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Evolution and Co-evolution in a Rugged Fitness Landscape

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Abstract

A variant of Kauffman's NKC-model for genetic evolution and adaption is analysed. First, a number of results are derived for species evolving in isolation. Next, it is shown that the evolution of interacting species belongs to one of two phases depending on the strength of the interaction. There is a *frozen* phase in which all species eventually reach local fitness maxima and stop evolving, and there is a *chaotic* phase in which a self-sustaining fraction of all species keep evolving. Individual species reach local fitness maxima also in the chaotic phase, but eventually their fitness is changed as a consequence of the evolution of other species, and they start evolving again.

The evolutionary activity of the steady state is a natural order parameter for the ecosystem. Closed expressions for the value of this order parameter and the system's relaxation time are given. The relaxation time diverges at the phase boundary, showing the system is critical there.

All results were obtained analytically for the maximally rugged case of $K + 1 = N$, and to leading order in N, the number of genes in a species.

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1 Introduction

We consider a variant of a simple, proto-typical model for biological evolution suggested by S. Kauffman [1, 2, 3, 4]: the co-evolution of abstract haploid organisms with a single copy of chromosomes. Evolution in this model is driven by random mutations of individual genes. Each species evolves in a fitness landscape which represents those aspects of its environment that remain unchanged on the time-scale of evolution. The fitness of any species depends on its position in its fitness landscape and on the state of other species. Species are, so to speak, part of each others *effective* landscapes. These may therefore change with time as species evolve.

It has been suggested [3] that this so-called *NKC*-model self-organizes dynamically to criticality [5] and thereby provides a very simple model for the intermittency of extinction events observed in biological evolution by Raup [6]. The purpose of our investigation of this model is to demonstrate its capacity for self-organization to criticality, if it is there in the model. This article reports on some progress towards this end, in-as-much as we show that the first prerequisite, critical behaviour, is there in the model. We may hope then that a more realistic version of the model, suggested by our results, may self-organize to criticality. Whether this is the case, is not addressed here.

The letters N, K, and C in the model's name, denote parameters for, respectively, the number of genes in the evolving organisms, the roughness of their fitness landscapes, and the strength of their mutual dependence. We study the model with maximally rugged fitness landscapes, obtained for $K = N - 1$, so K does not occur as an independent parameter in the present article. We demonstrate analytically that it possesses two phases, one phase with dynamics governed by attractive fixed points, and another phase with chaotic dynamics. The phases are separated by a critical line in the *(N,C)*-plane at $C \simeq N/\log N$. We have obtained closed expressions, valid anywhere in the two phases, for the system's relaxation time towards its asymptotic behaviour.

Some of the analytical results we give below for species evolving in isolation have been seen in numerical studies [7, 8], and derived in [9]. They represent a natural first insight, and are included to make the presentation self-contained. Different but related results have been obtained for the *NK*-model with general $K \gg 1$ in [10].

In the body of the present article, results are derived in a heuristic manner. In this way we, hopefully, give the reader a qualitative understanding of the dynamics of the *NKC*-model. More stringent derivations and other technical matters have been relegated to a number of appendices.

2 The system

We consider an ensemble of mutually dependent and evolving species, an *ecosystem*. At any time, the state of any species is given by the state of its genome. This genome contains N genes. We shall assume the genes are binary variables, *i. e.* there are only two alleles, $A = 2$. We do not expect our results to change in any significant way if the number of alleles is changed, as long as it is small compared with N in results based on expansion in $1/N$. We do not distinguish between phenotypes and genotypes, and also neglect variations in type within a species. In real life, variation is responsible for the very existence of evolution. In the NKC-model, however, only this consequence of variation is modelled: evolution takes place, and is driven by a constant rate of mutations of individual, randomly chosen genes. If a mutation increases the fitness of a species, it is accepted, and the entire species is changed. If a mutation does not increase the fitness, it is rejected, and the species remains unchanged. Tie situations, with two genetic configurations having the same fitness, do not occur (have measure zero), due to the way we assign fitness to genetic configurations: If the time-scale that selection works on is much faster than the time-scale for mutations, this lends some justification to our "all or nothing" dynamics neglecting variations [11]. Proliferation and extinction of species are both neglected in the present article, though the model could be adapted to accommodate their description.

The fitness f of any of the evolving species is a random function of its N genes *and* of C other genes belonging to other species [12]. These C other genes are chosen at random among the genes of other species. For a given sample of the kind of ecosystem described here, the particular choice for these C genes and the random fitness function define the sample, and remain fixed during evolution — the randomness is *quenched*.

The particular probability distribution $p(f)$ used to define the fitness function does not matter; we shall not even bother to introduce it in our considerations below, because it turns out that it disappears again by a transformation of variables to $F = \int_{-\infty}^{f} df' \, p(f')$. In the case where p is uniform on the interval $0 \leq f \leq 1$, we have $f = F$. So for convenience we shall refer to F as the fitness, although F in the general case really denotes the probability for fitness less than f. The elimination of $p(f)$ in equations expresses that the value f of the fitness is irrelevant; only the probability F of being less fit matters.

We have two reasons to consider random fitness landscapes; the first reason is a conjecture, the second is proven correct in the appendices:

1. Evolution in any fitness landscape having an effectively finite correlation length, will, when viewed at sufficiently coarse-grained scales of time and space (configuration space, i.e.) look like evolution in a

random fitness landscape. So evolution in a random fitness landscape describes the large-scale behaviour of evolution in a large class of landscapes. Consequently, with this choice of landscape we are avoiding the particular, while treating a quite general case.

2. It is technically convenient: the absence of correlations allows us to derive a number of analytical results.

Notice that from a mathematical point of view, N might as well be the number of positions in the primary sequence of a protein, with $A = 20$ denoting the 20 amino acids that potentially could occur at each position. Or $A = 4$ could denote the 4 nucleotides possible at each site in a DNA sequence of length N.

Alternatively, we may think of the N genes and their A alleles as N Potts spins and their A possible values in an A-state Potts model. With $V = -f$ denoting the *energy* of a spin-configuration, we recognize in each species a sample of Derrida's random energy model [13, 14], and these samples are asymmetrically coupled to each other for $C \neq 0$. In this language, the dynamics of mutations described above is the random-site Metropolis algorithm at zero temperature.

3 Estimating the length of walks

Evolution traces out a path in configuration space. At each time step, the path is either extended one step from its current end point to a nearest neighbor — when a mutation leading to higher fitness is offered to and accepted by evolution — or the path is *not* extended — because a mutation leading to lower fitness is offered and rejected. This path is often referred to as an *adaptive walk*.

In this section, we are not concerned with the temporal aspects of evolution, but only with the length ℓ of adaptive walks. This limitation simplifies the description a good deal. In subsequent sections, temporal aspects are treated.

Before we get involved with mathematics, let us estimate the average length of adaptive walks, and the average fitness they lead to. The qualitative picture thus obtained is confirmed by rigorous calculations in appendix B.

We assume N is large. The dimension of configuration space is N. We assume the length of adaptive walks is much smaller than $\sqrt{N}$, and find this assumption consistent with the results it leads to. Since the walk proceeds by random mutations, it proceeds in random directions in configuration space. There are many more directions than there are steps in the walk, by assumption. So each step in the walk has a different direction. In each step of the adaptive walk, the fitness F is increased. The value it increases to, is

uncorrelated — to leading order in $1/N$; see appendix A — with its previous value, except it is larger, of course. Consequently, in each step $1-F$ is halved, on the average. Thus, starting the walk with $F=0$, after ℓ steps the average fitness is $1-2^{-\ell}$. An adaptive walk stops when all neighbor positions have lower fitness than the current position. Since fitnesses are random and uncorrelated, this happens when N independent random numbers happen to be smaller than F. On the average, this occurs when $1-F \sim 1/N$. This is our estimate for the average final fitness, and, setting $1-F \sim 2^{-\ell}$, we have an estimate for the average length of an adaptive walk:

$$\bar{\ell} \simeq \log N / \log 2 \tag{1}$$

In the derivation of this result, we neglected correlations between fluctuations around the averages that we worked with. They do not change the logarithmic dependence on N in Eq. (1), but do change the coefficient of $\log N$; see appendix B.

In addition to a more precise result for the average length of adaptive walks, we want to know the probability distribution Q_ℓ for ℓ. In [8], "long upper tails containing little probability" were seen in numerical results for Q_ℓ. So one may wonder whether Q_ℓ decreases as a power of ℓ at large ℓ, or faster. We found that $(Q_\ell)_{\ell=0,1,2,\ldots}$ is a Poisson distribution to leading order in $1/\log N$; see appendix C and figure 1.

4 Estimating the duration of walks

Since we let the adaptive walk start out with fitness $F=0$, the probability Q_0 that it is at a local fitness maximum at time $t=0$ after the first step is

$$Q_0 = 1/N \tag{2}$$

This is a rigorous result.

