Evolutionary trajectories in rugged fitness landscapes

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Abstract. We consider the evolutionary trajectories traced out by an infinite population undergoing mutation-selection dynamics in static, uncorrelated random fitness landscapes. Starting from the population that consists of a single genotype, the most populated genotype jumps from one local fitness maximum to another and eventually reaches the global maximum. We use a strong selection limit, which reduces the dynamics beyond the first time step to the competition between independent mutant subpopulations, to study the dynamics of this model and of a simpler one-dimensional model which ignores the geometry of the sequence space. We find that the fit genotypes that appear along a trajectory are a subset of suitably defined fitness records, and exploit several results from the record theory for non-identically distributed random variables. The genotypes that contribute to the trajectory are those records that are not bypassed by superior records arising further away from the initial population. Several conjectures concerning the statistics of bypassing are extracted from numerical simulations. In particular, for the one-dimensional model, we propose a simple relation between the bypassing probability and the dynamic exponent which describes the scaling of the typical evolution time with genome size. The latter can be determined exactly in terms of the extremal properties of the fitness distribution.

Keywords: disordered systems (theory), models for evolution (theory), population dynamics (theory)
1. Introduction

The episodic nature of biological evolution has provided motivation for much work on the modelling of evolutionary dynamics in the statistical physics community [1, 2]; see [3–5] for a review. Evolution displays a punctuated pattern, with epochs of no or slow change interspersed with bursts of (relatively) rapid activity, on various levels ranging from the fossil record [6, 7] to experiments with microbial populations [8–11]. Punctuated behaviour is also seen in simulations of in vitro evolution of RNA molecules [12], optimization algorithms [13, 14], and artificial life [15]. It has been recognized for a long time that one possible scenario that is consistent with punctuated dynamics is the evolution of a population in a static fitness landscape with many peaks. In this picture, the two modes of evolution correspond to the extended periods of residence of the population at a local fitness maximum and the exploration of a new, higher lying peak, respectively, which entails the rapid crossing of a valley of lower fitness [16, 17]. In essence, this is the phenomenon of quantum evolution described by the palaeontologist Simpson 60 years ago [18], and more recently referred to in macroevolutionary theory as punctuated gradualism [6]. If the population is large, so that the distribution of individuals over the
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various phenotypes or genotypes can be modelled by a continuous field, the transition between fitness peaks described above displays analogies with physical processes such as quantum tunnelling [19], variable range hopping [20] or noise-driven barrier crossing.

Since this metastable behaviour seems ubiquitous in nature, it may be worthwhile to study a simple model where this can be analysed in detail. A convenient mathematical framework to address this issue is the quasispecies model, which was originally introduced to describe large populations of self-replicating macromolecules [21, 22]. The quasispecies model is a mutation–selection model whose steady state has been studied in great detail. For various choices of fitness landscapes, it exhibits the phenomenon of error threshold in which beyond a critical mutation rate the population delocalizes over the whole sequence space.

In this paper, we address the question of punctuated dynamics in the quasispecies model. To avoid complications associated with the error threshold phenomenon [4, 22], we work in a strong selection limit inspired by the zero-temperature limit of the statistical mechanics of disordered systems [23] (for a different kind of strong selection limit used in population genetics see e.g. [24]). In this limit, the location of the population in the space of genotypes can be identified with the most populated genotype at all times, and the evolutionary trajectories can be represented in a particularly transparent manner [25]. Since the population is located at a single genotype at any time, the evolutionary trajectory changes in a stepwise manner. To generate an evolutionary trajectory, a localized population is placed at a randomly chosen point in the space of all possible genotypes. Due to infinite population, in the next time step, all genotypes get occupied with non-zero population. As we describe later in detail, it turns out that the fit genotypes typically receive small initial population. Strong selection then reduces the problem to competition between these fit subpopulations struggling to overcome the poor initial conditions.

In the next section, we describe the quasispecies model and derive the reduced representation that arises in the strong selection limit. The bulk of the paper is then devoted to the analysis of the strong selection dynamics, which turns out to be rather closely related to the mathematical theory of records [26–29]. A relation between biological evolution and record statistics has been proposed previously [2, 30]; see also [31].

2. Quasispecies dynamics in the strong selection limit

The quasispecies model is defined on the space of genotypes represented by sequences \( \sigma \equiv \{\sigma_1, \ldots, \sigma_N\} \), where each of the \( N \) letters \( \sigma_i \) is taken from an alphabet of size \( \ell \geq 2 \). The number of individuals of genotype \( \sigma \) at time \( t \) is represented by a real variable \( Z(\sigma, t) \) that obeys the discrete time evolution equation

\[
Z(\sigma, t + 1) = \sum_{\sigma'} p(\sigma' \to \sigma) W(\sigma') Z(\sigma', t). \tag{1}
\]

Here the fitness \( W(\sigma) \) is defined [3] as the expected number of offspring produced by an individual carrying sequence \( \sigma \), and \( p(\sigma' \to \sigma) \) is the probability that genotype \( \sigma \) is created as offspring of genotype \( \sigma' \) due to copying errors in the genome. A simple choice
for the latter corresponds to independent point mutations occurring with probability $\mu$ per generation, so that $p(\sigma' \rightarrow \sigma) = (\mu/(\ell - 1))^{d(\sigma',\sigma)}(1 - \mu)^{N-d(\sigma',\sigma)}$, where

$$d(\sigma', \sigma) = \sum_{i=1}^{N} \left( 1 - \delta_{\sigma_i, \sigma'_i} \right),$$

(2)

is the Hamming distance between sequences $\sigma'$ and $\sigma$.

A constraint of fixed population size could be enforced by dividing the right-hand side of (1) by the population averaged fitness $\langle W \rangle$. This introduces an (inessential) nonlinearity into the problem [3], which is why we prefer to work with the un-normalized population variables $Z(\sigma, t)$. It is clear that within the quasispecies framework, which requires an infinite population from the outset, the actual population size cannot play any role.

To derive the strong selection limit [23], we write $Z(\sigma, t) = e^{\kappa E(\sigma, t)}$, $W(\sigma) = e^{\kappa F(\sigma)}$ and $\mu = e^{-\kappa}$ where $\kappa$ is the inverse selective temperature [3,32] and $E(\sigma, t)$ and $F(\sigma)$ are logarithmic population and fitness variables, respectively. Throughout this paper we take the fitness landscape to be completely uncorrelated, which implies that the fitnesses $F(\sigma)$ are independent, identically distributed (i.i.d.) quenched random variables chosen from a distribution $p(F)$ with support on interval $[F_{\text{min}}, F_{\text{max}}]$. The strong selection limit corresponds to $\kappa \rightarrow \infty$, which yields

$$E(\sigma, t + 1) = \max_{\sigma'} \left[ E(\sigma', t) + F(\sigma') - d(\sigma, \sigma') \right].$$

(3)

Starting with an initial condition $Z(\sigma, 0) = \delta_{\sigma, \sigma^{(0)}}$ in which only a single, randomly chosen sequence $\sigma^{(0)}$ has non-zero population, at the next time step each sequence is seeded with the logarithmic population

$$E(\sigma, 1) = F(\sigma^{(0)}) - d(\sigma, \sigma^{(0)}).$$

(4)

In terms of the original variables $Z(\sigma, t)$, this corresponds to a population distribution that decays exponentially with increasing Hamming distance from $\sigma^{(0)}$. Remarkably, it turns out that for the subsequent time evolution the mutations are unimportant for genotypes with high fitness. Since we are primarily interested in such genotypes, the dynamics of the model can be approximated by allowing each genotype to reproduce with its intrinsic rate $F(\sigma)$ for $t > 1$. In terms of the logarithmic variables, this leads to

$$E(\sigma, t) = E(\sigma, 1) + (t - 1) F(\sigma).$$

(5)

Thus, (3) reduces to a problem of non-interacting sequences whose population is growing linearly in time. The approximation of ignoring mutations after the seeding stage was tested numerically [25] and found to be in very good agreement with the full model described by (3).

