lie around mr_0 , therefore, we will first estimate the sum truncated on a certain neighborhood of mr_0 . We choose

$$\delta = m^{2/3}, \quad (30)$$

and we set $[i_-, i_+]$ to be the interval on which we will sum, where

$$i_- = \max \left(\lfloor mr_0 - \delta \rfloor, 0 \right) + 1,$$

$$i_+ = \lfloor mr_0 + \delta \rfloor.$$

Since $i_- \geq 1$ and $r_0 < 1/2$ asymptotically, since r_0 goes to 0, the interval $[i_-, i_+]$ is strictly included in $[1, m-1]$. Our goal is now to estimate the sum

$$S_m(\delta) = \sum_{i=i_-}^{i_+} \exp \left(mF\left(\frac{i}{m}\right) + G\left(\frac{i}{m}\right) \right). \quad (31)$$

Recalling that r_0 is the maximum of the function F , the truncated sum is related to the expression (29) through the inequalities

$$S_m(\delta) \leq S_m \leq S_m(\delta) + m \exp \left(mF(r_0) + \sup_{[\frac{1}{m}, \frac{m-1}{m}]} |G| \right).$$

We thus obtain, according to the inequality (23),

$$S_m = S_m(\delta) + \exp \left(mF(r_0) + O\left(\sup_{[\frac{1}{m}, \frac{m-1}{m}]} |G| \right) \right). \quad (32)$$

The Taylor-Lagrange formula at order 2 for F allows us to estimate the expression (31) of $S_m(\delta)$:

$$S_m(\delta) = \sum_{i=i_-}^{i_+} \exp \left(m \left(F(r_0) + \left(\frac{i}{m} - r_0 \right)^2 \frac{F''(\eta_i)}{2} \right) + G\left(\frac{i}{m}\right) \right), \quad (33)$$

where η_i , $i_- \leq i \leq i_+$ is a real number between i_-/m and i_+/m .

We will not need the precise value of $F''(r_0)$, we will only need to know that F'' is strictly smaller than a $-1/2$, as we shown with the expression (26). The function G will once more be uniformly bounded with Lemma 23. With this development, estimating the sum $S_m(\delta)$ reduces to estimating $T_m(\delta)$, where

$$T_m(\delta) = \sum_{i=i_-}^{i_+} \exp \left(m \left(\frac{i}{m} - r_0 \right)^2 \frac{F''(\eta_i)}{2} \right). \quad (34)$$

From the expression (33), we have

$$S_m(\delta) = \exp \left(mF(r_0) \right) T_m(\delta) \exp \left(O\left(\sup_{[\frac{1}{m}, \frac{m-1}{m}]} |G| \right) \right), \quad (35)$$

We will only need a rough approximation on $T_m(\delta)$. Since $F''(r_0)$ is negative, we first notice that

$$T_m(\delta) \leq m.$$

In order to bound from below $T_m(\delta)$, we need a lower bound on $F''(\eta_i)$, actually, we consider two cases.

If L_q is positive, then

$$F''(\eta_i) \geq F''(0) \geq -2\sigma.$$

If L_q is negative, then

$$F''(\eta_i) \geq F''\left(\frac{i_+}{m}\right) \geq F''\left(\frac{1}{2}\right) \geq -6.$$

In both cases, $F''(\eta_i)$ is greater than $-2(\sigma + 3)$. We can also bound the sum $T_m(\delta)$ from below by one of its terms: for example, the term of index $1 + \lfloor mr_0 \rfloor$

$$T_m(\delta) \geq \exp\left(-(\sigma + 3)m\left(\frac{1 + \lfloor mr_0 \rfloor}{m} - r_0\right)^2\right).$$

However, we have that

$$mr_0 - 1 \leq \lfloor mr_0 \rfloor \leq mr_0,$$

so

$$T_m(\delta) \geq \exp\left(\frac{\sigma + 3}{m}\right),$$

and this bound goes to 1.

Therefore, we have for m large enough

$$\frac{1}{2} \leq T_m(\delta) \leq m.$$

With the formula (35), we rewrite the sum (31) as

$$S_m(\delta) = \exp\left(mF(r_0)\right) R_5 e^{O\left(\sup_{[\frac{1}{m}, \frac{m-1}{m}]} |G|\right)}, \quad (36)$$

where

$$\frac{1}{2} \leq R_5 \leq m.$$

With the estimation (32), we finally obtain

$$S_m = e^{mF(r_0)} e^{O\left(\sup_{[\frac{1}{m}, \frac{m-1}{m}]} |G|\right)},$$

and we are done. □

6 Back to the persistence time

The expectation of the persistence time is

$$E(\tau_0) = K S_m e^R + T, \quad (37)$$

where, R is bounded by some constant and T is

$$T = \frac{K \psi\left(1 - \frac{1}{m}\right)}{\gamma_m} \exp\left(mF\left(1 - \frac{1}{m}\right) + G\left(1 - \frac{1}{m}\right) - \ln m + R\right).$$

Since γ_m tends towards a finite constant and so does $\psi(1 - \frac{1}{m})$, the remainder T is at most of the same order as the main term.