On the average, and to leading order in $1/N$, each step taken, including the first, reduces $1-F$ by a factor 2. Each step thereby doubles the probability that the ensuing step will be the last, while it halves the probability per unit of time that the next step is taken. Consequently, the probability per unit of time for the walk to terminate is constant during the walk. This means

$$Q_t = \frac{1}{\bar{t}} \exp(-t/\bar{t}) \tag{3}$$

Using the exact result in Eq. (2), we have the estimates

$$\bar{t} = N \tag{4}$$

and

$$Q_t = \frac{1}{N} \exp(-t/N) \tag{5}$$

This last equation shows that NQ_t remains a finite function of t/N in the limit $N \to \infty$, and its k'th moment is proportional to N^k. In particular we see that the standard deviation

$$\sigma(t) = N \tag{6}$$

scales like the average $\bar{t}$. This is in contrast to the scaling laws found for the average *length* of walks and *its* standard deviation; see appendices B and C.

In appendix D we show how this section's estimates are modified when we account properly for fluctuations and their correlations. The result for NQ_t is shown in figure 2.

5 Master Equation

Because each species evolves by mutation of randomly chosen genes in a random fitness landscape, its path of evolution through configuration space can be replaced by a random walk, to leading order in N; see appendix A. This observation causes vast simplifications in the description of the system's dynamics, which, on the other hand, is exact then only to leading order in N. But that is a small price to pay, as we imagine N is large anyway.

We include two additional simplifications in the description: instead of keeping fixed the C randomly chosen foreign genes that any species depends on, we re-choose them at random any time we need them, *i. e.* we exchange "quenched" randomness for "annealed". If the total number of species in the ecosystem is effectively infinite — and this assumption is the second simplification we add to the description — then there is no difference between results based on quenched, respectively annealed, randomness. This is because the set of species that any species depends on, directly or via other species, forms a C-branched tree, each node of the tree representing a species, each oriented branch a dependency. So while our exchange of quenched for annealed randomness amounts to a mean-field approximation, we nevertheless expect the mean-field theory to be exact, because the system effectively is infinite dimensional through its random connections.

The second assumption, an effectively infinite number of species in the ecosystem, makes a description in terms of density functions possible: let $\rho_M(F;t)$ denote the relative number of species which have fitness F and M less fit one-mutant neighbors at time t. A change in a random gene will then lead to higher fitness — and therefore be accepted — with probability

$$A(t) = \sum_{M=0}^{N} (1 - M/N) \int_0^1 dF \rho_M(F;t) \tag{7}$$

because $1 - M/N$ is the probability that the change of one random gene leads to higher fitness in a species which has M less fit one-mutant neighbors.

We note that $A(t)$ also is the rate at which mutations are accepted by the ecology from the constant rate of mutations offered. So $A(t)$ is a measure of the evolutionary activity in the ecology. We shall find it a useful quantity below, and refer to it as the *activity*.

The probability that such a mutation is accepted *and* results in fitness F for the changed species, is

$$\Phi(F;t) = \int_0^F dF' \phi(F';t), \tag{8}$$

where

$$\phi(F';t) = \frac{1}{1-F'} \sum_{M=0}^{N} (1 - M/N) \rho_M(F';t) \tag{9}$$

is the contribution to this probability from species with fitness F'. This contribution does not depend on F as long as $F \geq F'$. This is so because we have assumed the fitness landscape is uncorrelated. The factor $1/(1-F')$ in this expression is the normalization factor for the constant distribution for F with $F \geq F'$.

With this notation we can write down the master equation for $\rho_M(F;t)$:

$$\begin{aligned} \frac{\partial}{\partial t}\rho_M(F;t) &= -(1 - \frac{M}{N})\rho_M(F;t) + B_{M,N}(F)\Phi(F;t) \\ &\quad -\frac{C}{N}A(t)\rho_M(F;t) + \frac{C}{N}A(t)B_{M,N}(F) \end{aligned} \tag{10}$$

This non-linear integro-differential equation expresses that the relative number of species with fitness F, and M less fit 1-mutant neighbors, changes for four different reasons, corresponding to the four terms on the right-hand-side of Eq. (10). The time-scale in Eq. (10) has been chosen such that in one unit of time one mutation is offered per species — to be accepted or rejected.

The first term on the right-hand-side of Eq. (10) is the rate at which species with fitness F, and M less fit neighbors, mutate to higher fitness.

The second term on the right-hand-side is a rate of change of less fit species into species with fitness F and number of less fit neighbors M. The function $B_{M,N}(F)$ is the binomial distribution with mean F:

$$B_{M,N}(F) = \frac{N!}{M!\,(N-M)!} F^M (1-F)^{N-M} \tag{11}$$

It represents the probability that M out of N one-mutant neighbors to a genome with fitness F are less fit than F. This probability is binomially distributed because the fitness landscape is random, with fitness F equidistributed in the interval $[0,1]$ [20].

The third term is a rate of loss of species with fitness F, M. This loss is not caused by a change in the genes of the species lost, but by a change

in its fitness due to genetic changes in other species. Since the C genes in other species that any species depends on, are randomly chosen, this change is the product of the probability $A(t)$ that a mutation in a random species is accepted and the probability $C/N\rho_M(F;t)$ that the gene it occurs in is a gene on which a species with fitness F, M depends.

The fourth term on the right-hand-side of Eq. (10) is, like the second term, a rate of change of species into species with fitness F, M. It complements the third term: species that change fitness due to genetic changes in other species, can change their fitness to F with equidistributed F. When they have done that, they have M less fit neighbors with probability $B_{M,N}(F)$.

We note that Eq. (10) conserves the total probability, as it should:

$$\frac{\partial}{\partial t}\int_0^1 dF \sum_{M=0}^{N} \rho_M(F;t) = 0. \tag{12}$$

6 Estimating the Phase Structure

Clearly, a static solution to Eq. (10) is provided by

$$\rho_M(F;t) = \delta_{M,N}\rho(F), \tag{13}$$

for any distribution $\rho(F)$. This solution corresponds to all species being at local fitness maxima. In the language of [1, 2, 3], borrowed from economics, the system is at a Nash equilibrium. Whether this fixed point for the dynamics is attractive or repulsive with respect to perturbations of $\rho_M(F)$, depends on the value of C. For $C = 0$ it is attractive, since in this case each species evolves in a fixed landscape, and consequently arrives at a local maximum. At the other extreme, $C/N \gg 1$,

$$\rho_M(F;t) = B_{M,N}(F) \tag{14}$$

is a static solution to leading order in N/C. It corresponds to totally random fitness F, and maximum activity $A = 1/2$.

At intermediate values of C, we can easily imagine the existence of a static solution with a finite activity A corresponding to a certain fraction of all species being in states that evolve. The activity is maintained by a balance between the rate at which species evolve towards fitness maxima, and the rate at which species are set back in evolution by their dependence on other species. We expect the activity A to increase with C.

On the other hand, we can also imagine that C can be too small to sustain a finite activity. In appendix B we show that isolated species on the average change

$$\mu_1 = \log N + 0.09913... + \mathcal{O}(N^{-1}) \tag{15}$$

genes in their evolution to a local maximum. So do species in the NKC-model studied here, if they are not set back in evolution by their dependence on other species. Thus μ_1 is the minimal number of genetic changes per species by which the NKC-model can evolve to the fixed point Eq. (13). If, in doing so, each species on the average sets back less (or more) than one other species in evolution, the fixed point Eq. (13) will (or will not) be attractive.

We can make the argument more precise by making it perturbative: suppose for a given value of C the system has been arranged to be at the fixed point solution Eq. (13), and we change the fitness of one species to a random value. Since the other species do not evolve, the one singled out evolves as an isolated species, and arrives at a fitness maximum after having changed typically μ_1 of its genes. But the fitness of other species depend on the state of genes in the species that evolved; typically C other species will each depend on one gene. If any of these C genes were among the μ_1 genes that changed, the species depending on them were set back in evolution, and are now evolving, possibly setting back yet other species in their evolution. The question then is, if the chain reaction set off this way is sub- or super-critical. Will it die out or run away? The value for C which separates these two situations we call critical, and write it $C_{\rm crit}$. It is the value for which, on the average, one out of C randomly chosen genes is among the μ_1 changed genes. Thus $1 = C_{\rm crit}\mu_1/N$, or

$$C_{\rm crit} = N/\mu_1 \tag{16}$$

We conclude that the species collectively evolve each to their own local fitness maximum and remain there with vanishing activity A for $C < C_{\rm crit}$, while they evolve to a state with finite activity $A < 1/2$ for $C > C_{\rm crit}$. The asymptotic value of the activity A for $t \to \infty$ can consequently be used as an order parameter distinguishing the two phases.

The arguments used in this section were based on average values. While we would not expect fluctuations to change the qualitative picture, they might change the coefficient in a scaling law like Eq. (16). Actually they do not. The perturbative result is exact, as we see in appendix E, where we also find the activity as a function of $c = C/N$. This activity is shown in figure 3 for $N = 10$ and $N = 100$. In appendix F, the systems relaxation time to the steady state is calculated for both phases, and found to diverge with mean field exponent -1 at C_{crit}.