A further simplification can be made by noting that due to (4) the population $E(\sigma, 1)$ is the same for all the sequences that lie on a shell of constant Hamming distance $d(\sigma^{(0)}, \sigma)$ away from the sequence $\sigma^{(0)}$. Since we will be interested in the sequence with the largest population at any instant, only the sequence with the largest fitness within a shell needs to be considered. Labelling a shell by its Hamming distance $k = 0, 1, \ldots, N$ from the sequence $\sigma^{(0)}$, we arrive at the shell model [25] in which the population $E(k, t)$ of the fittest sequence in the shell $k$ with a total number of $\alpha_k$ sequences obeys

$$E(k, t) = -k + F(k)t.$$
Figure 1. Time evolution of the logarithmic population variable $E(k,t) = -k + F(k)t$. The fitnesses $F(k)$ of the sequences corresponding to thin green lines are not records whereas those corresponding to bold red lines are. The lines appearing in the upper envelope define the most populated sequence $k^*$; an evolutionary jump occurs when two such lines cross. Note that the sequences $k = 2$ and 6, although constituting fitness records, are bypassed as they do not satisfy the minimum crossing time constraint. The inset shows the punctuated evolution of the most populated sequence $k^*$ as a function of time.

Here $F(k)$ is the maximum of $\alpha_k$ i.i.d. random variables drawn from the fitness distribution $p(F)$; hence, the $F(k)$ are independent but non-identically distributed random variables. To arrive at the simple form (6), we have redefined the population as $E(k,t) + F(k) - F(0)$. The number of sequences in shell $k$ is given by the expression

$$\alpha_k = \binom{N}{k} (\ell - 1)^k,$$

as can be seen by noting that there are $\binom{N}{k}$ ways of choosing $k$ letters at which a sequence $\sigma$ differs from $\sigma^{(0)}$, and each of these $k$ letters can take $\ell - 1$ values. For large $N$, the majority of sequences is contained in a belt of width $\sim \sqrt{N}$ around the distance $k_{\text{max}} = N(\ell - 1)/\ell$ where (7) is peaked.

We will also consider an i.i.d. model for which the population $E(k,t)$ evolves according to (6) but the fitnesses $F(k)$ are i.i.d. random variables. This choice corresponds to a one-dimensional sequence space and we will see that our results are sensitive to the geometry of the sequence space. The i.i.d. model is closely related to the zero-temperature limit of the problem of directed polymers in the presence of columnar defects studied in [33] and a version of the parabolic Anderson model [34].

Figure 1 illustrates the geometric picture of the evolutionary process (6) that emerges after these simplifications and approximations. At a given time $t$, the most populated genotype $k^*$ for which $E(k^*, t) = \max_k \{E(k,t)\}$ leads until it is overtaken by a sequence...
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$k^*$ and so on. While the last leader is obviously located at the global fitness maximum, the identity of the previous leaders is non-deterministic. The inset of figure 1 shows the punctuated evolution of the leading sequence $k^*$. Our main interest in the present work is in the statistical properties of these leadership changes or evolutionary jumps. Initially, the sequence $\sigma^{(0)}$ with population $E(0, t)$ leads. A shell $k'$ can overtake the currently leading shell $k < k'$ at the crossing time $T(k, k')$ given by

$$T(k', k) = \frac{k' - k}{F(k') - F(k)},$$

which is positive provided $F(k') > F(k)$. In figure 1, only the shells $k = 1, 2, 6, 8, 15$ can overtake $k = 0$ (and only $k = 2, 6, 8, 15$ can overtake $k = 1, \ldots$) since $F(15) > F(8) > F(6) > F(2) > F(1) > F(0)$. Such a set of fitnesses in which each value is progressively larger than all the previous ones defines a sequence of records. However, in order to appear in the evolutionary trajectory, it is not sufficient to be a record. As shown in figure 1, the shell $k = 2$ is bypassed by shell $k = 8$ since $T(8, 1) = \min_{k>1} T(k, 1)$. In general, if the current leader is in shell $k$, then the next leader is in the shell $k'$ for which the crossing time (8) is minimized [13]. Thus, in principle, the properties of leadership changes can be formulated in terms of the extremal statistics of the matrix of crossing times. However, as will be explained in more detail in section 7, this minimization problem is too cumbersome to handle analytically and is further complicated by the presence of strong correlations among the crossing times.

The non-trivial dynamics of the change in leadership described above is due to the competition between the initial population at a sequence and its fitness. As discussed above, a potential leader must be a record and hence must occur at a large Hamming distance away from the sequence $\sigma^{(0)}$ but the initial population at such a sequence is small due to (4). Thus, the disadvantage due to poor initial condition may be overcome by a better fitness. Further, since the fitness of the leader is correlated to its Hamming distance from the sequence $\sigma^{(0)}$, the fitness $F(k^*)$ also shows punctuated evolution.

The rest of the paper is organized as follows. In sections 3 and 4, we define records and jumps precisely and study some of their statistical properties, both for the shell model and for the i.i.d. model. In section 5, we describe the dynamics of the approach to the global maximum of the fitness landscape. A conjecture concerning the probability of bypassing in the i.i.d. model, based on the results obtained in sections 4 and 5 along with numerical evidence, is presented in section 6. In section 7, we introduce and discuss a further simplification of the problem described by (6), which highlights the strong interdependence of the crossing times. Finally, we summarize our results and conclude with a brief discussion of the possible biological relevance of this work in section 8.

3. Record statistics in sequence space

In a sequence $\{X_k\}$ of random variables, an upper (or lower) record is said to occur at $m$ if $X_m > X_k$ (or $X_m < X_k$) for all $k < m$ [26]–[29]. Since only the upper records are pertinent to our study, we shall henceforth refer to them as records. In the following subsections, we study some characteristics of these records; in particular, we find the mean number of records and the typical spacing between them. The record statistics of i.i.d. variables is well studied and we briefly review some of the known results as they are

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useful for later discussion. We study the record statistics in the shell model, for which the random variables are not identically distributed, in some detail. An appealing general feature of record statistics is that the results are independent of the underlying probability distribution $p(F)$, which therefore does not need to be specified in this section.

### 3.1. Number of records

In this subsection, we calculate the average number $R_{\text{shell}}$ of records in the shell model. For i.i.d. random variables, it is well known that the average number of records among $N$ variables is $R_{\text{i.i.d.}} \approx \ln N$ for large $N$. To see this, note that the probability $P_{\text{i.i.d.}}(k)$ that the $k$th random variable is a record is equal to the probability that it is the largest among the first $k$ random variables. Since the location of the global maximum is uniformly distributed for i.i.d. variables, it follows that $P_{\text{i.i.d.}}(k) = 1/k$ for any choice of $p(F)$. Summing $P_{\text{i.i.d.}}(k)$ up to $k = N$ yields the average number $R_{\text{i.i.d.}}$ of records to be $\ln N$. In fact, it is known that the probability distribution of the number of records is a Poisson distribution with mean $\ln N$ [2].

The record statistics for non-i.i.d. variables is much less studied. A class of models in which records are obtained from a sequence $\{X_k\}$ where each $X_k$ itself is the maximum of a set of $\alpha_k$ i.i.d. random variables was considered by Nevzorov [35]. Such models have been used, for instance, in an (unsuccessful) attempt to account for the frequent occurrence of Olympic records due to an increasing world population [36]. The i.i.d. model is a special case corresponding to $\alpha_k = 1$ for all $k$ and the shell model is obtained by using $\alpha_k$ given by (7).