We have then

$$E(\tau_0) = K \exp\left(mF(r_0) + O\left(\sup_{[\frac{1}{m}, \frac{m-1}{m}]} |G|\right)\right). \quad (38)$$

We now develop this expression, remember that expression (19) of K yielded

$$K = \exp\left(\left(\frac{mf(q)}{\sigma M_{00}} + \frac{1}{2}\right)\left(\ln m - \ln(\sigma M_{11} + mf(q))\right) + m \frac{1-f(q)}{L_q} \ln(1-f(q)) + \frac{mf(q)}{L_q}\right).$$

Some terms in K are of order smaller than $(1 + mf(q)) \ln m$, we include them in the remainder term, and we get according to definition (25),

$$E(\tau_0) = \exp\left(m\varphi(M_{00}) + O\left(\left(1 + mf(q)\right) \ln m + \frac{mf(q)^2}{L_q}\right)\right).$$

with

$$\varphi(x) = \frac{\sigma(1-x) \ln \frac{\sigma(1-x)}{\sigma-1} + \ln(\sigma x)}{1 - \sigma(1-x)}.$$

Let us now estimate the asymptotic of function φ when the argument tends towards $1/\sigma$.

Its asymptotic will be given by the first non-zero derivative of φ at point $1/\sigma$. In order to expand φ around $1/\sigma$, we write

$$\varphi(x) = \varphi\left(\left(x - \frac{1}{\sigma}\right) + \frac{1}{\sigma}\right),$$

and we use the expression (25) of φ to get

$$\varphi(x) = \frac{\left(\sigma - (\sigma x - 1) - 1\right) \ln \frac{\sigma - (\sigma x - 1) - 1}{\sigma - 1} + \ln \left((\sigma x - 1) + 1\right)}{1 - \sigma(1 - x)}.$$

We develop the expression in powers of $\sigma x - 1$ and we get

$$\begin{aligned} \varphi(x) = & \frac{-(\sigma x - 1) + \left(\sigma - 1 - \frac{1}{2}(\sigma - 1)\right) \left(\frac{\sigma x - 1}{\sigma - 1}\right)^2 + O\left((\sigma x - 1)^3\right)}{1 - \sigma(1 - x)} \\ & + \frac{\sigma x - 1 - \frac{1}{2}(\sigma x - 1)^2 + O\left((\sigma x - 1)^3\right)}{1 - \sigma(1 - x)}. \end{aligned}$$

This shows that the function φ and its derivative vanish at $1/\sigma$ and

$$\varphi''\left(\frac{1}{\sigma}\right) = 2\sigma^2 \frac{\sigma - 1 - \frac{1}{2}(\sigma - 1) - \frac{1}{2}(\sigma - 1)^2}{(\sigma - 1)^2(1 - \sigma + 1)} = \sigma^2 \frac{(\sigma - 1)(2 - \sigma)}{(\sigma - 1)^2(2 - \sigma)} = \frac{\sigma^2}{\sigma - 1}.$$

Therefore, we have

$$m\varphi\left((1 - q)^\ell\right) = m\left((1 - q)^\ell - 1/\sigma\right)^2 \frac{\sigma^2}{2(\sigma - 1)} + O\left(m(\sigma(1 - q)^\ell - 1)^3\right).$$

Writing this expression with the help of the variable r_0 and replacing the first term with the estimates above, we obtain

$$m\varphi\left((1 - q)^\ell\right) = mr_0^2 \frac{\sigma - 1}{2} + O(mr_0^3).$$

7 Appendixes

7.1 Riemann Lemmas

Lemma 8. *For any function f of class C^2 on $[0, 1]$ and for every $i \in \{1, \dots, m\}$, we have*

$$\sum_{k=1}^i f\left(\frac{k}{m}\right) = m \int_0^{\frac{i}{m}} f(s) \, ds + \frac{1}{2} \left(f\left(\frac{i}{m}\right) - f(0) \right) + R,$$

with R bounded by

$$R \leq \frac{1}{m} \sup_{[0,1]} |f''|.$$

Because of the very small value of $\psi(0)$, we will need another formula that stays far from 0.