7 Summary. Discussion. Perspectives.

For species evolving in isolation, we have obtained rigorous results to leading order in $1/N$ for the length and duration of adaptive walks in a special case of Kauffman's NK-model. We found the average length scales as $\log N$, and so does the variance of the distribution of lengths. We have also obtained

analytical expressions for the prefactors in these scaling laws, and found that to leading order in $1/\log N$, lengths are Poisson distributed.

For the duration of adaptive walk, we found qualitatively different results. While the average duration is proportional to N with a constant of proportionality we have found analytically, the variance of the duration is proportional to N^2, again with analytically known coefficient. So while typical *lengths* of adaptive walks are relatively close to their average, typical *durations* vary over a range with magnitude equal to their average. We extended this result by showing analytically that in the limit $N \to \infty$, t/N has a finite distribution. Numerically, we found this distribution falls off exponentially for $t/N \geq 1$.

For co-evolving species, we have shown analytically that a variant of Kauffman's *NKC*-model has two phases; a *frozen* phase in which all species eventually stop evolving, because they all reach local fitness maxima, and a *chaotic* phase characterized by a balance between the number of species at local fitness maxima, and the number evolving towards such maxima, and changing the fitness landscape of other species in the process. As order parameter we used the asymptotic *activity*, the fraction of species changing genetically per unit of time. We gave a closed expression determining the asymptotic activity as an implicit function of the connectivity between species. We also gave expressions for the system's relaxation time to the asymptotic activity. On the line separating the two phases in the system's parameter space, the relaxation time diverges with mean field exponent -1.

We obtained these results in a mean field description of the model, keeping only leading terms in an expansion in $1/N$, N being the number of genes per species. Since N typically is very large, however, our leading-order approximation in N is very good. We do not expect any qualitative differences between our leading order $1/N$-expansion results and exact results as concerns the existence of the two phases, the location of the phase boundary, and the relaxation time. As for the exponent -1 for the divergence of the relaxation time, we have argued that it is an exact result. These results all depend on the number of species S being effectively infinite, and certainly much larger than both the number of genes N and the connectivity C.

It may well be possible to obtain other analytical results for the *NKC*-model, using the methods of the present paper. For example one may try to find the Lyapunov exponents of the chaotic phase.

As for the purpose of our investigation — the demonstration of self-organized criticality in the *NKC*-model — we see no way that the maximally rugged variant studied here can be driven with perturbations from its frozen phase into a "poised", critical state, as was done in [15] with Conway's *Game of Life*. The maximally rugged variant cannot be "pumped up" to a "poised" state — at least not in the mean field description — because after the model has responded to a perturbation it is back in the same state as it was before

the perturbation was applied. This is not necessarily a short-coming of the mean field description. It willingly describes for example the build-up of the self-organized critical state of conservative sand pile models [16]. Rather, it is due to the maximal ruggedness of the fitness landscape. Its total absence of correlations makes any perturbation of a species wipe out all memory of the fitness the species had acquired before the perturbation was applied. There is, so to speak, no such thing as a perturbation *of fitness* in the maximally rugged case. Genetic configurations may be perturbed by having just one or a few genes changed. But that typically results in a finite change of fitness in a maximally rugged landscape.

On the other hand, maximal ruggedness of the model's fitness landscape is crucial for our ability to derive analytical results, and these results are important in view of the difficulty of a numerical simulation of the model. So we are reluctant to abandon it. That leaves us with another, biologically appealing possibility: we can make the model more realistic (and computationally even more difficult) by treating N and C as dynamical parameters of the individual species, add criteria for their evolutionary change, and ask if evolution drives their averages onto the critical line found in the present paper. That study has yet to be done. Methods and results that appear to make such an undertaking feasible, were presented here.

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Appendix A: Adaptive and random walks

In this appendix we argue that if the dimension N of configuration space is sufficiently large compared to the length of a finite path in that space, we cannot distinguish, to leading order in N, between the path of a random walk and the path of an adaptive walk in a random fitness landscape:

Assume that the dimension N of configuration space is much larger than the length of adaptive walks in that space. Then we can neglect the fact that the adaptive walk avoids itself and all configurations previously probed by it. The reasoning goes as follows: Since mutations occur on random genes, a step is added to the walk by probing random directions in configuration space, until one leading to higher fitness is found. Then the walk is extended one step in that direction, and the procedure repeated from the new position

in configuration space. By this algorithm, correlations between successive directions chosen by the walk are of order $1/N$. So to leading order in an expansion in $1/N$ successive directions are uncorrelated, and we have a *random* walk at hand. Successive directions are also *different* to leading order. Consequently, if the length of the walk is much smaller than $\sqrt{N}$, *all* directions chosen by it are different, and it obviously does not self-intersect [17].

By assuming that the adaptive walk never probes a site in configuration space that it has probed before, we found, in section 3, that walks have length $\sim \log N$, which *is* much smaller than $\sqrt{N}$ for N large. We conclude that our assumption that the walk is short compared to N is self-consistent correct.

We may ask whether we can find all sub-leading terms in an expansion in $1/N$ without knowing the entire history of an adaptive walk. The answer is negative:

An adaptive walk does not back-track, while a random walk does with probability $\sim 1/N$ per step. We can handle a random walk without back-tracking analytically. But back-tracking is not the only $1/N$-effect distinguishing an adaptive walk from a random one, however. An adaptive walk also forms no closed loops, and does not visit sites in configuration space that were probed previously, but not visited for lack of fitness. Thus an adaptive walk is not only self-avoiding, but also avoids many one-mutant neighbors to itself. A short random walk visits such sites with probability $\sim 1/N$. This is seen as follows:

Self-intersection by a random walk requires the formation of a closed loop by the walk, i.e. at least two steps, of opposite orientation, must be taken in each dimension in which the loop extends. So the probability for the formation of a closed loop of length ℓ' on a random walk of length ℓ is, to leading order, suppressed by a factor $(\ell - \ell')/N^{\ell'/2}$, where $\ell' \geq 4$. Nearest neighbors to the walk can be visited in one step less, i.e. with probability $(\ell - \ell')/N^{\ell'/2-1}$. For $\ell' = 4$ this probability is $\sim \ell/N$. So to leading order in $1/N$ we can treat the adaptive walk as a random walk. We can also treat it as a random walk without back-tracking, thereby describing some of the $1/N$-effects at play. But a full description of $1/N$ effects requires more information than the walk's current position in configuration space.

In summary, to leading order in $1/N$ we may add a step to the adaptive walk by treating the one-mutant neighbors to the current configurations as if they had never been visited or probed before. Consequently, the probability that M of these N neighbors are less fit than the current configuration, is binomial, $B_{M,N}(F)$, where F is the fitness of the current configuration. If we take into account that the previous configuration is known to be less fit, the probability is $B_{M-1,N-1}(F)$, as given in Eq. (57).

When we forbid back-tracking, our treatment is exact for a configuration space which is a Cayley tree with coordination number N. It should not be

confused with an 'annealed' fitness landscape, as an approximation to the 'quenched' landscape we start out with. Not if 'annealed' means re-choosing the fitness of a configuration every time it is probed by the adaptive walk. If we did that, we would have no maxima, since a higher fitness could always be attained by sufficiently many trials. The picture of an 'annealed' fitness landscape applies only in the sense that the fitnesses of all N (or $N-1$) neighbors to a configuration are re-chosen every time that configuration is visited, *and kept fixed during the visit,* thereby possibly making the visit permanent.

Appendix B: The length of walks

When duration is not of interest, but length is, the simplest quantity to work with is the probability density $p_\ell(F)$ that an adaptive walk contains (at least) ℓ steps, and has fitness F after these ℓ steps. Evolution by random mutations through fitter one-mutant neighbors can be described approximately by a recursion relation:

$$p_{\ell+1}(F) = \int_0^F dF' \, \frac{1-F'^{N-1}}{1-F'} \, p_\ell(F') \quad \text{for} \quad \ell = 1, 2, \ldots \tag{17}$$

This recursion relation expresses that fitness F is acquired in $\ell+1$ evolutionary steps by acquiring any lower fitness F' in ℓ steps, and taking one more step to fitness F. Taking the last step requires that not all N one-mutant neighbors in configuration space are less fit. One is — the one that was reached after $\ell-1$ steps. The remaining $N-1$ neighbors have fitness less than F', each with probability F', since their fitness is random. Here we assume that they were not probed previously by the path of evolution. This assumption is only approximately true, so Eq. (17) is an approximation. Within this approximation, the probability that not all neighbors are less fit is $1-F'^{N-1}$. When this is the case, the $(\ell+1)$th evolutionary step will be taken, and leads to any fitness above F' with equal probability; hence to fitness F in the interval dF' with probability $dF'/(1-F')$.

