

EFFECTIVE FITNESS AS AN ALTERNATIVE PARADIGM FOR EVOLUTIONARY COMPUTATION I: GENERAL FORMALISM

March 21, 2006

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Keywords: Fitness landscape, Effective Fitness, Genotype-Phenotype Map,
Exact Evolution equations.

Abstract

In evolutionary computation the concept of a fitness landscape has played an important role, evolution itself being portrayed as a hill-climbing process on a rugged landscape. In this article we review the recent development of an alternative paradigm for evolution on a fitness landscape – effective fitness. It is shown that in general, in the presence of other genetic operators such as mutation and recombination, hill-climbing is the exception rather than the rule; a discrepancy that has its origin in the different ways in which the concept of fitness appears — as a measure of the number of fit offspring, or as a measure of the probability to reach reproductive age. Effective fitness models the former not the latter and gives an intuitive way to understand population dynamics as flows on an effective fitness landscape when genetic operators other than reproductive selection play an important role. Additionally, we will show that when the genotype-phenotype map is degenerate, i.e. there exists a synonym symmetry, it can be used to quantify the degree of symmetry breaking of the map, thus allowing for a quantitative explanation of phenomena such as self-adaptation, bloat and evolutionary robustness.

1 Introduction

Fitness landscapes, in spite of the fact that one can almost never draw a realistic one, have served as one of the chief organizing principles in the theory of evolutionary systems and, more recently, in a wider context in the theory of complex systems. In this first of two papers we critique the notion of a fitness landscape as it is most popularly understood and introduce and discuss an alternative concept, effective fitness, that allows for a more intuitive and thorough understanding of the dynamics of evolutionary systems. In the second paper [1] we will present several models, both analytic and numerical, that show why effective fitness is both qualitatively and quantitatively superior to that of standard reproductive fitness in explaining important phenomena that occur both in real evolving systems and in Evolutionary Computation (EC). Although for illustrative purposes we will concentrate attention on genetic algorithms (GAs), it will be clear that the general framework is equally applicable to other areas of EC such as Evolution strategies (ES) and Genetic Programming (GP).

The notion of a fitness landscape, as originally conceived by Sewall Wright [2] in evolutionary biology, gives an intuitive picture wherein natural selection can be understood in terms of population flows on a mountainous terrain. More recently it has been utilized to address the issue of the “origin of order” [3] in the biological world, offering another paradigm for such order — spontaneous ordering — as opposed to the traditional Darwinian view of order by selection. In EC the concept of a fitness landscape has played an important role (see for example [4] for an historical perspective and [5] for a recent account of the role of landscapes in EC).

Without doubt fitness landscapes have served as an important conceptual fixed point in the development of a qualitative understanding of evolutionary systems. However, quantitatively, landscape analysis is usually so difficult that one has to typically start at the level of very simple models. EC, on the other hand, is somewhat simulation driven and very much oriented towards solving complicated, real world problems, hence paradigmatically simple landscapes, such as the needle-in-the-haystack (NIAH) landscape considered by Eigen [6], do not generate a great deal of interest. In terms of population dynamics on fitness landscapes much attention has been paid to adaptive walks on the hyper-cubic configuration spaces of the Kauffman NK -models [3]. Such dynamics can be of interest biologically speaking, but do not seem to be of particular interest for EC. Thus, there has been an expectation gap between what theoretical biologists, physicists, and mathematicians have been able to achieve in landscape theory and what the EC community has traditionally found to be of interest.

Landscape analysis in GA theory, for instance, has tended to focus on the relation between problem difficulty and landscape modality; the assumption being that more modality signifies more difficulty. Obviously, a classification of landscapes into those that are difficult for an evolutionary algorithm and those that are easy would be immensely useful. As has been discussed however, [7, 8], things can be somewhat counter-intuitive. For instance, the NIAH landscape is unimodal yet, as is well known, is difficult for a GA, and for that matter just