Lemma 9. For any function f of class C^2 on $[0, 1]$ and for every $i \in \{1, \dots, m\}$, we have

$$\sum_{k=1}^i f\left(\frac{k}{m}\right) = m \int_{1/m}^{\frac{i}{m}} f(s) \, ds + \frac{1}{2} \left(f\left(\frac{i}{m}\right) + f\left(\frac{1}{m}\right) \right) + R,$$

with R bounded by

$$R \leq \frac{1}{m^2} \sum_{k=2}^m \sup_{[\frac{k-1}{m}, \frac{k}{m}]} |f''|.$$

For any function f of class C^2 on $[0, 1]$ and for $k \in \{1, \dots, m\}$, the Taylor-Lagrange formula applied to f between the points $s \in [\frac{k-1}{m}, \frac{k}{m}]$ and $\frac{k}{m}$ gives

$$\exists \eta_s^k \in \left] s, \frac{k}{m} \right[\quad f(s) = f\left(\frac{k}{m}\right) + \left(s - \frac{k}{m}\right) f'\left(\frac{k}{m}\right) + \left(s - \frac{k}{m}\right)^2 \frac{f''(\eta_s^k)}{2}.$$

Integrating this equality between the points $\frac{k-1}{m}$ and $\frac{k}{m}$ gives

$$\int_{\frac{k-1}{m}}^{\frac{k}{m}} f(s) \, ds = \frac{1}{m} f\left(\frac{k}{m}\right) - \frac{1}{2m^2} f'\left(\frac{k}{m}\right) + \int_{\frac{k-1}{m}}^{\frac{k}{m}} \left(s - \frac{k}{m}\right)^2 \frac{f''(\eta_s^k)}{2} \, ds. \quad (39)$$

The last term will be negligible, we call it R_2 :

$$R_2(k) = \int_{\frac{k-1}{m}}^{\frac{k}{m}} \left(s - \frac{k}{m}\right)^2 \frac{f''(\eta_s^k)}{2} \, ds. \quad (40)$$

We sum the expression (39) for k varying from 1 to i and we get

$$\int_0^{\frac{i}{m}} f(s) \, ds = \frac{1}{m} \sum_{k=1}^i f\left(\frac{k}{m}\right) - \frac{1}{2m^2} \sum_{k=1}^i f'\left(\frac{k}{m}\right) + \sum_{k=1}^i R_2(k). \quad (41)$$

Similarly, we apply the Taylor-Lagrange formula at order 1 to f' , we integrate and we sum to obtain

$$\int_0^{\frac{i}{m}} f'(s) \, ds = \frac{1}{m} \sum_{k=1}^i f'\left(\frac{k}{m}\right) + \sum_{k=1}^i \int_{\frac{k-1}{m}}^{\frac{k}{m}} \left(s - \frac{k}{m}\right) f''(\zeta_s^k) \, ds, \quad (42)$$

for some ζ_s^k between s and $\frac{k}{m}$. We set

$$R_1(k) = \int_{\frac{k-1}{m}}^{\frac{k}{m}} \left(s - \frac{k}{m}\right) f''(\zeta_s^k) \, ds.$$

We combine the two formulas (41) and (42) and we obtain

$$\sum_{k=1}^i f\left(\frac{k}{m}\right) = m \int_0^{\frac{i}{m}} f(s) \, ds + \frac{1}{2} \int_0^{\frac{i}{m}} f'(s) \, ds - \frac{1}{2} \sum_{k=1}^i R_1(k) - m \sum_{k=1}^i R_2(k).$$

To control the remainder terms, we uniformly bound the second derivative of the function f :

$$\left| R_1(k) \right| \leq \frac{1}{2m^2} \sup_{\left[\frac{k-1}{m}, \frac{k}{m}\right]} |f''|,$$

and for $R_2(k)$ from expression (40),

$$\left| R_1(k) \right| \leq \frac{1}{6m^3} \sup_{\left[\frac{k-1}{m}, \frac{k}{m}\right]} |f''|.$$

Finally, the total remainder term is bounded by

$$\left| \sum_{k=1}^i R_1(k) + m \sum_{k=1}^i R_2(k) \right| \leq \frac{1}{m^2} \sum_{k=1}^m \sup_{\left[\frac{k-1}{m}, \frac{k}{m}\right]} |f''|.$$