The approximation we have made with Eq. (17) relies on N being large. While the power $N-1$ on F' excludes evolutionary back-tracking, Eq. (17) does not exclude that the path of evolution *intersects* itself or visits other points in configuration space that it probed and rejected at an earlier time. Such intersections are forbidden by the dynamics, which forces the path to always higher degrees of fitness in a fixed landscape, or to stop at a local maximum. But in Eq. (17), the $N-1$ one-mutant neighbors which are not a state's immediate predecessor in evolution, are all treated as if they were never probed before by the evolutionary process. Which some of them may have been, in which case we know that their fitness is lower than the current one. So Eq. (17) yields an upper bound for the true value of $p_\ell(F)$, because

the exact relation has a power lower than or equal to $N-1$, where Eq. (17) has $N-1$. This exact power depends on the entire path of evolution up to the currents state, so the approximation made with Eq. (17) causes a vast simplification of the problem. In the appendix we give arguments that this approximation is correct to leading order in an expansion in $1/N$.

In view of the further approximation considered below, all we really need are results to leading order in N. But since we can solve Eq. (17) as it stands — i.e. with back-tracking forbidden, and self-intersection permitted — we shall do that for definiteness.

Introducing the monotonic function

$$H_N(F) = \sum_{k=1}^{N} \frac{1}{k} F^k \tag{18}$$

a change of variable to $H = H_{N-1}(F)$ in Eq. (17) gives

$$p_{\ell+1}(H) = \int_0^H dH'\, p_\ell(H') \quad \text{for} \quad \ell = 1, 2, \ldots, \tag{19}$$

which is easily iterated to give

$$p_\ell(H) = \frac{1}{(\ell-1)!} \int_0^H dH'\, (H-H')^{\ell-1} p_1(H'). \tag{20}$$

For definiteness and notational convenience, we let all adaptive walks begin in the least fit state, characterized by $F = 0$. Since there is zero probability for this state being a local maximum of fitness, the first step of the adaptive walk is always taken. For notational convenience, we let ℓ denote the number of steps taken *in excess* of this first step. Then the initial condition reads

$$p_{-1}(F) = \delta(F) \tag{21}$$

This rather eccentric choice of initial condition assures that the walk has a predecessor for all values of $\ell \geq 0$. This makes formulas look simpler, and makes Eq. (17) and Eq. (19) valid also for $\ell = -1$. They have the unique solution

$$p_\ell(F) = \frac{1}{\ell!} H_{N-1}(F)^\ell \quad \text{for} \quad \ell = 0, 1, 2, \ldots \tag{22}$$

Obviously, for fixed $F < 1$

$$H_N(F) \to -\log(1-F) \quad \text{for} \quad N \to \infty, \tag{23}$$

while for $F = 1$, $H_N(1)$ are the *harmonic numbers* discussed by Knuth in [18]

$$H_N(1) = \sum_{k=1}^{N} \frac{1}{k} = \psi(N+1) + \gamma_E = \log N + \gamma_E + \mathcal{O}(N^{-1}), \tag{24}$$

where $\psi(x) = d\log\Gamma(x)/dx$, and $\gamma_E = 0.57721566...$ is Euler's constant. For general F we note that

$$H_N(F) = \mathrm{li}(F^{N+1}) - \log(-\log(F)) + \mathcal{O}(N^{-1}) \tag{25}$$

where *li* is the logarithmic integral. We shall need that

$$H_N(1-x/N) = \log N + \gamma_E - \mathrm{Ein}(x) + \mathcal{O}(N^{-1}) \quad \text{for} \quad x \sim \mathcal{O}(1), \tag{26}$$

where *Ein(x)* is an entire function related to the exponential integral [19]:

$$\mathrm{Ein}(x) = \int_0^x dt \frac{1-e^{-t}}{t} = \mathrm{E}_1(x) + \log x + \gamma_E \tag{27}$$

As stated above, Eq. (17) is the simplest relation we can write down for a probability describing the length of the adaptive walks considered here, in the approximation specified. The probability that a walk contains (at least) ℓ steps is obtained from $p_\ell(F)$ by integration over F:

$$\begin{aligned} P_\ell &= \int_0^1 dF p_\ell(F) = \frac{1}{\ell!}\int_0^1 dF H_{N-1}(F)^\ell \\ &= \frac{1}{\ell!}\sum_{k_1,\ldots,k_\ell=1}^{N-1} \frac{1}{k_1\cdots k_\ell(k_1+\cdots+k_\ell+1)} \quad \text{for} \quad \ell = 0,1,2,\ldots \end{aligned} \tag{28}$$

Integration over F on both sides in Eq. (17) gives

$$P_{\ell+1} = P_\ell - \int_0^1 dF F^{N-1} p_\ell(F) \tag{29}$$

which obviously cannot be made into a closed equation for P_ℓ. The remaining integral in Eq. (29) is the probability that an adaptive walk contains *exactly* ℓ steps. This is a quantity of interest. We introduce the notation Q_ℓ for it, and $q_\ell(F)$ for the corresponding probability density that a walk stops with fitness F after exactly ℓ steps:

$$q_\ell(F) = F^{N-1}p_\ell(F) = F^{N-1}\frac{1}{\ell!}H_{N-1}(F)^\ell \quad \text{for} \quad \ell = 0,1,2,\ldots \tag{30}$$

$$\begin{aligned} Q_\ell &= \int_0^1 dF\, q_\ell(F) = \frac{1}{\ell!}\int_0^1 dF F^{N-1} H_{N-1}(F)^\ell \\ &= \frac{1}{\ell!}\sum_{k_1,\ldots,k_\ell=1}^{N-1} \frac{1}{k_1\cdots k_\ell(k_1+\cdots+k_\ell+N)} \quad \text{for} \quad \ell = 0,1,2,\ldots \end{aligned} \tag{31}$$

From Eq. (29) follows

$$Q_\ell = P_\ell - P_{\ell+1} \tag{32}$$

Since Eq. (21) implies

$$Q_{-1} = 0, \quad P_0 = 1, \tag{33}$$

normalization of $q_\ell(F)$ and Q_ℓ follows trivially from Eq. (32):

$$\sum_{\ell=0}^{\infty} \int_0^1 dF\, q_\ell(F) = \sum_{\ell=0}^{\infty} Q_\ell = \sum_{\ell=0}^{\infty} (P_\ell - P_{\ell+1}) = P_0 = 1 \tag{34}$$

Here we have used $\lim_{\ell\to\infty} P_\ell = 0$, and we have set the upper limit on the sum over ℓ to infinity for convenience. Strictly speaking, this upper limit is A^N, the number of points in configuration space. We shall see below that typical values for ℓ are of order $\log N$, and much larger values of ℓ occur with probabilities that are more than exponentially suppressed. So the effect of this change in upper limit is truly negligible.

Inserting Eq. (30) in Eq. (34) and summing over ℓ, we see that normalization means

$$\int_0^1 dF F^{N-1} \exp\left(H_{N-1}(F)\right) = 1 \tag{35}$$

for any positive integer N. This identity is exact, and may also be proven directly; we leave that for the reader's entertainment.

The generating function for the probabilities Q_ℓ reads

$$\tilde{Q}(\lambda) = \sum_{\ell=0}^{\infty} \lambda^\ell Q_\ell = \int_0^1 dF F^{N-1} \exp\left(\lambda H_{N-1}(F)\right). \tag{36}$$

Despite our ability to evaluate the integral in Eq. (35) we have not been able to evaluate the integral in Eq. (36) for general λ. But as we have already neglected terms of sub-leading order in $1/N$, we may continue to do so with no further loss of generality. To this end we write $F = 1 - x/N$, and observe that $F^N = \exp(-x) + \mathcal{O}(x^2/N)$. Consequently, the integrand in Eq. (36) is negligible unless $x \sim 1$, and, to leading order in $1/N$, we have for $\tilde{Q}(\lambda)$, Q_ℓ, and its first moment μ_1:

$$\tilde{Q}(\lambda) = N^{\lambda-1} \int_0^\infty dx\, e^{-x-\lambda(\mathrm{Ein}(x)-\gamma_E)} \tag{37}$$

$$\tilde{Q}(1) = 1 \tag{38}$$

$$\begin{aligned} Q_\ell &= \frac{1}{N\ell!} \int_0^\infty dx\, e^{-x} \left(\log N + \gamma_E - \mathrm{Ein}(x)\right)^\ell \\ &= \frac{1}{N\ell!} \left((\log N)^\ell + \mathcal{O}((\log N)^{\ell-1})\right) \end{aligned} \tag{39}$$

$$\mu_1 = \sum_{\ell=0}^{\infty} \ell Q_\ell = \frac{dQ}{d\lambda}(1) = \log N + \mu_1^{(\mathrm{finite})} + \mathcal{O}(N^{-1}). \tag{40}$$

Here

$$\mu_1^{(\mathrm{finite})} = \int_0^\infty dx \left(\gamma_E - \mathrm{Ein}(x)\right) e^{-x+\gamma_E-\mathrm{Ein}(x)} = 0.09913... \tag{41}$$

is a constant that we have not been able to express in terms of known constants. Our results for μ_1, and for μ_2 given in Eq. (34), agree with the two-digit numerical results given in [8].