about anything else. On the other hand a maximally modal function, such as the porcupine function [9], can be easy. The moral here is that modality is not the same thing as ruggedness. Of more importance is the degree of correlation in the landscape. Correlation structure is obviously of the highest importance in search as it is a rough measure of the mutual information available between two points of the landscape. The correlation length, ξ , of the landscape is a characteristic measure of the degree and extent of such correlations. There are various methods to define correlation length, one of the most natural being in terms of the connected two-point correlation function or variance defined by $G(i, j) = \langle f(i)f(j) \rangle - \langle f(i) \rangle \langle f(j) \rangle$ where $\langle \rangle$ represents an average over the statistical ensemble of interest. One may define the corresponding correlation length as $\xi = -\ln G(i, j)/|i - j|$. Obviously this requires the definition and existence of a metric on the landscape. A fuller discussion of correlation lengths on fitness landscapes can be found in [10].

The key intuition behind the correlation length is that points separated by a distance $> \xi$ will be essentially uncorrelated, while points at a distance $< \xi$ will be substantially correlated. In the NIAH landscape the natural correlation length is zero, there being no indication anywhere in the landscape of the existence of the isolated global optimum. That the NIAH landscape has zero correlation length might seem a bit counterintuitive but is associated with the fact that the correlation length is defined from $G(i, j)$ and not $\langle f(i)f(j) \rangle$. In other words it is more concerned with correlations between fluctuations about the mean than with persistence, which is more appropriately measured by $\langle f(i)f(j) \rangle$.

When talking about fitness landscapes it is important to distinguish between static and dynamic landscape properties. The degree of ruggedness is a static concept. However, what is of importance in biology, as well as EC, is how a population flows on a given landscape. In fact, one might argue that the whole problem of evolution can be understood from the point of view of flows on fitness landscapes. Obviously, to specify a flow one has to specify a dynamics. There is then an important question: what properties are robust, i.e. universal, under a change in the dynamics and which are sensitive?

It would clearly be of enormous interest to have a more general theory of landscapes, though this is an extremely ambitious task. The work of [10] (see also references therein) is of particular interest in this context. The majority of previous work has been restricted to dynamics generated by one or both of the two genetic operators reproductive selection and mutation, some celebrated results being Fisher's fundamental theorem of natural selection [11] and the concept of an error threshold [6]. In particular, adaptive walk models for Kauffman NK landscapes [3] offer an arena wherein some analytical progress can be made. Work that includes the effect of recombination has been less forthcoming, especially in terms of analytical work.

A fundamental question is: how do the different genetic operators such as reproductive selection, mutation and recombination affect population flows? Here, we define a genetic operator to be any operation H such that $P(t+1) = HP(t)$, where $P(t)$ is the population at time t . A lot of the power behind the standard

visualization of a fitness landscape has been associated with the view that evolution is a hill-climbing process on such a landscape. This intuition however is linked to a particular class of dynamics — principally reproductive selection. In the presence of other genetic operators it is quite generic that population flows are not simple hill climbing processes. What is required is a more democratic approach that treats the various genetic operators on a more equal footing. Thus, one is led to enquire as to whether there exist other ways of thinking of landscapes so as to restore an intuitive picture of landscape dynamics in the presence of genetic operators other than reproductive selection.

Of course, it is all fine and well to talk about fitness landscapes. This presupposes an understanding of what fitness means. Fitness, almost everyone would agree, is a measure of reproductive success. In EC, following the lead of population genetics, fitness, f , directly measures the strength of the reproductive selection operator, be it proportional selection, tournament selection or whatever. One of the principal themes of this paper, which will be illustrated throughout using both analytic and numerical models, is that f , i.e. pure reproductive selection, quite generically is not a good measure of reproductive success.

In fact, this will always be the case when the genotype-phenotype map is degenerate, i.e. certain genotypes are equivalent in terms of reproductive selection. We call such equivalence a “symmetry”. Such genotypes are by definition selectively neutral with respect to each other. However, inevitably some genotypes experience more reproductive success than others. It might be that this is a purely stochastic or finite population effect. In such circumstances one may argue that the symmetry is spontaneously broken. However, in the presence of other genetic operators such as mutation and crossover one observes consistent preferences for some genotypes over others. In this case the other operators themselves are affecting the reproductive success in a highly non-trivial fashion. In this case one may speak of an induced symmetry breaking, induced by the action of operators other than reproductive selection.