To analyse the Nevzorov model, we define a binary random variable $Y_k$ which takes value unity if a record occurs in the $k$th set and zero otherwise. Since the distribution $p_k(F)$ of the maximum of $\alpha_k$ i.i.d. random variables is given by [37]

$$p_k(F) = \alpha_k p(F) \left( \int_{F_{\min}}^{F} p(x) \, dx \right)^{\alpha_k - 1}, \quad (9)$$

we have

$$\text{Prob}(Y_k = 1) = \int_{F_{\min}}^{F_{\max}} dF \prod_{i=0}^{k-1} q_i(F) p_k(F) = \frac{\alpha_k}{(\alpha_0 + \cdots + \alpha_k)}, \quad (10)$$

where $q_k(F)$ is the cumulative distribution corresponding to $p_k(F)$. The above equation expresses the fact that the $k$th record value is a global maximum amongst $\sum_{j=0}^{k} \alpha_j$ variables and there are $\alpha_k$ ways in which it can occur in the $k$th set. Further, the joint probability $\text{Prob}(Y_{k_1} = 1, Y_{k_2} = 1)$ for $k_1 < k_2$ is given by

$$\text{Prob}(Y_{k_1} = 1, Y_{k_2} = 1) = \int_{F_{\min}}^{F_{\max}} dF \prod_{i=0}^{k_1-1} q_i(F) p_{k_1}(F) \int_{F}^{F_{\max}} dG \prod_{j=k_1+1}^{k_2-1} q_j(G) p_{k_2}(G)$$

$$= \frac{\alpha_{k_1} \alpha_{k_2}}{(\alpha_0 + \cdots + \alpha_{k_1})(\alpha_0 + \cdots + \alpha_{k_2})}. \quad (11)$$

In a similar manner, it can be shown that $\text{Prob}(Y_{k_1} = 1, \ldots, Y_{k_m} = 1) = \prod_{j=1}^{m} \text{Prob}(Y_{k_j} = 1)$ for any $m \geq 2$. Thus, the $Y_k$s are independent, non-identically distributed variables [27]–[29].
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For the shell model, due to (7) and (10), the probability $\hat{P}_{\text{shell}}(k, N)$ that a record occurs in the $k$th shell is given by

$$\hat{P}_{\text{shell}}(k, N) = \text{Prob}(Y_k = 1) \approx 1 - \left( \frac{1}{\ell - 1} \right) \frac{a}{1 - a}, \quad a = \frac{k}{N} < \frac{\ell - 1}{\ell} = \frac{k_{\text{max}}}{N},$$

where we have used that $\left( \frac{N}{k-m} \right) / \left( \frac{N}{k} \right) \approx [a/(1-a)]^m$ for $k, N \gg 1$ with $k/N$ fixed. Since it is easier to break records in the beginning, the probability of finding a record is near unity for $k \ll N$. However, it vanishes beyond $k_{\text{max}}$ because the global maximum typically occurs in the shell $k_{\text{max}}$. The average number $R_{\text{shell}}$ of records can be obtained by simply integrating $\hat{P}_{\text{shell}}(k, N)$ over $k$ and we find

$$R_{\text{shell}} \approx \frac{(\ell - \ln \ell - 1)}{\ell - 1} N.$$

Thus, $R_{\text{shell}}$ increases with $\ell$, and as $\ell \to \infty$, $R_{\text{shell}} \to N$ because the population in each shell becomes infinite. Since the $Y_k$ are independent random variables with finite mean and variance, the number of records satisfies the central limit theorem and becomes Gaussian for large $N$. Specifically, for large $N$, the variance of the number of records is

$$\nu_{\text{shell}} = \sum_{k=0}^{N} \text{Prob}(Y_k = 1)[1 - \text{Prob}(Y_k = 1)] \approx \frac{N}{\ell - 1} \left( \frac{\ell + 1}{\ell - 1} \ln \ell - 2 \right),$$

which is maximal for $\ell = 5$ and vanishes for large $\ell$. The ratio $\nu_{\text{shell}}/R_{\text{shell}}$ is always considerably smaller than unity, which implies that the distribution is much sharper than the log-Poisson distribution obtained in the i.i.d. case.

3.2. Inter-record spacings

For the discussion of the spacings between records, it is convenient to label the records ‘backwards’ in time, with $r_1$ denoting the position of the last record (i.e., the global maximum), $r_2 < r_1$ the penultimate record, and so on. In this way the pathologies associated with the fact that the expected waiting time for the next record to occur is infinite in the i.i.d. case [26] can be avoided. The probability $\hat{P}(r_j)$ that the $j$th record occurs at location $r_j$ can be found for the Nevzorov model in a manner analogous to (11). We obtain

$$\hat{P}(r_j) = \sum_{r_1, \ldots, r_{j-1}} \prod_{k=0}^{j-1} \frac{\alpha_{r_{k+1}}}{\alpha_0 + \cdots + \alpha_{r_{k-1}}},$$

with $N \geq r_1 > \cdots > r_{j-1} > r_j$ and $r_0 = N + 1$. The factors on the right-hand side of the above equation simply reflect the fact that the record at location $r_{k+1}$ remains the maximum until the next record occurs at $r_k > r_{k+1}$.

For the i.i.d. model, using $\alpha_k = 1$ for all $k$ in (15), the average location $\langle r_j \rangle = \sum r_j \hat{P}(r_j)$ can be calculated. One finds that the average inter-record distance $\hat{\Delta}_{\text{i.i.d.}}(j) = \langle r_j \rangle - \langle r_{j+1} \rangle$ between the $j$th and $(j+1)$th records behaves as [28, 29]

$$\hat{\Delta}_{\text{i.i.d.}}(j) \approx \frac{N}{2} \left( \frac{1}{2} \right)^j, \quad j = 1, 2, \ldots .$$

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A simple argument, useful for later discussion, can also be employed to obtain the above equation. The record labelled by \( j = 1 \), being the global maximum, is equally likely to occur anywhere between 1 and \( N \). Thus, on average, it is located at \( N/2 \). Similarly, the record labelled by \( j = 2 \) is a global maximum in the range \([1, r_1]\) with uniformly distributed location, which gives the average location \( \langle r_2 \rangle = (1/2) \langle r_1 \rangle = N/4 \). Repeating this argument, we obtain the result in (16).

For the shell model, since the most likely position of the global maximum is in the shell with the largest number \( \alpha_k \) of sequences, we have \( \langle r_1 \rangle = k_{\text{max}} \). For sake of simplicity, we consider binary sequences (\( \ell = 2 \)) in the following but the scaling behaviour obtained below holds for \( \ell > 2 \) as well. We find that for \( j \geq 2 \) the average location \( \langle r_j \rangle \) of the \( j \)th record is given by

\[
\langle r_j \rangle = \langle r_1 \rangle - \frac{1}{\pi} \sqrt{\frac{N}{2}} \left( \frac{2}{\sqrt{\pi}} \right)^{j-2} \int_{-\infty}^{\infty} dx_{j-1} \frac{e^{-x_{j-1}^2}}{\text{erfc}(x_{j-1})} \int_{x_{j-1}}^{\infty} dx_{j-2} \frac{e^{-x_{j-2}^2}}{\text{erfc}(x_{j-2})} \\
\times \cdots \times \int_{x_2}^{\infty} dx_1 \frac{e^{-2x_1^2}}{\text{erfc}(x_1)}, \quad j \geq 2, \tag{17}
\]

where we have used equations (A.1)–(A.3) and performed a Gaussian integral. The average location \( \langle r_2 \rangle \) of the second record is given by \( \langle r_2 \rangle = \langle r_1 \rangle - 2.0064\sqrt{N/\pi\sqrt{2}} \). Thus, the second record (and in fact, \( j \)th record for \( j \) of order unity) can be found within \( \mathcal{O}(\sqrt{N}) \) distance of the global maximum since \( \alpha_k \) has width \( \sim \sqrt{N} \) about \( k_{\text{max}} \). For \( j > 2 \), after repeated integration by parts, (17) can be rewritten as

\[
\langle r_j \rangle = \langle r_1 \rangle - \frac{1}{\pi} \sqrt{\frac{N}{2}} \sum_{m=1}^{j-2} \frac{(\ln 2)^{j-2-m}}{(j-2-m)!} G(m), \quad j > 2, \tag{18}
\]

where

\[
G(m) = (-1)^m \int_{-\infty}^{\infty} dx \frac{e^{-2x^2}}{\text{erfc}(x)} \frac{(\ln \text{erfc}(x))^m - (\ln 2)^m}{m!}. \tag{19}
\]