Eq. (39) shows that to leading order in $\log N$, Q_ℓ is a Poisson distribution. This simple results has a simple explanation: the Poisson distribution is obtained because all adaptive walks terminate with essentially the same fitness F. F belongs to an interval of width $\sim 1/N$ at $F = 1$. This is seen from our rewriting $\int^1 dF F^{N-1}$ as $1/N \int_0 dx \exp(-x)$. Thus, in the interval $[0,1]$, NF^{N-1} is almost a δ-function with support at $F \simeq 1$. If we replace it with that in the formulas above, we arrive at a Poisson distribution.

Appendix C: Q_ℓ's Poisson behaviour

In this appendix we elaborate on Q_ℓ's similarity with a Poisson distribution, and compare it with such distributions for various values of N.

With the notation

$$\langle \ldots \rangle = \int_0^1 dF\, q(F) \ldots, \tag{42}$$

where

$$q(F) = \sum_{\ell=0}^{\infty} q_\ell(F) = F^{N-1}\, e^{H_{N-1}(F)} \tag{43}$$

is the probability density that an adaptive walk terminates at a local fitness maximum with fitness F, we have a positive measure on the fitness interval $[0,1]$. Eq. (35) shows that this measure is normalized. We write the integral in Eq. (36) in terms of this measure and cumulant-expand it:

$$\begin{aligned} \tilde{Q}(\lambda) &= \langle e^{(\lambda-1)H_{N-1}} \rangle \\ &= \exp\left(\langle e^{(\lambda-1)H_{N-1}} - 1 \rangle_c \right) \\ &= \exp\left((\lambda-1)\mu_1 + \frac{1}{2}(\lambda-1)^2 \langle H_{N-1}^2 \rangle_c + \frac{1}{3!}(\lambda-1)^3 \langle H_{N-1}^3 \rangle_c \ldots \right) \end{aligned} \tag{44}$$

where the first cumulants are

$$\langle H_{N-1} \rangle_c = \langle H_{N-1} \rangle = \mu_1 = \log N + \mu_1^{(\text{finite})} + \mathcal{O}(N^{-1}) \tag{45}$$

$$\left\langle H_{N-1}^2 \right\rangle_c = \left\langle (H_{N-1} - \mu_1)^2 \right\rangle = 0.16733... + \mathcal{O}(N^{-1}) \tag{46}$$

$$\left\langle H_{N-1}^3 \right\rangle_c = \left\langle (H_{N-1} - \mu_1)^3 \right\rangle = -0.08370... + \mathcal{O}(N^{-1}) \tag{47}$$

$$\begin{aligned} \left\langle H_{N-1}^4 \right\rangle_c &= \left\langle (H_{N-1} - \mu_1)^4 \right\rangle - 3 \left\langle (H_{N-1} - \mu_1)^2 \right\rangle^2 \\ &= 0.03815... + \mathcal{O}(N^{-1}) \end{aligned} \tag{48}$$

$$\ldots$$

Here we have used that to leading order in $1/N$ these expectation values receive contributions only from values of F obeying $F = 1 - x/N$ with $x \sim 1$, i.e. where $H_{N-1}(F) - \mu_1 = \gamma_E - \mathrm{Ein}(x) - \mu_1^{(\text{finite})}$. Consequently, all cumulants beyond the first are ~ 1, while the first, μ_1, is $\sim \log N$. Neglecting cumulants

higher than the first in Eq. (44), we arrive at the generating function for a Poisson distribution with the same mean, μ_1, as Q_ℓ has:

$$\tilde{Q}(\lambda) = \exp((\lambda - 1)\mu_1) \tag{49}$$

Figure 1 shows Q_ℓ against ℓ for $N = 10$, 100, 1000, and 10,000 as open symbols connected by lines. The lines are only meant to guide the eye. Q_ℓ was found by numerical integration of the expressions for Q_ℓ deriving from Eq. (36). The values for the Poisson distributions with the same mean values are shown as filled circles, which in most cases fall within the open symbols. This agreement is rather striking. It is *not* just due to the central limit theorem making both Q_ℓ and the Poisson distribution well approximated by the same Gaussian distribution, hence by each other. This is illustrated in figure 1 for the case of $N = 10$: the dashed line shows the Gaussian distribution with the same mean and variance as Q_ℓ has. Clearly, it does not approximate Q_ℓ, shown as open circles, as well as the Poisson distribution with the same mean as Q_ℓ, shown as filled circles. In addition to that it has non-negligible support for negative values of ℓ.

We can also compare Q_ℓ's moments, μ_n, with the moments of the Poisson distribution with the same mean, μ_1:

$$\begin{aligned}
\mu_1 &= \langle H_{N-1} \rangle = \log N + \mu_1^{(\text{finite})} && (50)\\
\mu_2 &= \mu_1 + \langle H_{N-1}^2 \rangle_c = \mu_1 + 0.16733... && (51)\\
\mu_3 &= \mu_1 + \langle H_{N-1}^2 \rangle_c + \langle H_{N-1}^3 \rangle_c = \mu_1 + 0.08363... && (52)\\
\mu_4 &= \mu_1 + \langle H_{N-1}^2 \rangle_c + 3(\mu_1 + \langle H_{N-1}^2 \rangle_c)^2 + \langle H_{N-1}^3 \rangle_c + \langle H_{N-1}^4 \rangle_c \\
&= \mu_1 + 0.16733... + 3(\mu_1 + 0.16733...)^2 + 0.12215... && (53)
\end{aligned}$$

As expected from Eq. (44), we see that when we neglect cumulants beyond the first, the n'th moment, μ_n, depends on the first moment, μ_1, as the n'th moment of a Poisson distribution does. We also see that this neglect introduces an error of just a few percent in the moments shown for $N \geq 100$. We expect this error to increase with the order n of the moment μ_n, and know that it decreases as $1/\log N$.

Appendix D: The duration of walks

Let $p_{\ell,M;t}(F)$ denote the probability that an adaptive walk at time t has proceeded ℓ steps, thereby reaching a point in configuration space having fitness F and M less fit neighbors. The time-evolution of $p_{\ell,M;t}(F)$ is found as follows. As above, we neglect the fact that an adaptive walk cannot intersect itself or any site that was previously probed by its evolution and discarded for being less fit. As explained in the appendix, this is a leading order approximation in an expansion in $1/N$. Within this approximation,

but explicitly forbidding back-tracking, $p_{\ell,M;t}(F)$'s development in time is given by

$$p_{\ell,M;t+1}(F) = \frac{M}{N} p_{\ell,M;t}(F) + B_{M-1,N-1}(F)\Phi_{\ell-1;t}(F) \tag{54}$$

where

$$\Phi_{\ell;t}(F) = \int_0^F dF'\, \phi_{\ell;t}(F') \tag{55}$$

and

$$\phi_{\ell;t}(F) = \frac{1}{1-F} \sum_{M=0}^{N} \left(1 - \frac{M}{N}\right) p_{\ell,M;t}(F) \tag{56}$$

Eq. (54) expresses that an adaptive walk has length ℓ, fitness F, and number of less fit neighbors M at time $t+1$ for one of two mutually exclusive reasons: it was either characterized by these values at time t, and took no step between time t and time $t+1$ — this happens with the probability given as the first term on the right-hand-side in Eq. (54) — *or* a step *was* taken between time t and time $t+1$, and the adaptive walk arrived at values (ℓ, F, M) with that step — this happens with the probability given as the second term on the right-hand-side of Eq. (54). $\Phi_{\ell-1;t}(F)$ is the transition probability density at time t to fitness F from less fit one-mutant neighbor configurations arrived at in $\ell - 1$ steps. It is an integral over $F' < F$ of $\phi_{\ell-1;t}(F')$, the transition probability density at time t from fitness F' arrived at in $\ell - 1$ steps to any more fit one-mutant neighbor configuration.

A configuration with fitness F, arrived at from a less fit configuration, will have a total of M less fit neighbor configurations, when $M-1$ of the $N-1$ new neighbor configurations are less fit. This happens with binomially distributed probability,

$$B_{M-1,N-1}(F) = \left(\begin{array}{c} N-1 \\ M-1 \end{array} \right) F^{M-1}(1-F)^{N-M}, \tag{57}$$

when we treat the landscape's quenched randomness as if the one-mutant neighborhood of any configuration arrived at is "annealed", thereby allowing the adaptive walk to self-intersect, with the exception that back-tracking remains forbidden.

As initial condition for Eq. (54) we choose as before, with no essential loss of generality, to let the adaptive walk start out in the least fit configuration, at a time that is chosen to be -1 for notational convenience. We let ℓ denote the number of steps taken *in excess* to the first step, which is always taken. Then the initial condition reads

$$p_{\ell,M;-1}(F) = \delta_{\ell,-1}\, \delta_{M,0}\, \delta(F). \tag{58}$$

Inserted in Eq. (54), this initial condition gives the equivalent initial condition

$$p_{\ell,M;0}(F) = B_{M-1,N-1}(F)\, \delta_{\ell,0} \tag{59}$$

Again our rather eccentric choice of initial condition assures that the walk has a predecessor at $t = 0$, as at all later times. This makes formulas look simpler.