Such induced symmetry breaking one can interpret as leading to a self-organization of the genotype-phenotype map. What we mean by self-organization here is that, as there is no selective preference for one synonym versus another in terms of f , one would expect, modulo finite size effects, to see a random distribution of synonyms, i.e. a lack of organization or structure. We will present later many examples where organization does occur and that such organization is an intrinsic property of the system and not something imposed externally, hence the term self-organization. We wish to emphasize that this is not some esoteric phenomenon but is at the heart of any evolving system. Some important examples of this phenomenon are bloat in GP, self-adaptation in GAs and the emergence of algorithmic language in genetic systems.

If selection isn't a good measure of reproductive success then what is? Effective fitness, denoted by f_{eff} , is as we shall see a much more direct measure of reproductive success and offers a qualitative and quantitative framework within which population dynamics can be intuitively understood as a population flow on an effective fitness landscape. Effective fitness treats all genetic operators

on an equal footing and can be computed algorithmically if one has access to an evolution equation for the population dynamics. In the context of effective fitness phenomena such as bloat, self-adaptation and evolutionary robustness can be not only qualitatively understood but also quantitatively.

The concept of effective fitness was introduced first in the context of GP [12, 13] to take into account the destructive effect of crossover and mutation in the context of an evolution inequality, i.e. an inequality that gives only a lower bound on the expected number of individuals of a certain genotype in the next generation, and importantly does not take into account the important contribution to effective fitness due to string and/or schema creation. A similar concept, “adjusted fitness” and the corresponding concept of an “adjusted” Walsh coefficient, were introduced in [14, 15] in the context of deceptive landscapes. Once again however, it was in the context of an evolution inequality.

Effective fitness was introduced independently in the context of GAs in [16, 17], and discussed more formally in [18, 19, 20]. One motivation for the introduction of effective fitness there was the recognition that the effects of operators such as mutation and crossover could be naturally reinterpreted via a “renormalization”, or redefinition, of the reproductive fitness. More importantly it was defined with respect to an exact evolution equation for strings and/or schemata that took into account exactly the effects of string/schema creation. In distinction to the Nordin-Banzhaf formulation [12, 13] where $f > f_{\text{eff}}$ always in the Stephens-Waelbroeck formulation [16, 17] quite generically $f < f_{\text{eff}}$. In fact, for every genotype where $f > f_{\text{eff}}$ there is another where $f < f_{\text{eff}}$.

Following the lead taken in [16, 17] Poli [21] has recently extended this definition of effective fitness to GP where it quite clearly offers the possibility to understand quantitatively the phenomenon of bloat. It can also be used to understand how evolutionary robustness, as measured by effective fitness, arises and thus offers a path to understanding how to overcome the “brittleness” problem.

The plan of the paper is as follows: in section 2 we discuss some relevant issues related to the definition of fitness drawing in particular a strong distinction between the concepts of selective or reproductive fitness and effective fitness which measures the complete reproductive success of an individual. In section 3, we discuss landscape statics and dynamics showing that a realistic landscape is almost always explicitly time dependent. We further consider population flows generated by the standard genetic operators: reproductive selection, mutation and crossover, and present dynamical equations that exactly describe the population evolution in the presence of these operators. In section 4 we define effective fitness and, in terms of the evolution equations presented in section 3, give an algorithm for computing it in a generic class of evolutionary models. Finally, in section 5, we draw some conclusions.

2 What is fitness?

Unfortunately, there is no general consensus on what fitness is physically, although most people would agree that it is in its broadest sense a measure of “reproductive success”. Mathematically, however, it is rather simply defined: $f_Q : Q \rightarrow R^+$ where Q is the space of phenotypes. The real domain of f_Q of course may be different from R^+ ; e.g. the integers over a finite interval.

It is conventional to consider fitness as a function of the phenotype, the latter being the physical expression of the genotype and hence the object on which natural selection is most naturally seen to act. However, the raw material of an evolutionary system is the genotype. This is certainly true in EC, where more often than not the genotype-phenotype relation is quite simple, hence, one needs to know how fitness manifests itself at the genotypic level. To do this one defines a map between genotype and phenotype, $\phi : G \rightarrow Q$, where G is the space of genotypes. The existence of the two functions ϕ and f_Q allows one to define on G a fitness function, $f_G = f_Q \circ \phi$, induced by the action of ϕ and f_Q .