As outlined in appendix A, the integral \( G(m) \) can be estimated by the saddle point method and we find \( G(m) \approx \sqrt{\pi m/2} \) for large \( m \). Since the leading contribution to the sum in (18) comes from the \( m = j - 2 \) term, we have

\[
\tilde{\Delta}_{\text{shell}}(j) \approx \sqrt{\frac{N}{4\pi j}}, \quad j \gg 1. \tag{20}
\]

Thus, while the inter-record spacing decays exponentially with \( j \) for the i.i.d. model, it falls as a power law for the shell model. The spacing between the first few records (\( j = \mathcal{O}(1) \)) is of order \( \sqrt{N} \), while for the bulk of the records with \( j = \mathcal{O}(N) \) the spacing is of order unity; this is consistent with the vanishing of the record occurrence probability (12) near \( k = k_{\text{max}} \).
4. Jump statistics

As we described in section 2, in our model evolutionary jumps are a subset of records, and if a jump occurs at $k'$ the next jump is said to occur at $k > k'$ if (i) $F(k)$ is a record and (ii) the overtaking time $T(k,k') = \min_{j \geq k'} \{T(j,k')\}$. By convention, the first jump and the first record occurs at $k = 0$. Due to the second condition, some of the records can be bypassed and fail to appear in the set of jumps. In this section, we find the mean number of jumps and the inter-jump spacing for both the i.i.d. and the shell model. In contrast to the properties of records, the statistics of jumps depends explicitly on the fitness distribution $p(F)$ and we will consider distributions for which the tail behaviour corresponds to the three universality classes of standard extreme value theory [38] and which also appear in a very similar form in the theory of records [27]–[29].

4.1. Mean number of jumps

We begin by discussing numerical results for the average number of jumps in the i.i.d. model. It was found in [25] that the average number $J_{i.i.d.}$ of jumps grows as $\beta \ln N$ where the prefactor $\beta < 1$, and was conjectured to be

$$
\beta \approx \begin{cases} 
1/2, & \text{if } p(F) = 1 \\
(\delta - 1)/(2\delta - 1), & \text{if } p(F) \sim e^{-F} \\
(2+\nu)/(3+2\nu), & \text{if } p(F) \sim (F_{\text{max}} - F)^\nu, \quad \nu > -1.
\end{cases}
$$

(21)

Figure 2 shows $J_{i.i.d.}$ increasing linearly with $\ln N$ and slope $\beta$ for some distributions in accordance with (21). Thus, in the i.i.d. model the jumps can be viewed as ‘diluted’
records, in the sense that the mean numbers of records and jumps differ only up to a prefactor and the probability $P_{i \text{i.d.}}(k, N)$ that a jump occurs at $k$ is given by $\beta/k$. In this picture, the probability for a given record to be bypassed is simply $1 - \beta$. However, bypassing is not completely random, as the variance of the number of jumps is found consistently to be smaller than the mean. This implies a certain amount of ‘anti-bunching’ among the jumps, which can also be detected by the direct measurement of correlation $C_{i \text{i.d.}}(k_1, k_2) = P_{i \text{i.d.}}(k_1, k_2) - P_{i \text{i.d.}}(k_1)P_{i \text{i.d.}}(k_2)$ where $P_{i \text{i.d.}}(k_1, k_2)$ is the joint distribution of having a jump at $k_1$ and $k_2$, as shown in the inset of figure 4. Some further discussion of the conjecture (21) will be provided in section 6.

Estimates for the mean number of jumps in the shell model were also given in [25], but the range of sequence lengths was too limited to allow for a definite statement. Here we present the results of our simulations for large values of $N$ obtained using the approximation described below. Since the shell fitness $F(k)$ is the maximum of $\alpha_k$ i.i.d. random variables drawn from the distribution $p(F)$, it can be obtained from a uniform random variable $u$ using the relation

$$\int_{F_{\text{min}}}^{F(k)} p(x) \, dx = u^{1/\alpha_k}. \quad (22)$$

However, the binomial coefficient $\binom{N}{k}$ increases exponentially with $N$ for large $k$ and the distribution of $u^{1/\alpha_k}$ approaches a delta-function centred at unity for $k \gg 1$ making it difficult to determine the distribution $p_k(F)$ of $F(k)$ accurately when $N$ is large. For the exponential fitness distribution, the relation (22) becomes

$$F(k) = -\ln(1 - e^{\ln u/\alpha_k}) \simeq -\ln[\ln(1/u)] + \ln(\alpha_k). \quad (23)$$

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Figure 3. Data collapse for the scaled jump distribution $\sqrt{N}P_{\text{shell}}(k, N)$ versus $k/N$ for the shell model with $\ell = 2$ and $p(F) = e^{-F}$. Inset: scaled inter-jump spacing $\Delta_{\text{shell}}(j)/\sqrt{N}$ versus $j/\sqrt{N}$ to show that jumps are roughly equally spaced in the shell model.
Since the last expression only involves the logarithms of binomial coefficients, \( F(k) \) can be easily generated up to large values of \( N \). While a similar approximation can be employed for other distributions with unbounded tails, we have not been able to obtain reliable results for bounded distributions.

In figure 3, we show simulation results for the probability \( P_{\text{shell}}(k, N) \) that a jump occurs in the \( k \)th shell, for a binary alphabet (\( \ell = 2 \)) and two different values of \( N \). The data collapse onto the scaling form

\[
P_{\text{shell}}(k, N) \approx N^{-1/2} f(k/N), \quad x < \frac{\ell - 1}{\ell} = \frac{k_{\text{max}}}{N},
\]

where the scaling function behaves as \( f(x) \sim x^{-1/2} \) for small \( x \). This has the interesting consequence that \( P_{\text{shell}} \sim 1/\sqrt{k} \) is independent of \( N \), and hence the number of jumps grows as \( \sqrt{k} \) for \( k \ll k_{\text{max}} \). The scaling function appears to be independent of the alphabet size \( \ell \), which therefore only changes the cut-off at \( k = k_{\text{max}} \) [31]. Thus, the average number \( J_{\text{shell}} \) of jumps obtained by integrating \( P_{\text{shell}}(k, N) \) over \( k \) grows with \( N \) as

\[
J_{\text{shell}} \sim \sqrt{\frac{(\ell - 1)N}{\ell}}.
\]

Our simulations indicate that the above dependence of \( J_{\text{shell}} \) on \( N \) is also true for normal-distributed fitness and we expect it to hold for all distributions decaying more rapidly than any power law [31]. Further, the distribution of the number of jumps is a Gaussian (as in the case of records) with both mean and variance scaling as \( \sqrt{N} \).

For the power law case, we find that \( J_{\text{shell}} \to 1 \) for large \( N \). As we shall see in section 5, the globally fittest sequence takes over the leadership in a time of order unity in
this case, which explains the above behaviour of $J_{\text{shell}}$. In summary, unlike the i.i.d. model, most of the records are bypassed in the shell model for both exponential and power law distributions.