The simpler Eq. (17) is contained in Eq. (54): the probability that an adaptive walk reaches length ℓ and fitness F at time t is $\Phi_{\ell-1;t-1}(F)$. Consequently, the probability that it reaches length ℓ and fitness F at all, denoted $p_\ell(F)$ in appendix B, is

$$p_\ell(F) = \sum_{t=0}^{\infty} \Phi_{\ell-1;t-1}(F) \quad \text{for} \quad \ell \geq 0. \tag{60}$$

Using this with Eq. (54), one obtains an equation for $p_\ell(F)$, Eq. (17).

Eq. (54) is a linear integro-difference equation. The fact that it is non-local in F does not prevent its solution, since it can be made local by appropriate differentiation after F. Introducing the generating function

$$\tilde{p}_M(\lambda, F; \tau) = \sum_{\ell=0}^{\infty} \lambda^\ell \sum_{t=0}^{\infty} \tau^t \, p_{\ell,M;t}(F) \tag{61}$$

and the corresponding generating functions for transition probability densities

$$\tilde{\phi}(\lambda, F; \tau) = \frac{1}{1-F} \sum_{M=0}^{N} (1 - M/N) \tilde{p}_M(\lambda, F; \tau) \tag{62}$$

and

$$\tilde{\Phi}(\lambda, F; \tau) = \int_0^F dF' \, \tilde{\phi}(\lambda, F'; \tau), \tag{63}$$

the initial condition, Eq. (59), reads

$$\tilde{p}_M(\lambda, F; 0) = B_{M-1,N-1}(F) \tag{64}$$

and Eq. (54) itself, after a minor rearrangement, reads

$$\tilde{p}_M(\lambda, F; \tau) = \frac{N}{N - \tau M} B_{M-1,N-1}(F) \left(1 + \lambda\tau \tilde{\Phi}(\lambda, F; \tau)\right). \tag{65}$$

Consequently,

$$\tilde{\phi}(\lambda, F; \tau) = h_{N-1}(F; \tau)(1 + \lambda\tau \tilde{\Phi}(\lambda, F; \tau)), \tag{66}$$

where we have introduced

$$\begin{aligned} h_{N-1}(F; \tau) &= \frac{1}{1-F} \sum_{M=0}^{N-1} \frac{N-M}{N-\tau M} B_{M-1,N-1}(F) \\ &= \sum_{M=1}^{N-1} \frac{N-1}{N-\tau M} B_{M-1,N-2}(F) \\ &= \frac{N-1}{N-\tau} \frac{1}{1-F} \, {}_2F_1(2-N, 1; 2-N/\tau; F). \end{aligned} \tag{67}$$

Here ${}_2F_1$ is Gauss' hypergeometric function. For later use, we note that

$$\tau h_{N-1}(1-x/N;\tau) = (N-1)x^{-1-N(\tau^{-1}-1)}e^{-x}\gamma(1+N(\tau^{-1}-1);x)+\mathcal{O}(N^{-1}), \tag{68}$$

where γ is the incomplete gamma-function. We shall also need the function

$$H_N(F;\tau) = \int_0^F dF' h_N(F';\tau) \tag{69}$$

and make contact with appendix B by noting that

$$H_N(F;1) = H_N(F). \tag{70}$$

For later use, we note that

$$\tau H_{N-1}(1-x/N;(1+z/N)^{-1}) = \log N - \psi(1+z) - \gamma_E - \mathcal{I}(x;z) + \mathcal{O}(N^{-1}), \tag{71}$$

when $x \sim 1$ and $z \sim 1$, and we have introduced:

$$\mathcal{I}(x;z) = \int_0^1 dy\, y^z\, \frac{1-e^{-x(1-y)}}{1-y} - \gamma_E \tag{72}$$

$$\mathcal{I}(x;0) = \mathrm{Ein}(x) - \gamma_E. \tag{73}$$

Eq. (66) is solved by

$$\tilde{\phi}(\lambda,F;\tau) = h_{N-1}(F;\tau)\exp(\lambda\tau H_{N-1}(F,\tau)), \tag{74}$$

and consequently

$$\tilde{p}_M(\lambda,F;\tau) = \frac{NB_{M-1,N-1}(F)}{N-\tau M}\exp(\lambda\tau H_{N-1}(F,\tau)). \tag{75}$$

In this result λ only occurs multiplied by τ. This is because in the series expansion of this result each power of λ represents one step taken in configuration space by the adaptive walk, and each such step takes one unit of time, represented by one power of τ. Powers of τ not occurring in conjunction with λ, on the other hand, represent time-steps during which the adaptive walk did not progress.

The relation between length and duration of adaptive walks is contained in

$$p_{\ell;t} = \int_0^1 dF \sum_{M=0}^{N} p_{\ell,M;t}(F) \tag{76}$$

and therefore in

$$\tilde{p}(\lambda;\tau) = \int_0^1 dF \sum_{M=0}^{N} \tilde{p}_M(\lambda,F;\tau) = \frac{1}{\lambda\tau}\left(\frac{1}{(1-\tau)^\lambda}-1\right)+\mathcal{O}(N^{-1}) \tag{77}$$

The generating function at time $t \geq 0$,

$$\tilde{p}_t(\lambda) = \sum_{\ell=0}^{\infty} \lambda^\ell \, p_{\ell;t} \, , \tag{78}$$

is obtained from $\tilde{p}(\lambda;\tau)$ via the relation

$$\begin{aligned} \tilde{p}_t(\lambda) &= \frac{1}{2\pi i} \oint \frac{d\tau}{\tau^{t+1}} \, \tilde{p}(\lambda;\tau) = \frac{1}{2\pi i \lambda} \oint \frac{d\tau}{\tau^{t+2}} \left(\frac{1}{(1-\tau)^\lambda} - 1 \right) + \mathcal{O}(N^{-1}) \\ &= \frac{\sin(\pi\lambda)}{\pi\lambda} B(1-\lambda, \lambda+t+1) + \mathcal{O}(N^{-1}), \end{aligned} \tag{79}$$

where the closed path of integration in the complex τ-plane encircles $\tau = 0$ once in the positive direction. Using Cauchy's theorem, the last identity was established by moving the path to lie along the integrand's branch cut on the real axis, $\tau \geq 1$. The function $B(x,y)$ is the beta-function, Euler's integral of the first kind. Notice that the normalization condition

$$\tilde{p}_t(1) = \sum_{\ell=0}^{\infty} p_{\ell;t} = 1 \;\; \forall \, t \geq 0 \tag{80}$$

is satisfied by the result in Eq. (79). The same result gives, to leading order in $1/N$, that

$$\begin{aligned} (\bar{\ell})_t &= \sum_{\ell=0}^{\infty} \ell \, p_{\ell;t} = \frac{d\tilde{p}_t(1)}{d\lambda} = \psi(t+2) + \gamma_E - 1 \\ &= \log t + \gamma_E - 1 + \mathcal{O}(t^{-1}) \end{aligned} \tag{81}$$

and

$$\begin{aligned} \sigma_t^2(\ell) &= (\bar{\ell^2})_t - (\bar{\ell})_t^2 = \psi(t+2) + \gamma_E + \sum_{k=1}^{t+1} \frac{1}{k^2} \\ &= \log t + \gamma_E + \pi^2/6 + \mathcal{O}(t^{-1}) \end{aligned} \tag{82}$$

Thus we see our estimate confirmed: the average length of an adaptive walk grows logarithmically with time. Furthermore, we see that the variance of the length grows like the average length, like for a biased random walk. This similarity is no coincidence, since the adaptive walk in many respects resembles a simple, biased random walk.

In the last identity in Eq. (77) it was tacitly assumed that N itself was the only quantity of order N. Consequently, the time-dependence found from this identity is reliable only when t is far from being of order N. This restriction needs not prevent t from being large and the asymptotic forms in Eq. (81) and Eq. (82) from being valid.