Whenever the genotype-phenotype map is non-injective (many-to-one) the function f_G will be degenerate, many genotypes corresponding to the same fitness value, and hence non-invertible. This may also occur for other reasons. Thus, fitness defines an equivalence relation on G , many genotypes being equivalent selectively. We will refer to the equivalence of a set of genotypes under the action of reproductive selection (i.e. they’re all equally fit) as a “symmetry” between them. Obviously, by definition, reproductive selection preserves this symmetry. A simple example of this would be the standard synonym symmetry of the genetic code.

To what extent there exists a non-trivial genotype-phenotype map is very much area, and indeed problem, dependent. By non-trivial here we mean that it is many-to-one and exhibits some degree of self-organization. As mentioned, it appears in the genetic code, a given amino acid corresponding to more than one triplet codon. It also appears very naturally in GP where programs of variable structure and size can all be equally fit. We can thus pose the question: is there a selective advantage in having a non-trivial versus a trivial genotype-phenotype map?

Having defined fitness as a mathematical relation we must now understand it conceptually, in particular in its relation to other genetic operators. In its simplest, and perhaps most intuitive, form [22] fitness and selection are measured by the number of fertile offspring produced by one genotype versus another. We will call the fitness that measures the complete reproductive success of a particular genotype “effective” fitness for reasons that will become clear momentarily and which will be discussed extensively in sections 4 and 7.

A criticism that can be aimed against describing fitness in terms of the number of offspring is its tautological nature as manifested in the phrase “survival of the fittest”. If one defines effective fitness via a relation of the type

$$n_i(t+1) \propto f_{\text{eff}}^i n_i(t) \tag{1}$$

where $n_i(t)$ is the number of individuals of type i present in the population at time t it is of no predictive value if our only means of evaluating it is to measure n_i in two successive generations unless, for example, we know it is a constant in time. However, if one can provide an algorithm to calculate it then one can obviously use it to predict the population dynamics. One of the key objectives of this paper besides introducing and reviewing the concept of effective fitness is to show how to calculate it in a generic class of evolutionary models.

In EC, which follows the lead of population genetics, another notion of fitness is prevalent. Here it is a measure of the probability that an individual survives to reproductive age [23]. Obviously, such reproduction could be biological or algorithmic. This reproductive fitness is clearly a property of an individual, in that it does not depend on other genotypes, even though the reproductive fitness function may reflect environmental effects. Clearly the two concepts of fitness are quite different. We denote the latter for a genotype c_i by $f(c_i, t)$ or $f(c_i)$, depending on whether or not the fitness landscape is explicitly time dependent, and the effective fitness by $f_{\text{eff}}(c_i, t)$. In terms of genetic operators reproductive fitness takes into account only reproductive selection while effective fitness takes into account all genetic operators.

We will see below, using several model examples, that the effects of the other operators is such that very often population flows on the standard reproductive fitness landscape cannot be understood with any degree of intuition. When the effects of other genetic operators are small, selection being dominant, it is quite likely that the two fitnesses are quite close numerically. However, to take another extreme — neutral evolution, where all genotypes have the same probability to reach maturity — the two will be quite different.

Having discussed fitness we now come to the idea of a fitness landscape. One can intuitively think of a mountainous landscape where fitness is the height function above some D_Q or D_G -dimensional space where D_Q and D_G are the dimensions of the spaces Q and G respectively. However, the idea of a mountainous landscape carries with it the intuitive idea of a Euclidean metric. In evolutionary systems such a metric can be quite unnatural. However, in order to think of graphing a fitness landscape one indeed does need a distance function, or at the very least a notion of neighborhood and closeness, in order to have an ordering relation for G and Q . The visualization of the landscape will intimately depend on this metric, as indeed will the naturalness of the flows on the space.