4.2. Inter-jump spacings

We now turn to a discussion of the inter-jump spacings $\Delta(j)$ defined in analogy to the inter-record spacings. We denote by $s_j$ the position of the $j$th jump, with $j = 1$ referring to the last jump, which is also the last record (the global maximum), and define the inter-jump spacing as $\Delta(j) = \langle s_j \rangle - \langle s_{j+1} \rangle$ where $\langle s_j \rangle$ is the average location of the $j$th jump. For the i.i.d. model, an approximate calculation of $\Delta_{\text{i.i.d.}}(j)$ can be carried out by assuming jumps to be randomly diluted records. The position $s_j$ of the $j$th jump equals the position $r_k$ of the $k$th record, where $k \geq j$ because of the possibility of bypassing. If the record $k + 1$ is not bypassed, then $s_{j+1} = r_{k+1}$ and $s_{j+1} = (1/2)s_j$ on average due to the argument given after (16) for the inter-record spacings. In the diluted record picture, this is true with probability $\beta$. With probability $\beta(1 - \beta)$, record $k + 1$ is bypassed and $s_{j+1} = r_{k+2}$ so that $s_{j+1} = (1/4)s_j$ on average. Similarly, with probability $\beta(1 - \beta)^l$, $l$ records are bypassed and the ratio $s_{j+1}/s_j = (1/2)^{l+1}$ on average. Summing over all possibilities, we find that $\langle s_{j+1} \rangle = b(s_j)$ with

$$b = \sum_{l=0}^{\infty} 2^{-(l+1)} \beta(1 - \beta)^l = \frac{\beta}{1 + \beta}. \quad (26)$$

Taking into account that the sum over all inter-jump spacings adds up to $\langle s_1 \rangle = \langle r_1 \rangle = N/2$, we obtain

$$\Delta_{\text{i.i.d.}}(j) \approx \frac{N}{2} (1 - b) b^{j-1}, \quad j = 1, 2, \ldots. \quad (27)$$

The numerical data shown in figure 4 support the general form of this expression, but with the coefficient $b \approx \beta/2$ rather than $\beta/(1 + \beta)$. This is another indication of correlations that are not accounted for in the random dilution picture.

For the shell model, as shown in figure 3, the data for $\Delta_{\text{shell}}(j)$ for various $N$ collapses onto a monotonically decreasing curve if we assume $\Delta_{\text{shell}}(j)$ to be of the scaling form

$$\Delta_{\text{shell}}(j) \approx \sqrt{N} h(j/\sqrt{N}). \quad (28)$$

The scaling with $\sqrt{N}$ follows naturally from the scaling form (24) for the jump occurrence probability. The latter implies that the density of jumps on the $k$-axis is of order $1/\sqrt{N}$ for finite $k/N$, hence the spacing is of order $\sqrt{N}$, and the argument of the scaling function is $j/\sqrt{N}$ because the total number of jumps is also of order $\sqrt{N}$. However, the tail of the scaling function $h$ does not obey the scaling form (28) and approaches zero with increasing $N$. Thus, while for finite $k/N$, the jumps are roughly equally spaced with spacing $\sqrt{N}$, the spacing is of $O(N^s)$ with $s < 1/2$ for $k/N \to 0$.  

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5. Approach to the global fitness maximum

So far, we have discussed the statistics on the $k^*$ axis of the inset of figure 1 and now we focus on the temporal statistics. As explained in section 2, a fit sequence $k^*$ leads until it is overtaken by an even fitter one and eventually the globally fittest sequence emerges as the leader at typical time $T^*$. In this section, we find this typical time $T^*$ required for the population to reach the global maximum of the fitness landscape and the distribution of the evolution times to jump from one local maximum to another.

5.1. Dynamic scaling

The location $k^*(t)$ of the most populated sequence at time $t$ for which the logarithmic population is $E(k^*, t) = \max_k \{E(k, t)\}$ increases with time until the global maximum is reached. In appendix B, the distribution $P_t(k^*)$ is explicitly calculated for the i.i.d. model in the limit of infinite genome size ($N \to \infty$). This distribution is usually of the scaling form

$$P_t(k^*) = t^{-1/z} \Phi(k^*/t^{1/z}),$$

where the scaling function $\Phi$ depends on the underlying fitness distribution and the dynamic exponent $z$ is given by

$$z = \begin{cases} 
1, & p(F) \sim e^{-F} \\
(2 + \nu)/(1 + \nu), & p(F) \sim (F_{\text{max}} - F)^\nu, \quad \nu > -1 \\
(\delta - 1)/\delta, & p(F) \sim F^{-1-\delta}, \quad \delta \geq 1,
\end{cases}$$

for the three classes of fitness distributions introduced in section 4. The corresponding behaviour $k^*(t) \sim t^{1/z}$ of the mean location has been derived previously using Flory-type arguments [20,33] and can also be seen using (29). As we have already discussed, the global maximum is reached when $k^*(t) \approx N/2$, which defines a total evolution time $T^* \sim N^z$. One thus expects a scaling form

$$k^*(t, N) \approx t^{1/z} \varphi(t/T^*),$$

where the scaling function $\varphi(x)$ is a constant for $x \ll 1$ and decays as $x^{-1/z}$ for $x \gg 1$.

An alternative approach [23,25] to estimating the typical time $T^*$ required by the population to reach the global maximum starts from the observation that $T^*$ is of the order of the time $T_1$ at which the globally fittest sequence at typical location $r_1 = s_1$ and fitness $F(r_1)$ overtakes the penultimate leader with respective quantities $s_2$ and $F(s_2)$ (refer to section 4.2). From (8), we have

$$T_1 = \frac{s_1 - s_2}{F(s_1) - F(s_2)},$$

where the inter-jump spacing in the numerator is given by (27). The estimation of the denominator involves a subtlety—in previous works [23,25], it was assumed that $F(s_1) - F(s_2)$ is of the order of the fitness gap $\epsilon$, which was defined as the difference $1$. This scaling form is not true for power law distributed fitness with $1 < \delta \leq 2$, because the scaling function $\Phi$ in (29) does not possess a first moment in this case (see (B.10)). Nevertheless, the timescale $T^* \sim N^z$ with $z$ given in (30) for all $\delta > 1$. 

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between the values of the global maximum and the second largest fitness of the fitness landscape. Because the second largest fitness does not necessarily appear in the record sequence, $\epsilon$ is only a lower bound on $F(r_1) - F(r_2)$, which in turn is clearly a lower bound on the fitness difference of interest, $\epsilon \leq F(r_1) - F(r_2) \leq F(s_1) - F(s_2)$. However, our explicit calculations show that $F(r_1) - F(r_2)$ is of the same order as $\epsilon$; moreover, at least for the i.i.d. model, we know that at most a few records are bypassed between $s_1$ and $s_2$, and hence the assumption that $F(s_1) - F(s_2) \sim \epsilon$ seems justified.

The calculation of the distribution of fitness gap $\epsilon$ is a standard exercise in extreme value statistics [37]. In a system with a total number $S$ of sequences, the typical value of the fitness gap increases as $S^{1/\delta}$ for the unbounded power law distribution, decreases as $S^{-1/(1+\nu)}$ for the bounded distribution, and is of order unity for the exponential distribution. For the i.i.d. model, using $s_1 - s_2 \sim N$ (see (27)) and $S = N$ in (32), we recover $T_1 \sim T^* \sim N^z$ with $z$ given in (30). The other fitness distributions can be treated in a similar manner.

For the shell model, $S = \ell^N$ and due to (28), the numerator is of order $\sqrt{N}$ so that $T^* \sim \sqrt{N}$ for the case of exponentially distributed fitness. Presumably, the time $T_j$ at which the $j$th jump occurs is also of order $\sqrt{N}$ for $j \sim O(1)$. Since the total number of jumps is of the same order, it follows that initially there are many, quick jumps followed by a few jumps that take $O(\sqrt{N})$ time. This result agrees qualitatively with that seen in experiments (discussed later) concerning the pace of evolution which is initially rapid and later slows down considerably. For the bounded distributions, $T^*$ increases exponentially with $N$ whereas it decreases exponentially for the fat-tailed power law distributions. The latter result implies that, for large $N$, the global maximum takes over in a single time step, which explains why the mean number of jumps tends to unity for the power law distributions (see section 4.1).