When $t \sim N$, walks reach local maxima and terminate, according to our estimate for their duration. This, of course, is an average result. For example

there is a probability $\sim 1/N$ that an adaptive walk terminates already after its first step. Now let us substantiate the estimate: the probability that a walk terminates with length ℓ and fitness F at time t is

$$q_{\ell;t}(F) = p_{\ell,N;t}(F) - p_{\ell,N;t-1}(F). \tag{83}$$

Contact is made with appendix B by observing

$$q_\ell(F) = \sum_{t=0}^{\infty} q_{\ell;t}(F) = \lim_{t\to\infty} p_{\ell,N;t}(F). \tag{84}$$

We introduce

$$Q_{\ell;t} = \int_0^1 dF\, q_{\ell;t}(F) \tag{85}$$

and

$$\tilde{Q}(\lambda;\tau) = \sum_{\ell=0}^{\infty} \lambda^\ell \sum_{t=0}^{\infty} \tau^t Q_{\ell;t} \tag{86}$$

and have

$$\begin{aligned} \tilde{Q}(\lambda;\tau) &= (1-\tau)\int_0^1 dF \tilde{p}_N(\lambda,F;\tau) = \int_0^1 dF\, F^{N-1} \exp(\lambda\tau H_{N-1}(F;\tau)) \\ &= e^{-\lambda(\psi(1+z)+\gamma_E)}\mathcal{F}(\lambda;z) + \mathcal{O}(N^{-1}), \end{aligned} \tag{87}$$

where Eq. (75) was used in the second identity, and $F = 1 - x/N$, $\tau = (1+z/N)^{-1}$, $x, z \sim 1$, in the third. We have introduced the N-independent function

$$\mathcal{F}(\lambda;z) = \int_0^\infty dx\, e^{-x-\lambda\mathcal{I}(x;z)}. \tag{88}$$

Eq. (87) is the time-dependent extension of Eq. (36). From the generating function in Eq. (87) we derive the average time it takes for an adaptive walk to reach a local maximum:

$$\begin{aligned} \bar{t} &= \sum_{\ell,t=0}^{\infty} t Q_{\ell;t} = \frac{\partial\tilde{Q}}{\partial\tau}(1;1) \\ &= \langle H_{N-1}(F;1) + \frac{\partial H_{N-1}}{\partial\tau}(F;1)\rangle \\ &= \langle \int_0^F dF' \sum_{M=1}^{N-1} \frac{N(N-1)}{(N-M)^2} B_{M-1,N-2}(F')\rangle \qquad (89) \\ &= N\left(\frac{\pi^2}{6} - \frac{\partial\mathcal{F}}{\partial z}(1;0)\right) + \mathcal{O}(1) \\ &= 1.22398\ldots N + \mathcal{O}(1) \\ \bar{t^2} - \bar{t}^2 &= N^2\left(2\zeta(3) + \frac{\partial^2\mathcal{F}}{\partial z^2}(1;0) - \left(\frac{\partial\mathcal{F}}{\partial z}\right)^2(1;0)\right) + \mathcal{O}(N) \qquad (90) \\ &= 1.71788\ldots N^2 + \mathcal{O}(N) \qquad (91) \end{aligned}$$

where ζ is Riemann's zeta-function. We have not been able to relate the derivatives of $\mathcal{F}$ in these equations to known mathematical constants.

Comparing this appendix's results with those of appendix B, we notice a big difference between the length and the duration of adaptive walks in a random fitness landscape: while typical lengths are relatively closer to the average length, the larger the system size N is, typical durations can differ from the average by an amount the size of this average. This picture is confirmed by the following expression for Q_t, the probability that a walk has duration t:

$$\begin{aligned} Q_t &= \frac{1}{2\pi i}\oint \frac{d\tau}{\tau^{1+t}}\tilde{Q}(1;\tau) \\ &= \frac{1}{2\pi i N}\oint dz\, e^{\frac{t}{N}z-\psi(1+z)-\gamma_E}\mathcal{F}(1;z). \end{aligned} \tag{92}$$

Here the closed path of integration in the complex τ-plane encircles $\tau = 0$ once in the positive direction, while a similar path of integration in the complex z-plane, obtained by the substitution $z = N(\tau^{-1} - 1)$, has been moved to lie along the negative real axis. That is the only place in the z-plane, where $\mathcal{F}(1;z)$ is not analytic. We have not found a more closed analytical expression for Q_t in the large-N limit than Eq. (92). Eq. (92) suffices, however, since it shows that for $t/N \sim 1$ we have $Q_t \sim N^{-1}$. Hence, in the limit $N \to \infty$, NQ_t is a finite function of the variable t/N. We have found this function numerically. Its graph is shown in figure 3 as the fully drawn line. The dashed line shows the graph for the estimate in Eq. (3) with the exact value in Eq. (89) used for $\bar{t}$. From the figure it seems that for $t/N \geq 1$, Q_t is essentially an exponential function, or at least exponentially bounded, though other possibilities cannot be eliminated on the basis of the figure.

Appendix E: Calculating the Phase Structure

Let us denote a stationary, or fixed point, solution to Eq. (10) by $\rho^*_M(F)$. With the notation $A^* = A[\rho^*]$, $\phi^* = \phi[\rho^*]$, $\Phi^* = \Phi[\rho^*]$, and $c = C/N$, the time-independent version of Eq. (10) can be rewritten

$$\rho^*_M(F) = \frac{N}{N - M + CA^*} B_{M,N}(F)(cA^* + \Phi^*(F)) \tag{93}$$

Since A^* and Φ^* both depend on ρ^*, Eq. (93) is a non-linear integral equation for $\rho^*_M(F)$. We can solve it, nevertheless, by temporarily treating A^* as a constant, to be determined by self-consistency in the end. This is done in the following way: By multiplying both sides in Eq. (93) with $(1-M/N)/(1-F)$, and summing over M, one finds

$$\phi^*(F) = g(F; cA^*)(cA^* + \Phi^*(F)), \tag{94}$$

where we have introduced the function [21]

$$g(F;x) = \frac{1}{1-F}\sum_{M=0}^{N-1}\frac{N-M}{N-M+Nx}B_{M,N}(F) = N\sum_{M=0}^{N-1}\frac{B_{M,N-1}(F)}{N-M+Nx}. \quad (95)$$

For later use we also introduce

$$G(F;x) = \int_0^F dF'\, g(F';x) \quad (96)$$

and

$$\mathcal{G}(x) = \int_0^1 dF\, e^{G(F;x)}. \quad (97)$$

Since g and G have simple poles at $x = -1, -1+1/N, -1+2/N, \ldots, -1/N$, the function $\mathcal{G}$ has essential singularities at these points. The graph for $\mathcal{G}(x)$ is shown in figure 4 for the case of $N = 10$. For $x \gg \mathcal{O}(1/N)$ or $x < -1$, $\mathcal{G}$ simplifies to

$$\mathcal{G}(x) = (1+x)\log(1+x^{-1}) \quad (98)$$

to leading order in $1/N$. The graph for this approximation is shown as the dotted curve in figure 4. The approximation has a cut in the interval $[-1,0]$ where $\mathcal{G}(x)$ has N essential singularities.

Now, remembering $\phi^*(F) = \frac{d}{dF}\Phi^*(F)$, we see Eq. (94) is solved by

$$\Phi^*(F) = cA^*(e^{G(F;cA^*)} - 1). \quad (99)$$

Inserting this solution in the definition Eq. (7) of the activity, we finally arrive at a self-consistency equation for A^*, given c:

$$A^* = cA^*(-1 + \mathcal{G}(cA^*)) \quad (100)$$

This equation is solved by $A^* = 0$ and by A^* satisfying

$$c^{-1} = -1 + \mathcal{G}(cA^*). \quad (101)$$

The last equation gives A^* as an implicit function of c. It has a real, positive solution A^* only for

$$c > c_{\rm crit} = (-1 + \mathcal{G}(0))^{-1} = \mu_1^{-1} \quad (102)$$

where μ_1 is given in Eq. (15). For $cA^* \gg \mathcal{O}(1/N)$, Eq. (101) simplifies to leading order in $1/N$ to another implicit expression for $A^*(c)$,

$$c^{-1} = -1 + (1+cA^*)\log(1+(cA^*)^{-1}). \quad (103)$$

According to Eq. (101), $A^* \propto c - c_{\rm crit}$ for $c \sim c_{\rm crit}$, *i. e.* the critical exponent for the order parameter A^* is 1. At the other extreme, for $c \to \infty$, Eq. (101) gives $A^* = 1/2$, as we expect from section 6. Figure 3 shows $A^*(c)$

for $N = 10$ and $N = 100$ as fully drawn curves. The approximate expression in Eq. (103) is shown as the dotted curve.

For $c > c_{\rm crit}$, Eq. (93) then gives

$$\rho^*_M(F) = \frac{CA^*}{N - M + CA^*} B_{M,N}(F) \exp(G(F; cA^*)), \tag{104}$$

while for $c < c_{\rm crit}$ we have

$$\rho^*_M(F) = \delta_{M,N} F^N \exp(G(F; 0)). \tag{105}$$

So, as already seen in section 6, the long-term dynamics of the co-evolving species can be of two qualitatively different kinds, depending on whether the parameters C and N have values making $c = C/N$ smaller or larger than $c_{\rm crit}$ given above. In the first case, the activity $A(t)$ dies out because all species stop evolving as they reach local fitness maxima. This is *frozen* dynamics, characterizing the *frozen phase.* In the second case the activity converges to a non-zero value A^*, signalling *chaotic* dynamics, characterizing the chaotic phase. In this phase species also evolve towards local maxima in fitness, but in the process of doing so, they change the fitness of other species, typically setting them back in evolution. After a transient time, a balance is reached where a certain fraction of species evolve, while another fraction remains at local fitness maxima, with individual species passing from one fraction to the other every so often.

The line $C/N = c_{\rm crit}$ dividing the (C, N)-plane into two phases is critical in the sense that the relaxation time to asymptotic behaviour diverges on this line, as shown in appendix F.