A very common distance function is the Hamming distance, d_{ij} , between two genotypes c_i and c_j . Closeness is here defined by the bit by bit similarity between two strings. For a binary representation the domain for the fitness function is a hypercube where every vertex represents a possible string and every edge between two adjacent vertices represents a one-mutation jump. If one considers crossover rather than mutation it may be argued that Hamming distance is not the most natural of metrics and one may seek another more appropriate one. This thinking leads to the “One operator One landscape” philosophy advocated in [5]. However, there is only one dynamics, even though it may be induced by many different operators acting simultaneously, thus it

complicates matters unnecessarily using many landscapes to describe only one population flow, especially given the highly non-linear relationships between the different operators.

If the fitness function is an explicit function of time the corresponding landscape will be a dynamical not a static object. Almost invariably, landscape analysis has been restricted to landscapes associated with a static *reproductive* fitness. Such landscapes, as we shall see, are the exception rather than the rule. In particular, given that the number of offspring of a genotype will almost inevitably be a function of time a landscape based on f_{eff} will likewise be time dependent.

We may ask how does symmetry, such as the standard synonym symmetry alluded to above, affect the form of the fitness landscape? In this case fitness as a function of genotype will exhibit flat “directions” associated with the fact that there is no selective gradient between synonyms. The word “direction” here would be most appropriate in the case where synonyms are neighbors, although as previously emphasized neighbor depends both on the metric and the operators involved. In the presence of only reproductive selection one would expect the population to perform a random walk in this flat subspace. However, as we shall see this is not the case when other operators are present. In fact, this phenomenon is one of the possible causes of bloat [12, 13] in GP and related phenomena.

Another key idea associated with selection is the idea of order whose most salient characteristic for present purposes is that in the presence of selection a finite population will evolve into a subspace $U \subset G$ such that $\int_U \rho(x) \gg \int_{G-U} \rho(x)$ where $\rho(x)$ is the population density function normalized such that $\int_G \rho(x) = 1$. The population density function for a discrete model is $\rho(i) = \text{Limit}_{n \rightarrow \infty} (n(C_i, t)/n)$ where n is the population size. One may consider a continuous limit in a similar manner to as is done in fluid mechanics or field theory. Thus, the more ordered a system is the smaller the subspace into which it dynamically evolves. Such a point of view of evolution as an ordering process is implied by the idea that on a fitness landscape populations flow to fitness peaks. Intuitively, it is clear that selection will induce order in this sense. For example, in the presence of pure reproductive selection the dynamical attractor is typically of dimension zero.

In the presence of mutation, such as in the Eigen model [6], the quasi-species represents the dynamical attractor. i.e. if one starts with a disordered random state then the effect of selection is to arrive at a more ordered state — the quasi-species. As is well known, however, for a large class of fitness landscapes there exists a critical mutation rate above which there is no dynamical reduction onto a smaller dimension attractor, i.e. reproductive selection has its limits. The crucial point to emphasize here is that the system fails to order despite the presence of reproductive selection. In fact, considering the Eigen model with a NIAH landscape, even in the presence of an arbitrarily large fitness differential between the optimum and the rest there will exist some critical mutation rate beyond which there are no more offspring associated with the optimum than

with any other genotype.

In the case of systems with a degenerate genotype-phenotype map one would not expect to see ordering, other than by finite size effects, associated with the flat directions of the genotypic fitness landscape. However, the examples of sections 5 and 6 will show that other operators can induce such an ordering and that this ordering can be readily understood in terms of effective fitness.

3 Landscape Statics and Dynamics

As mentioned above, a fitness landscape is normally thought of as a static concept, the reproductive fitness assigned to a given configuration being independent of time. It is clear that generally this will be a crude oversimplification. Relatively speaking there has been little work dedicated to time dependent problems though this situation is changing rapidly.

Of course, under certain circumstances and over certain time scales a static landscape may be a good approximation to the actual one. In this case a key concept is the ruggedness of the landscape, which one can partially think of as being a measure of the density of local optima but, more importantly, is a measure of the degree of correlation in the landscape.