### 5.2. Universal tails of the evolution time distribution

In the last subsection, we found the typical time $T^*$ to reach the global maximum and now we consider the distribution $P(T_1, N)$ of the time $T_1$ at which the final jump occurs. For the i.i.d. model, since the typical $T_1$ also grows as $N^z$, we may expect the normalized distribution $P(T_1, N)$ to be of the scaling form $P(T_1, N) \approx N^{-z}g_1(T_1/N^z)$. In general, for $j \sim O(1)$, the distribution $P(T_j, N)$ of the time $T_j$ at which the $j$th jump occurs is of the scaling form

$$P(T_j, N) \approx N^{-z}g_j(T_j/N^z).$$

(33)

Although the dynamic exponent $z$ depends on the underlying fitness distribution, we shall now show that the tail of the distribution $P(T_j, N)$ is universal. The events contributing to large $T_1$ are the ones for which $F(s_1) - F(s_2)$ is small; in these cases we expect the general bound $F(s_1) - F(s_2) \geq F(r_1) - F(r_2)$ to be saturated, i.e. the second record is not bypassed and $s_2 = r_2$. Thus, using (32), we obtain

$$P(T_1, N) \approx \left| \frac{d\epsilon_1}{dT_1} \right| \text{Prob}(\epsilon_1 = \Delta_{i,i.d.}(1)/T_1) \approx \frac{\Delta_{i,i.d.}(1)}{T_1^2} \text{Prob}(\epsilon_1 = 0),$$

(34)

for large $T_1$, where $\epsilon_1 = F(r_1) - F(r_2)$. The probability distribution of $\epsilon_1$ can be obtained along the lines of the derivation of the distribution of the fitness gap $\epsilon$ in [23], and it is found
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Figure 5. Log–log plot for the ratios $P(T_2)/P(T_1)$ and $P(T_3)/P(T_2)$ of evolution time distributions for the i.i.d. model with $p(F) = e^{-F}$. The ratios decay as $1/T$ for large $T$, as the line with slope $-1$ indicates.

that the probability for a near-vanishing difference between two successive record values is non-zero for any $p(F)$. We conclude that $P(T_1, N)$ has a power law tail with exponent $-2$ for any underlying fitness distribution [25]. This is an example of the generation of a power law through a change of variables (from $\epsilon_1$ to $T_1 \sim 1/\epsilon_1$) as described in [38].

Similarly, the events contributing to the tail of $P(T_2, N)$ are the ones in which the record at $r_2$ is the penultimate leader and the record at $r_3$ is the leader previous to it. Thus, we demand that neither of these two records should be bypassed; in particular, $r_2$ should not be bypassed, which requires that $T(r_1, r_2) > T(r_2, r_3)$. This condition can be written as $\epsilon_1 < C \epsilon_2$, where $\epsilon_2 = F(r_2) - F(r_3)$ and $C$ is the average value of $(r_1 - r_2)/(r_2 - r_3)$, a number of order unity. Thus we obtain

$$P(T_2, N) \approx \frac{\Delta_{i.i.d., (2)}(N)}{T_2} \int_0^{C \Delta_{i.i.d., (2)}(N)/T_2} d\epsilon_1 \text{Prob}(\epsilon_1, \epsilon_2, N)$$

$$\approx \frac{C \Delta_{i.i.d., (2)}(N)^2}{T_2^3} \text{Prob}(\epsilon_1 = 0, \epsilon_2 = 0, N).$$

(35)

Since $\text{Prob}(\epsilon_1 = 0, \epsilon_2 = 0, N)$ can be shown to be non-zero, we conclude that $P(T_2, N) \sim T_2^{-3}$ for large $T_2$. Extending the above arguments in a similar fashion to the next evolution times, we find that the scaling functions in (33) behave as $g_j(x) \sim x^{-1-j}$ for $x \gg 1$. Interestingly, this implies that the expected time $\langle T_j \rangle$ is finite for $j \geq 2$ and infinite for $j = 1$. In figure 5, the prediction $P(T_j, N) \sim T^{-1-j}$ for $j = 1, 2, 3$ is compared with data obtained using Monte Carlo simulations for the i.i.d. model. The behaviour of the universal tails of $P(T_j)$ discussed above is true for the shell model as well.
6. Bypassing probability and dynamic exponent: a conjecture

As we have seen in the previous sections, the jump statistics are not analytically tractable due to the constraint of minimal overtaking time. For the i.i.d. model, the jumps differ from the records only up to a prefactor $\beta$ conjectured to be given by (21). Comparing the expressions in equations (21) and (30), we observe that the bypassing probability $1 - \beta$ appears to be related to the dynamic exponent $z$ by the following universal relation:

$$\beta = (1 - \beta)z. \quad (36)$$

A derivation of this relation (which eludes us so far) would constitute a proof of the conjecture (21).

Interestingly, the relation (36) can be interpreted in terms of a kind of duality between the $k$- and the $t$-axis of the inset of figure 1. So far we have identified each jump with the position on the $E$-axis where the line that takes over the leadership when the jump occurs originates, but we may just as well identify the jump with the corresponding crossing time $T(k, k')$ at which the leadership shifts from $k'$ to $k$. Clearly, there is a one-to-one correspondence between the jumps defined on two axes and the average number $\mathcal{J}_{i.i.d}^\prime$ of jumps on the time axis is equal to $\mathcal{J}_{i.i.d}$ discussed in earlier sections. Thus, $\mathcal{J}_{i.i.d}^\prime = \mathcal{J}_{i.i.d} \approx \beta \ln N$ and since the typical time $T^\ast$ to reach the global maximum scales as $N^z$ we have $\mathcal{J}_{i.i.d}^\prime \approx \beta' \ln T^\ast$ with $\beta' = 1 - \beta$ due to the conjecture (36). This leads us to expect that the probability $P_{i.i.d}(t, N)$ that a jump occurs at time $t$ decays as $\beta' / t$ for $t \ll N^z$ and as $1 / t^2$ for $t \gg N^z$; the latter behaviour is the universal $t^{-2}$ tail explained in...
section 5. We conclude that the sum of the jump probabilities along the $k$- and the $t$-axes should sum up to a universal function, i.e.

$$P_{\text{i.i.d.}}(t = X, N) + P_{\text{i.i.d.}}(k = X, N) = 1/X,$$

(37)

for any choice of fitness distribution. The numerical evidence supporting this claim is shown in figure 6. Furthermore, in analogy to the jump spacing $\Delta_{\text{i.i.d.}}(j)$ along the $k$-axis, one can also consider the quantity $\Delta'_{\text{i.i.d.}}(j) = \langle T_j \rangle - \langle T_{j+1} \rangle$ which is the spacing between the successive jumps on the time-axis. Replacing $N$ by $T^*$ and $b = \beta/2$ by $\beta'/2 = (1-\beta)/2$ in (27), we expect

$$\Delta'_{\text{i.i.d.}}(j) \sim N^z \left( \frac{1-\beta}{2} \right)^{j-1}, \quad j = 1, 2, \ldots$$

(38)

Numerical results consistent with this expression are shown in the inset of figure 6 for some distributions. The deviations seen in the data for the first jump ($j = 1$) reflect the fact that, because of the $1/T^*_2$-tail derived in equation (34), the average of $T_1$ is not defined and hence grows with the number of disorder realizations.

7. A model based on record times

In this section, we introduce a further simplification of the i.i.d. model. As we have discussed already, a sequence $k$ may occur in the set of jumps provided $F(k)$ is a record. Thus, it is sufficient to consider only the subset of sequences whose fitness is a record. Here it is convenient to label the records forward in time, so we denote by $R_j$ the location of the $j$th record with $j = 1$ labelling the first record ($R_1 = 1$ by convention), $R_2 > R_1$ the second record, and so on. Note that there are two sources of randomness in the problem—one arising from the record locations $R_j$ and the other due to record values $F(R_j)$. For
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exponentially distributed fitness, it is known that the differences between successive record values are independent and exponentially distributed random variables [39]. Thus, the fitness of two successive records differs by unity on average. These considerations allow us to eliminate the randomness associated with the record values by replacing the i.i.d. model of (6) with exponentially distributed fitness by a simpler model for which the population evolves as

$$\bar{E}(j, t) = -R_j + jt.$$ (39)

As in the original i.i.d. model, we find numerically that the average number $\bar{J}$ of jumps grows logarithmically with $N$ with a prefactor $\bar{\beta} \approx 0.63$ (see figure 7). This is distinctly different from the value $\beta \approx 1/2$ found for the i.i.d. model with exponential fitness distribution, indicating that the randomness in the record values is relevant. Somewhat surprisingly, in contrast to the conjectured values of $\beta$ for the full i.i.d. problem given in (21), $\bar{\beta}$ does not seem to be a simple rational number.