Appendix F: Relaxation Times

In order to find the relaxation time to asymptotic values, we linearize Eq. (10) at its fixed point solution. We write

$$\begin{aligned}
\rho_M(F;t) &= \rho^*_M(F) + \Delta\rho_M(F;t), && (106)\\
A(t) &= A^* + \Delta A(t), && (107)\\
\Phi(F;t) &= \Phi^*(F) + \Delta\Phi(F;t), && (108)\\
\phi(F;t) &= \phi^*(F) + \Delta\phi(F;t), && (109)
\end{aligned}$$

and insert these expressions in Eq. (10). By using Eq. (93) and keeping only terms linear in Δ...., we arrive at the linearized master equation

$$\begin{aligned}
\frac{\partial}{\partial t}\Delta\rho_M(F;t) &= -(1 - \frac{M}{N} + cA^*)\Delta\rho_M(F;t) \qquad (110)\\
&\quad + c(B_{M,N}(F) - \rho^*_M(F))\Delta A(t) + B_{M,N}(F)\Delta\Phi(F;t).
\end{aligned}$$

This equation is more easily solved by writing $\Delta\rho_M(F;t)$ as a Laplace transform:

$$\Delta\rho_M(F;t) = \int_0^\infty d\lambda\, e^{-t\lambda} \Delta\tilde{\rho}_M(F;\lambda). \tag{111}$$

$\Delta A(t)$ and $\Delta\Phi(F;t)$ are linear functionals of $\Delta\rho_M(F;t)$ and therefore commute with Laplace transformation. So with a self-explanatory notation, the inverse Laplace transform of Eq. (110) reads, slightly rewritten:

$$\Delta\tilde{\rho}_M(F;\lambda) = \frac{c\Delta\tilde{A}(\lambda)(B_{M,N}(F) - \rho^*_M(F)) + B_{M,N}(F)\Delta\tilde{\Phi}(F;\lambda)}{1 - M/N + cA^* - \lambda} \tag{112}$$

By multiplying both sides of this equation with $(1 - M/N)/(1 - F)$, and summing over M, one finds

$$\begin{aligned} &\Delta\tilde{\phi}(F;\lambda) = \\ &\quad c\Delta\tilde{A}(\lambda)(g(F;cA^* - \lambda) - g_1(F;cA^* - \lambda)) + g(F;cA^* - \lambda)\Delta\tilde{\Phi}(F;\lambda), \end{aligned} \tag{113}$$

where the function $g(F;x)$ was introduced in the previous appendix, and the function g_1 has a similar definition:

$$\begin{aligned} g_1(F;x) &= \frac{1}{1-F}\sum_{M=0}^{N-1} \frac{N-M}{N-M+Nx}\rho^*_M(F) \\ &= \frac{cA^*}{x - cA^*}(g(F,cA^*) - g(F,x))\exp(G(F,cA^*)) \end{aligned} \tag{114}$$

Eq. (113) is solved by

$$\begin{aligned} &\Delta\tilde{\Phi}(F;\lambda) = \\ &\quad c\Delta\tilde{A}(\lambda)e^{G(F;cA^*-\lambda)} \int_0^F dF'\, e^{-G(F';cA^*-\lambda)} \left(g(F';cA^* - \lambda) - g_1(F';cA^* - \lambda)\right) \\ &\quad = c\Delta\tilde{A}(\lambda)\left(-1 + \frac{cA^*}{\lambda}e^{G(F;cA^*)}\right) \end{aligned} \tag{115}$$

where we have used the definition, Eq. (114), for g_1 to obtain the last equality. Using

$$\Delta\tilde{A}(\lambda) = \int_0^1 dF\, \Delta\tilde{\Phi}(F;\lambda), \tag{116}$$

integration over F on both sides of Eq. (115) gives an equation for $\Delta\tilde{A}(\lambda)$ which is solved by $\Delta\tilde{A}(\lambda) = 0$, as we might expect, and by

$$\frac{cA^* - \lambda}{\lambda}(\mathcal{G}(cA^* - \lambda) - \mathcal{G}(cA^*)) = 0 \tag{117}$$

The smallest value for λ solving this equation contributes with the longest relaxation time

$$t^{\text{chaotic}}_{\text{relax}} = \lambda^{-1} \tag{118}$$

to $\Delta\rho_M(F;t)$ in Eq. (111). An obvious solution is

$$\lambda = cA^*. \tag{119}$$

A survey of $\mathcal{G}(x)$'s graph shows there are $N-1$ other solutions to Eq. (117), one in each interval $]cA^*+M/N, cA^*+(M+1)/N[$, where $M = 1, 2, \ldots, N-1$. So all these solutions correspond to contributions to $\Delta\rho_M(F;t)$ which decay faster in time than the mode corresponding to $\lambda = cA^*$. We conclude that the relaxation time in the chaotic phase is

$$t_{\rm relax}^{\rm chaotic} = \frac{1}{cA^*}, \tag{120}$$

where A^* is a function of c given implicitly by Eq. (101).

Since $A^* \sim c - c_{\rm crit}$ for $c - c_{\rm crit} \sim 0^+$, we see from Eq. (120) that the relaxation time diverges with exponent -1 at the critical connectivity. This typical mean-field value for the exponent comes as no surprise; it is after all a mean-field description we are developing. The value for this exponent is exact, however, in the limit $S = \infty$ of infinitely many species, which we are considering. The only requirement is that each species depends on a vanishing fraction of other species — i.e. $C/S = 0$ — and that the species which a given species depends on were chosen at random. Whether this randomness is quenched or annealed does not matter. This point has been explained in detail in [22, 23] for an in this respect identical problem.

In the frozen phase, where the order parameter $A^* = 0$, Eq. (117) shows

$$c^{-1} + 1 = \mathcal{G}(-\lambda) \tag{121}$$

which for a given value of $c < c_{\rm crit}$ has N positive solutions for λ, one in each interval $]cA^* + M/N, cA^* + (M+1)/N[$, where $M = 0, 1, \ldots, N-1$. The smallest solution, which determines the relaxation time, grows from $\lambda = 0$ to $\lambda = 1/N$ for c decreasing from $c_{\rm crit}$ to 0. So the relaxation time grows from N to infinity when c grows from 0 to $c_{\rm crit}$. This result agrees with the average relaxation time for isolated species found in appendix D, and the expected increase in relaxation time with increasing coupling.

We can summarize our results for the relaxation time in the following implicit expressions for it:

$$c^{-1} + 1 = \mathcal{G}(-t_{\rm relax}^{-1}) \quad \text{for} \quad c < c_{\rm crit} \tag{122}$$

$$c^{-1} + 1 = \mathcal{G}(t_{\rm relax}^{-1}) \quad \text{for} \quad c > c_{\rm crit} \tag{123}$$

where the solution for $t_{\rm relax}$ is obtained by using the branch of $\mathcal{G}^{-1}$ characterized by $-1/N < x < \infty$.

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[12] At this point we differ slightly from Kauffman's own definition of the *NKC*-model. He defines the fitness function of a species as the sum of N random functions, one for each gene, depending on the gene and on K other genes in the species *plus* on C genes in other species. For $K = N - 1$, a species' fitness function is therefore an entirely random function of the N genes in the species, but a rather correlated function of the foreign genes it depends on. There is no good reason that the fitness function should be this way; it is just an accidental consequence of its parametrization. So for convenience we have simply assumed that the fitness function is a random function of *all* its variables.

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[20] Strictly speaking, this probability for M less fit neighbors is $B_{M',N'}(F)$, with $N' < N$ and $M' = M - (N - N')$, because we already know that one or more 1-mutant neighbor configurations are less fit. But we can neglect this difference in calculations to leading order in $1/N$ for reasons similar to those given in appendix A.

[21] Contact is made with appendix B by observing that $g(F;0)$ essentially is equal to the function $h_{N-1}(F;1)$ defined there. The two functions differ only because in appendix B we chose to account explicitly for the impossibility of back-tracking in adaptive walks, though this is an effect of sub-leading order in $1/N$. In the present appendix, formulas are simpler when we neglect sub-leading terms from the start. Thus the difference between $g(F;0)$ and $h_{N-1}(F;1)$.

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Figure Captions

Fig. 1 Q_ℓ versus ℓ for $N = 10$ ($\circ$), 100 (∇), 1000 ($\triangle$), and 10,000 ($\square$). The connecting dashed lines are only meant to guide the eye. Poisson distributions with the same mean values are shown with the symbol $\bullet$. In the case of $N = 10$, the Gaussian distribution with same mean and variance as Q_ℓ is shown as a solid line.

Fig. 2 NQ_t versus t/N for $N = \infty$. Fully drawn curve: exact result from Eq. (92). Dashed curve: estimate from Eq. (3) with exact value for $\bar{t}$ taken from Eq. (89).

Fig. 3 The asymptotic activity A^* versus the connectivity c for $N = 10$ and $N = 100$ according to Eq. (101) (full curves) and according to Eq. (103) (dotted curve).

Fig. 4 Graph of the function $\mathcal{G}(x)$ defined in Eq. (97) in the case of $N = 10$ (full curve), and its approximation given in Eq. (98) (dotted curve).