Naturally, there are situations, especially in global optimization, such as the traveling salesman problem, where the landscape is strictly static. However, here as well a time-dependent landscape emerges in a very natural way. Consider any microscopic configuration, c_i , that we can represent by a set s of N elements $\{s_k\}$, $k \in [1, N]$. Such a configuration could represent, for example, the genotype of an organism, or a possible solution to a combinatorial problem. The fitness of such a configuration, $f(c_i)$, we assume to be independent of time. Considering another configuration, $c_j \neq c_i$, of fitness $f(c_j)$ it is natural to ask: what common characteristics do the two configurations have? If they have N_2 elements in common, represented by a set $\{\bar{s}\} \subset \{s_k\}$, then we may ask if one may assign a fitness to those common characteristics? This can be simply done by defining

$$f(\xi, t) = f(c_i)P(c_i, t) + f(c_j)P(c_j, t) \quad (2)$$

where $P(c_i, t)$ is the probability of finding the configuration c_i at time t .

The above is very familiar to people working in GAs as ξ is just a schema. We mention it here as it is also of fundamental importance in biology, or indeed in any other area of EC. Why? Because, except in a computer simulation, one can never keep track of the evolution of all microscopic configurations, and even in this case it may neither be necessary nor desirable. Typically, what are of interest are more coarse-grained variables. For example, the fitness of a species, S , we can consider as

$$f(S, t) = \frac{\sum_{c_i \in S} f(c_i)P(c_i, t)}{\sum_{c_i \in S} P(c_i, t)} \quad (3)$$

where the sum is over those genotypes that are members of the species. The moral here is that any coarse graining whatsoever will introduce a time dependence into the fitness function for the coarse grained effective degrees of freedom. Thus, in general the concept of a dynamic landscape is of more relevance than a static one. Certainly fitness as measured in terms of number of offspring will be time dependent, hence, any landscape portrayal of this function will also be time dependent.

We now come to the crucial question of how to impose a dynamics on the fitness landscape. A population $\mathcal{M}(t) \equiv \{g(t)\} \subset G$, where $\{g(t)\}$ is the set of genotypes present in the population at time t , flows according to

$$\mathcal{M}(t+1) = \mathcal{H}(\{f(c_i)\}, \{\mathcal{M}(t)\}, \{p_k\}, t)\mathcal{M}(t) \quad (4)$$

where \mathcal{H} is an evolution operator that depends on the reproductive fitness landscape, $\{f(c_i)\}$, the population $\{\mathcal{M}(t)\}$ and the set of parameters, $\{p_k\}$, that govern the other genetic operators; e.g. mutation and recombination probabilities.

There are very many choices by which one can implement a population dynamics. A simple one, applicable in both biology and EC, is that of pure proportional selection which gives the following equation, in the case of an infinite population, for the mean proportion, $P(c_i, t)$, of genotype c_i

$$P(c_i, t+1) = (f(c_i)/\bar{f}(t))P(c_i, t) \quad (5)$$

where we assume the reproductive fitness landscape to be time independent. For a finite population the equation relates the expectation value of $P(c_i, t+1)$ to the actual proportion at time t . In this case $P(c_i, t) = n(c_i, t)/n$.

In this case it is clear how the population flows — monotonically towards the global optimum of the landscape (neglecting of course finite size effects). It is precisely such intuitive flows, according to the gradient of the landscape, that have lent such power to the concept of evolution as a flow on a fitness landscape. It should be fairly clear, and will be shown explicitly in section 4, that in this dynamics reproductive and effective fitnesses are equal due to the fact that the only operator present is reproductive selection.

A more general dynamics for proportional selection, mutation, and one-point crossover (the equations are easily generalized to more general crossover operators) can be described by the equation [16, 17]

$$P(c_i, t+1) = \mathcal{P}(c_i)P_c(c_i, t) + \sum_{c_j \neq c_i} \mathcal{P}(c_j \rightarrow c_i)P_c(c_j, t) \quad (6)$$

where the effective mutation coefficients $\mathcal{P}(c_i)$ and $\mathcal{P}(c_j \rightarrow c_i)$ represent the probabilities that the genotype c_i remains unmutated and the probability that the genotype c_j mutates to the genotype c_i respectively. $P_c(c_i, t)$ is the proportion of strings c_i at time t after selection and recombination. Explicitly