Since f is a primitive of f' , we get the Lemma 9. For any function f of class C^2 on $[0, 1]$ and for every $i \in \{1, \dots, m\}$, we have

$$\sum_{k=1}^i f\left(\frac{k}{m}\right) = m \int_0^{\frac{i}{m}} f(s) \, ds + \frac{1}{2} \left(f\left(\frac{i}{m}\right) - f(0) \right) + R,$$

with R bounded by

$$R \leq \frac{1}{m} \sup_{\left[\frac{k-1}{m}, \frac{k}{m}\right]} |f''|.$$

If we choose to bound uniformly the function $|f''|$, we get the Lemma 4

7.2 Solving the cubic

Let us study the function ζ where

$$\zeta\left(\frac{k}{m}\right) = \delta_{k-1} - \gamma_k.$$

For the probabilities of our model, the denominators add some complications. Under the same denominators that we didn't write, we have

$$\begin{aligned} \zeta(x) = & \left((\sigma - 1)x + 1 \right) \left(1 - x + \frac{1}{m} \right) \left(f(q) + \sigma M_{00} \left(x - \frac{1}{m} \right) \right) \\ & - \left((\sigma - 1) \left(x - \frac{1}{m} \right) + 1 \right) x \left(1 - f(q) + L_q x \right). \end{aligned}$$

We factorise what we can and find that

$$\begin{aligned} \zeta(x) = & \left((\sigma - 1)x + 1 \right) \left(-(\sigma - 1)x^2 + \left(-1 + \sigma M_{00} \left(1 + \frac{2}{m} \right) \right) x \right. \\ & \left. + \left(1 + \frac{1}{m} \right) \left(f(q) - \frac{\sigma M_{00}}{m} \right) \right) + \frac{\sigma - 1}{m} x \left(1 - f(q) + L_q x \right). \end{aligned}$$

After developing, we finally obtain

$$\begin{aligned}\zeta(x) = & -(\sigma - 1)^2 x^3 + (\sigma - 1) \left(-1 + (\sigma - 1)r_0 + \frac{\sigma}{m} + R_2 \right) x^2 \\ & + \left((\sigma - 1)r_0 + \frac{2}{m} + (\sigma - 1)f(q) + R_1 \right) x + f(q) - \frac{1}{m} + R_0,\end{aligned}$$

where

$$R_2 = (\sigma - 1) \frac{r_0}{m},$$

$$R_1 = \frac{r_0}{m} - \frac{r_0 + 1}{m^2},$$

and

$$R_0 = -\frac{r_0}{m} + \frac{1}{m} \left(f(q) - \frac{\sigma M_{00}}{m} \right).$$

Now that we have the equation, we follow the strategy and notations of [14]. First, we compute the center of symmetry x_N of the polynomial. If $P = ax^3 + bx^2 + cx + d$, the general expression is $x_N = -b/3a$, here we have

$$x_N = \frac{1}{3} \left(-\frac{1}{\sigma - 1} + r_0 + \frac{\sigma}{m(\sigma - 1)} \right) + o\left(r_0 + \frac{1}{m}\right). \quad (43)$$

We will need the image of that point $y_N = P(x_N)$

$$y_N = P(x_N) = \frac{2}{3^3} \frac{b^3}{a^2} - \frac{bc}{3a} + d.$$

Let us compute each terms independently

$$\frac{2}{3^3} \frac{b^3}{a^2} = \frac{2}{3^3(\sigma - 1)} \left(-1 + 3(\sigma - 1)r_0 + \frac{3\sigma}{m} - 3(\sigma - 1)^2 r_0^2 + o\left(r_0^2 + \frac{1}{m}\right) \right),$$

and

$$\frac{bc}{3a} = \frac{r_0}{3} - \frac{\sigma - 1}{3} r_0^2 + \frac{2}{3m(\sigma - 1)} + \frac{f(q)}{3} + o\left(r_0^2 + \frac{1}{m} + q\right).$$

After factorising, we obtain

$$\begin{aligned}y_N = & -\frac{2}{3^3(\sigma - 1)} \left(1 + \frac{3(\sigma - 1)}{2} r_0 + 3 \frac{7\sigma - 3}{2} \frac{1}{m} - 3^2(\sigma - 1)f(q) \right. \\ & \left. - \frac{3(\sigma - 1)^2}{2} r_0^2 + o\left(r_0^2 + \frac{1}{m} + q\right) \right).\end{aligned}$$

Another interesting quantity we will need is δ , with

$$\delta^2 = \frac{b^2 - 3ac}{9a^2}.$$

Let us take both terms separately, we have

$$\frac{b^2}{9a^2} = x_N^2 = \frac{1}{9} \left(\frac{1}{(\sigma - 1)^2} - 2 \frac{r_0}{\sigma - 1} - \frac{2\sigma}{m(\sigma - 1)^2} + r_0^2 \right),$$

and

$$-\frac{3ac}{9a^2} = -\frac{c}{3a} = \frac{1}{3(\sigma-1)} \left(r_0 + \frac{2}{m(\sigma-1)} + f(q) \right).$$