Our primary motivation for introducing this simplified model is to gain further insight into the mathematical structure of bypassing. For the model defined by (39), the crossing time $\bar{T}(j, j')$ at which the line associated with the $j$th record overtakes that associated with record $j'$ is given by

$$\bar{T}(j, j') = \frac{R_j - R_{j'}}{j - j'}.$$ (40)

Then the probability $\bar{\beta}_2$ that the second record is not bypassed can be written as

$$\bar{\beta}_2 = \text{Prob} \left[ R_2 - 1 = \min \left( R_2 - 1, \frac{R_3 - 1}{2}, \frac{R_4 - 1}{3}, \ldots \right) \right].$$ (41)

The evaluation of the condition on the right hand side using the joint probability distribution for the record times [27]–[29]

$$\text{Prob}(R_2, R_3, \ldots, R_n) = \frac{1}{(R_2 - 1)(R_3 - 1)(R_4 - 1)\cdots (R_n - 1)R_n}$$ (42)

is clearly a difficult task. An upper bound on $\bar{\beta}_2$ is obtained by requiring that the record at $R_2$ is not bypassed by the one at $R_3$, i.e. that $\bar{T}(2, 1) < \bar{T}(3, 1)$. This gives

$$\bar{\beta}_2 \leq \text{Prob}(R_3 > 2R_2 - 1) = \sum_{R_2=2}^{\infty} \frac{1}{R_2 - 1} \frac{1}{2R_2 - 1} = 2(1 - \ln 2) \approx 0.613706.$$ (43)

In our simulations on a large system, we find $\bar{\beta}_2 \approx 0.600786$, showing that bypassing of $R_2$ by the records beyond $R_3$ is rather unimportant.

Consider next the behaviour of the crossing times (40) when $j$ and $j'$ are large. Williams [40] has shown that the sequence of record times can be generated from the recursion relation [26]–[29]

$$R_{j+1} = [e^{X_j}R_j] + 1,$$ (44)

where the $X_j$ are independent, exponentially distributed random variables with mean one, and $[a]$ is the integer part of $a$. For large $j$, the integer constraint can be ignored, and hence

$$\bar{T}(j, j') \approx \frac{R_j}{j - j'} \left[ \exp \left( \sum_{i=j'+1}^{j} X_i \right) - 1 \right].$$ (45)
Recalling that the choice of the next non-bypassed record involves finding the minimum among all crossing times $\tilde{T}(j, j')$ with $j > j'$, we see that the current location $R_j$ cancels in the comparison between two such crossing times. The problem thus acquires translation invariance in the record space, in the sense that the position of the next non-bypassed record depends only on $j - j'$ and on the random variables $X_i$ associated with the records between $j'$ and $j$. It is therefore plausible that the bypassing probability tends to a constant for large $j$, and one is tempted to describe the process by a Markov chain on the set of records with the transition probability

$$P_{j', j} = \text{Prob} \left[ \tilde{T}(j, j') = \min_{n > j'} \tilde{T}(n, j') \right].$$

(46)

This is the conditional probability that the next jump occurs at $j$, given that the preceding jump was at $j'$, averaged over all realizations of record times. Using the representation (45), the $P_{j, j'}$ are manifestly translationally invariant for large $j, j'$, depending only on $j - j'$. Even in the asymptotic limit in which the expression (45) can be used, the evaluation of (46) is cumbersome, but an analytic upper bound on $P_{j, j+1}$ can be obtained along the lines of (43). In the limit of large $j$, we can write

$$P_{j, j+1} \leq \text{Prob}[\tilde{T}(j + 1, j) < \tilde{T}(j + 2, j)] = \text{Prob}[e^{X_{j+1}} + e^{-X_j} > 2] = \ln 2,$$

(47)

where $X_j$ and $X_{j+1}$ are the independent exponential random variables used in the representation (44). The numerical evaluation of (46) yields $P_{j, j+1} \approx 0.669$, $P_{j, j+2} \approx 0.225$ and $P_{j, j+3} \approx 0.075$, indicating a roughly exponential decay of the transition probability. From the $P_{j', j}$, the mean density of jumps (non-bypassed records) can be computed according to

$$\tilde{\beta}_{\text{Markov}} = \left( \sum_{n=1}^{\infty} n P_{j, j+n} \right)^{-1} \approx 0.676,$$

(48)

which is significantly larger than the direct numerical estimate $\tilde{\beta} \approx 0.63$ (see figure 7). This shows that the transition probability (46) is not an exact representation of the process. The reason is that (46) is an annealed average, whereas in the full problem the record times (or, equivalently, the exponential random variables in (44)) must be treated as quenched: Minimizing the crossing times $\tilde{T}(j, j')$ for a given $j'$ involves, in principle, all $j > j'$, and the same set of random variables is used every time this minimization is repeated for different $j'$.

We thus have to conclude that the range of attainable analytic results, even for the simplified problem (39), is very limited. An extension of the bound (43) to the full i.i.d. model should be feasible using the representation of the joint distribution of record times and record values through a Markov chain [28, 29]; however, as such a bound is unlikely to provide much insight into the conjectured relation (36), we have not pursued this approach.

8. Conclusions

In this paper, we have characterized the evolutionary trajectories traced out by a quasispecies population in an uncorrelated rugged fitness landscape. These trajectories approach the global fitness maximum through a sequence of jumps which mark a change
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in the identity of the most populated genotype. The statistics of these evolutionary jumps has been studied mainly numerically. However, useful insights were provided by a study of record statistics which could be handled analytically. It was found that the jump statistics are qualitatively similar to records, but there are quantitative differences because, as shown in figure 1, a record breaking genotype can be bypassed by a superior one before it can acquire dominance in the population (i.e. qualify to be a jump).

The statistics of records and jumps depends strongly on the geometry of the space of genotypes. The natural setting for genotype evolution is the Hamming space of sequences of fixed length N. However, computational effort could be greatly reduced by lumping together the sequences within a shell of constant Hamming distance with respect to the initial population [25]. Complementary to this shell model, we also considered a model of i.i.d. shell fitnesses, which corresponds effectively to a one-dimensional sequence space. While for the i.i.d. model, the average number of jumps differs from the number of records only through the prefactor β of the logarithm of N, for the shell model the ratio of the two numbers $J_{\text{shell}}/R_{\text{shell}} \to 0$ as $N \to \infty$. For fat-tailed fitness distributions the evolutionary trajectories in the shell model may even degenerate, in the sense that the global fitness maximum is reached in a single step. For distributions decaying faster than a power law, like the exponential and normal distributions, we find numerically that $J_{\text{shell}} \sim \sqrt{N}$; an analytic understanding of this result would be very desirable.

A universal feature of the evolutionary trajectories, which is independent of the geometry of genotype space as well as of the fitness distribution, is the hierarchy of power law tails for the distributions of the times at which the jumps occur. In particular, the $T^{-2}$-tail for the total evolution time implies that the average of $T$ is infinite. The dependence of the typical evolution time on the size of the sequence space can be characterized by a dynamic exponent $z$, which was obtained exactly in terms of the extremal properties of the fitness distribution. On a mathematical level, perhaps the most intriguing result of this work is the conjectured relation (36) between β and $z$ for the i.i.d. model. It would be extremely interesting to understand how such a simple relation arises from the properties of the matrix of crossing times (8); however, in view of the difficulties encountered even in the analysis of the simplified problem (39), we do not see at present how further progress in this direction can be achieved.