$$P_c(c_i, t) = (1 - p_c) P'(c_i, t) + \frac{p_c}{N-1} \sum_{k=1}^{N-1} P'(c_i^L(k), t) P'(c_i^R(k), t) \quad (7)$$

where $P'(c_i, t) = (f(c_i, t)/\bar{f}(t))P(c_i, t)$, $\bar{f}(t)$ being the average population fitness. p_c is the crossover probability and k the crossover point which ranges over the entire string. The quantities $P'(c_i^L(k), t)$ and $P'(c_i^R(k), t)$ are defined analogously to $P'(c_i, t)$ but refer to coarse grained variables, i.e. schemata, c_i^L and c_i^R . c_i^L is of order $N_2 = k$ and defining length $l = k$ while c_i^R is of order $N_2 = N - k$ and defining length $l = N - k$. Note that here and throughout we are taking the defining length to be the total number of bits between and including the outermost defining positions. Hence, $l = \delta(\xi) + 1$ where $\delta(\xi)$ is the standard definition. In the case of complete strings, as opposed to schemata as examined below, $l(c_i^L) = N_2(c_i^L)$ and $l(c_i^R) = N_2(c_i^R)$. One can illustrate the content of the equation with a simple example: 0110100|0101010010. The crossover point is at $k = 7$ hence $c_i^L = 0110100*****$ has $N_2 = l = 7$ while $c_i^R = *****0101010010$ has $N_2 = l = 10$.

An analogous equation, identical in functional form, for the case of a general schema ξ can also be derived [16, 17]

$$P(\xi, t + 1) = \mathcal{P}(\xi)P_c(\xi, t) + \sum_{\xi_i} \mathcal{P}(\xi_i \rightarrow \xi)P_c(\xi_i, t) \quad (8)$$

where

$$P_c(\xi, t) = P'(\xi, t) - \frac{p_c}{N-1} \sum_{k=1}^{l-1} (P'(\xi(k), t) - P'(\xi_L(k), t)P'(\xi_R(k), t)) \quad (9)$$

and the sum in (8) is over all schemata ξ_i that differ by at least one bit from ξ in one of the N_2 defining bits of ξ . In other words any schema competing with ξ and belonging to the same partition. All other quantities are the schema analogs of quantities defined in (6) and (7). Note that the sum over crossover points here is only over the within schema points, i.e. over the defining length, l , of the schema not over the entire string. Equation (8) obviously can also be interpreted as a schema theorem [18].

Both these equations will be found to be very useful in trying to quantify effective fitness. Both equations can be understood as describing the evolution of the mean proportion of strings or schemata in the infinite population limit or more generally the relation between the expected proportions at time $t + 1$ and the actual proportions at time t . These equations can also be generalized to the case of GP [24, 25].

4 Effective fitness and effective fitness landscapes

In section 2 we emphasized the difference between reproductive landscape fitness and effective fitness. We will now define mathematically the latter. There are several possibilities for such a quantity. For instance, based on the thermodynamic analogy [26] between an inhomogeneous two-dimensional spin model

and a population evolving with respect to reproductive selection and mutation, one could define quite naturally the free energy per row as an effective measure of fitness. Here, however, we will use another definition, more directly related to the traditional idea of fitness in biology and EC.

We define the effective fitness in the case of strings as [16, 17, 18, 20]

$$P(c_i, t+1) = \frac{f_{\text{eff}}(c_i, t)}{\bar{f}(t)} P(c_i, t) \quad (10)$$

and analogously in the case of schemata by

$$P(\xi, t+1) = \frac{f_{\text{eff}}(\xi, t)}{\bar{f}(t)} P(\xi, t) \quad (11)$$

One may think of the effective fitness as representing the effect of all genetic operators in a single reproductive selection factor. $f_{\text{eff}}(c_i, t)$ is the fitness value at time t required to increase or decrease $P(c_i, t)$ by pure reproductive selection by the same amount as all the genetic operators combined in the context of a reproductive fitness $f(c_i)$. If $f_{\text{eff}}(c_i, t) > f(c_i, t)$ the effect of the genetic operators other than selection is to enhance the reproductive success of genotype c_i . Obviously, the converse is true when $f_{\text{eff}}(c_i, t) < f(c_i, t)$.