Therefore,

$$\begin{aligned} \delta^2 = \frac{1}{3^2(\sigma-1)^2} & \left(1 + (\sigma-1)r_0 + \frac{-2\sigma+6}{m} \right. \\ & \left. + 3(\sigma-1)f(q) + (\sigma-1)^2r_0^2 + o(r_0^2 + \frac{1}{m} + q) \right). \end{aligned}$$

Thus, δ expands as

$$\begin{aligned} \delta = \frac{1}{3(\sigma-1)} & \left(1 + \frac{\sigma-1}{2}r_0 + \frac{-\sigma+3}{m} \right. \\ & \left. + \frac{3(\sigma-1)}{2}f(q) + \frac{3(\sigma-1)^2}{8}r_0^2 + o(r_0^2 + \frac{1}{m} + q) \right). \end{aligned}$$

We will also need $h = 2a\delta^3$, we deduce h

$$\begin{aligned} h = -\frac{2}{3^3(\sigma-1)} & \left(1 + \frac{3}{2}(\sigma-1)r_0 + \frac{-3\sigma+9}{m} \right. \\ & \left. + \frac{9(\sigma-1)}{2}f(q) + \frac{15(\sigma-1)^2}{8}r_0^2 + o(r_0^2 + \frac{1}{m} + q) \right). \end{aligned}$$

If $y_N > h$, the equation admits 3 real roots. From these quantities, we define θ with the equation $\cos(3\theta) = -\frac{y_N}{h}$,

$$\cos(3\theta) = -1 - \frac{y_N - h}{h}.$$

where

$$y_N - h = -\frac{1}{m} + f(q) + \frac{(\sigma-1)}{4}r_0^2 + o(r_0^2 + \frac{1}{m} + q),$$

this difference already tells us how many roots the polynomial have. If $mr_0^2 > 1$, then $y_N - h$ is positive which implies $y_N^2 < h^2$, so there are 3 distinct roots. In the other case, there is only one only one root. Let us place ourselves in the former case and compute the roots. We have that,

$$\cos(3\theta) = -1 + \frac{3^3(\sigma-1)}{2} \left(-\frac{1}{m} + f(q) + \frac{(\sigma-1)}{4}r_0^2 + o(r_0^2 + \frac{1}{m} + q) \right).$$

Since $\cos(3\theta)$ is close to -1 , the parameter θ must be close to π , let us set $\theta = \frac{\pi}{3} + u$ which leads to

$$\cos(3\theta) = -1 + \frac{3^2u^2}{2},$$

it means that

$$u = \frac{\sqrt{3}(\sigma-1)}{2}r_0 - \frac{\sqrt{3}}{mr_0} + \frac{\sqrt{3}f(q)}{r_0}.$$

We now have everything we need to express the solutions, the first is $\alpha = x_N + 2\delta \cos \theta$. First, let us develop

$$\cos \theta = \frac{1}{2} - \frac{\sqrt{3}}{2}u.$$

The product $2\delta \cos \theta$ is equivalent to

$$2\delta \cos \theta = \delta(1 - \sqrt{3}u + O(u^2)) = \frac{1}{3(\sigma - 1)} - \frac{r_0}{3} + \frac{1 - mf(q)}{(\sigma - 1)mr_0}.$$

Therefore

$$\alpha = \frac{1 - mf(q)}{(\sigma - 1)mr_0}.$$

The second is $\beta = x_N + 2\delta \cos(\theta + \frac{2\pi}{3})$, the development for the cosine is then

$$\cos\left(\theta + \frac{2\pi}{3}\right) = \frac{1}{2} + \frac{\sqrt{3}}{2}u.$$

In that case, the product $2\delta \cos(\theta + \frac{4\pi}{3})$ is equivalent to

$$2\delta \cos \theta = \delta(1 + \sqrt{3}u + O(u^2)) = \frac{1}{3(\sigma - 1)} + \frac{2r_0}{3} - \frac{1 - mf(q)}{(\sigma - 1)mr_0},$$

thus

$$\beta = r_0 - \frac{1 - mf(q)}{(\sigma - 1)mr_0}.$$

The third root is $\gamma = x_N + 2\delta \cos(\theta + \frac{2\pi}{3})$, for which we have

$$\cos\left(\theta + \frac{2\pi}{3}\right) = -1 + \frac{u^2}{2},$$

hence

$$\gamma = -\frac{1}{\sigma - 1}.$$

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