In this paper, we have worked in the limit of infinite population and strong selection. However, we expect our results to hold, at least qualitatively, for finite selective temperature as well. The jumps appear instantaneous in the strong selection limit; at finite selective temperature they take a finite amount of time in which the peak associated with the new leader catches up with the currently dominating peak and the population distribution briefly becomes bimodal [13, 19, 33]. Although the quasispecies theory, which works in the infinite population limit, is inadequate to address the fluctuation effects that become important when small mutant populations cross a fitness valley [41], for the related problem of episodic behaviour in evolutionary computation [14], some of the finite population behaviour has been understood on the basis of the infinite population limit. Thus we expect our investigation to give some insight into the behaviour of finite populations in rugged fitness landscapes [42, 43] as well.

We close with some remarks on the applicability of the present work to the evolution of biological populations. A realization of asexual mutation–selection dynamics in a static fitness landscape that is believed to be quite rugged is provided by the
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long-term experiments on populations of Escherichia coli carried out by Lenski and collaborators [8,9,11]. These experiments show evidence for punctuated behaviour both in the fitness and in the morphological features (such as cell size) of the evolving populations, which is attributed to the emergence and fixation of beneficial mutations. Fixation implies that a mutation which is initially present only in a single individual is inherited by a growing fraction of the population and eventually acquires dominance.

At least on a qualitative level, this process corresponds in our model to that in which a subpopulation residing in a distant shell of sequence space takes over the leadership of the population, as described by (6) and illustrated in figure 1. The bypassing of one subpopulation by another is analogous to the phenomenon of clonal interference, in which one beneficial mutation is superseded by another one before reaching fixation [44]. The key difference between our model and the behaviour of real asexual evolution is that in the latter case beneficial mutants arise through the stochastic search of a finite population in an immensely large sequence space, while in the quasispecies model all possible mutants are present (in extremely small numbers) after the first time step. It is, therefore, mandatory to include the stochastic finite population dynamics into the model. Nevertheless, some features of the competition between the mutant populations (however they may have arisen) could well survive in a more complete, realistic treatment.

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Appendix A. Inter-record spacing for the shell model

Using the Stirling formula \( r! \approx \sqrt{2\pi r} (r/e)^r \) in the binomial coefficient \( \binom{N}{r} \) for \( r, N \gg 1 \) with \( r/N \) fixed and expanding \( \binom{N}{r} \) about its maximum at \( r = N/2 \), we have

\[
\frac{1}{2^N} \binom{N}{r} \approx \sqrt{\frac{2}{\pi N}} \exp \left[ -\frac{(N/2 - r)^2}{N/2} \right].
\]  

This expression can be used to show that

\[
\frac{1}{2^N} \sum_{r=0}^{y} \binom{N}{r} \approx \frac{1}{2} \text{erfc}(\alpha)
\]  

by approximating the sum on the left-hand side by an integral. In the above expressions, \( \alpha = (N/2 - y)/\sqrt{N/2} \) and \( \text{erfc}(x) = (2/\sqrt{\pi}) \int_x^\infty dt e^{-t^2} \) is the complementary error function. One can derive (17) for the average location \( \langle r_j \rangle = \sum r_j \hat{P}(r_j) \) where \( \hat{P}(r_j) \) is given by (15) using equations (A.1)–(A.3) and replacing the sums by integrals.

The integral \( G(m) \) in section 3.2 can be estimated by the saddle point method as follows. We have

\[
G(m) = (-1)^m \int_{-\infty}^{\infty} dx \frac{e^{-2x^2}}{\text{erfc}(x)} = \frac{(\ln \text{erfc}(x))^m}{m!} - \frac{(\ln 2)^m}{m!} \approx (-1)^m \int_{-\infty}^{\infty} dx \frac{e^{-G(x)}}{m!},
\]  

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where $G(x) \approx x^2 - \ln(x(2m + 1 + x^{-2}))$ for large $m$. Here we have used that erf$(x) \approx e^{-x^2}/(\sqrt{\pi}x)$ for $x \gg 1$. Expanding $G(x)$ about its minimum $x_0 \approx m - \ln \sqrt{m}$ up to $O(x - x_0)^2$ and doing the Gaussian integral, we obtain $G(m) \approx \sqrt{\pi m}/2$ for large $m$.

**Appendix B. Distribution of the most populated sequence**

Our goal is to compute the probability $P_t(k^*)$ that the sequence $k^*$ has the maximum population at time $t$ in the i.i.d. model. This distribution is given by

$$P_t(k^*) = \int_{E_{\min}(k^*,t)}^{E_{\max}(k^*,t)} dE p_t^{(k^*)}(E) \prod_{k \neq k^*} q_t^{(k)}(E),$$  

(B.1)

where

$$p_t^{(k)}(E) = t^{-1}p[(E + k)/t]$$  

(B.2)

is the distribution of $E(k,t)$ obtained from the fitness distribution $p(F)$ via the variable transformation (6). The limits of the support of $p_t^{(k)}(E)$ are $E_{\min}(k,t) = -k + F_{\min}t$ and $E_{\max}(k,t) = -k + F_{\max}t$, and $q_t^{(k)}(E) = \int_{E_{\min}}^{E} dE p_t^{(k)}(E)$ is the corresponding cumulative distribution for $E > E_{\min}$ and zero otherwise. In the following, we show that the distribution $P_t(k^*)$ is of the scaling form $P_t(k^*) \approx t^{-1/2} \Phi(k^*/t^{1/2})$ for various choices of fitness distribution.

(i) $p(F) = e^{-F}$:

$$P_t(k^*) = \frac{1}{t} \int_0^{\infty} dx e^{-(x+k^*)/t} \prod_{k \neq k^*} (1 - e^{-(x+k)/t}) \approx \frac{1}{t} e^{-k^*/t},$$  

(B.3)

where the last expression is obtained by exponentiating the product and evaluating the resulting sum as an integral for an infinite system. Thus in this case $z = 1$ and the scaling function is given by $\Phi_1(y) = e^{-y}$.

(ii) $p(F) = (1 + \nu)(1 - F)^\nu$, $\nu \geq -1$:

$$P_t(k^*) = \frac{1 + \nu}{t} \int_0^{t^{-k^*}} dx \left(1 - \frac{x + k^*}{t}\right)^\nu \prod_{k \neq k^*} \left[1 - \left(1 - \frac{x + k}{t}\right)^{1+\nu}\right]$$  

(B.4)

$$\approx \frac{1 + \nu}{t} \int_0^{t^{-k^*}} dx \left(1 - \frac{x + k^*}{t}\right)^\nu \exp\left[-\frac{t}{2 + \nu}\left(1 - \frac{x}{t}\right)^{2+\nu}\right]$$  

(B.5)

$$\approx \frac{1}{t^{1/2}} \Phi_2\left(y = \frac{k^*}{t^{1/2}}\right),$$  

(B.6)
where \( z = (2 + \nu)/(1 + \nu) \) and the scaling function \( \Phi_2(y) \) is given by

\[
\Phi_2(y) \approx \frac{1 + \nu}{(2 + \nu)^{1/z}} \int_{y^{2(1+\nu)/(2+\nu)}}^\infty dx \, e^{-x} x^{-1/z} \left( y + ((2 + \nu)x)^{1/(2+\nu)} \right)^\nu. \quad (B.7)
\]

(iii) \( p(F) = \delta F^{-1-\delta}, \delta > 1: \)

\[
P_t(k^*) = \frac{\delta}{t} \int_t^\infty dx \left( \frac{t}{x + k^*} \right)^{1+\delta} \prod_{k\neq k^*} \left[ 1 - \left( \frac{t}{x + k} \right)^\delta \right] \quad (B.8)
\]

\[
\approx \frac{1}{t^{1/z}} \Phi_3 \left( y = \frac{k^*}{t^{1/z}} \right), \quad (B.9)
\]

where \( z = (\delta - 1)/\delta \) and the scaling function \( \Phi_3(y) \) is given by

\[
\Phi_3(y) \approx \delta (\delta - 1)^{1/(\delta-1)} \int_0^\infty dx \frac{e^{-x} x^{1/(\delta-1)}}{(1 + ((\delta - 1)x)^{1/(\delta-1)}y)^{1+\delta}}. \quad (B.10)
\]

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