The exact functional form of the effective fitness obviously depends on the set of genetic operators involved. For the fairly general case of equation (6) we have

$$f_{\text{eff}}(c_i, t) = \left(\frac{\mathcal{P}(c_i)P_c(c_i, t) + \sum_{C_j \neq c_i} \mathcal{P}(c_j \rightarrow c_i)P_c(C_j, t)}{P(c_i, t)} \right) \bar{f}(t) \quad (12)$$

Note that it is time dependent and depends on the actual composition of the population. Effective fitness also naturally extends to schemata via equation (11) and equation (8) and takes a form analogous to that above showing that it is form invariant under a coarse graining. Explicitly

$$\begin{aligned} f_{\text{eff}}(\xi, t) &= \mathcal{P}(\xi)\bar{f}(\xi, t) + \sum_{\xi_i} \mathcal{P}(\xi_i \rightarrow \xi) \frac{P(\xi_i, t)}{P(\xi, t)} \bar{f}(\xi_i, t) \\ &- \frac{p_c}{N-1} \mathcal{P}(\xi)\bar{f}(t) \sum_{k=1}^{l-1} \left(\frac{P'(\xi(k), t) - P'(\xi_L(k), t)P'(\xi_R(k), t)}{P(\xi, t)} \right) \\ &- \frac{p_c}{N-1} \sum_{\xi_i} \mathcal{P}(\xi_i \rightarrow \xi)\bar{f}(t) \sum_{k=1}^{l-1} \left(\frac{P'(\xi_i(k), t) - P'(\xi_{i_L}(k), t)P'(\xi_{i_R}(k), t)}{P(\xi, t)} \right) \end{aligned} \quad (13)$$

where $\bar{f}(\xi, t)$ is the average fitness of the schema ξ . In the limit $p \rightarrow 0$, $p_c \rightarrow 0$ (or in more generic circumstances when the strengths of operators other than reproductive selection $\rightarrow 0$) $f_{\text{eff}}(\xi, t) \rightarrow \bar{f}(\xi, t)$.

One is also naturally led to the idea of an effective selection coefficient, $s_{\text{eff}} = f_{\text{eff}}(\xi, t)/\bar{f}(t) - 1$, that measures directly effective selection pressure. If

we think of s_{eff} as being approximately constant in the vicinity of time t_0 , then $s_{\text{eff}}(t_0)$ gives us the exponential rate of increase or decrease of growth of the schema ξ at time t_0 . In the limit of a continuous time evolution the solution of the evolution equation (11) is

$$P(\xi, t) = P(\xi, 0)e^{\int_0^t s_{\text{eff}} dt'} \quad (14)$$

We emphasized previously that the evolution equations are valid for both finite and infinite populations. In the case of a finite population one must interpret differently the right hand side of the equation. One may say that effective fitness applies to a finite population if we interpret in equation (12) the string proportions as being the actual proportions in the population rather than as expected values. In other words that the evolution equations relate the actual population proportions at time t to the expected value at time $t + 1$. However, this can lead to pathological behavior such as $f_{\text{eff}}(C_i, t) \rightarrow \infty$ when $P(C_i, t) = 0$ and $P(C_i, t + 1) \neq 0$. Additionally, in this case the effective fitness landscape will change stochastically in time. This is not something intrinsic to the reproductive landscape, or the other operators themselves, but is a finite size effect arising from the limited stochastic sampling. For these reasons we prefer to think of the effective landscape as being defined in the infinite population limit where its evolution is completely deterministic. In this case the effective fitness landscape will give information about the expected evolution of a population. Of course, the ‘‘experimental’’ effective fitness can be determined by measuring the proportion of individuals of a given type in two successive generations. This will not generically compare well with theoretical estimates for small population sizes due to stochastic sampling effects.

We do not wish to propagate the point of view that definition (12) is unique, nor even the best definition under all possible circumstances. For instance, in [16, 17] another natural definition was presented which follows from the split into those terms of the evolution equation that are linear in $P(\xi, t)$ and those source terms that are independent of it. For instance, in the case of reproductive selection and crossover we have

$$P(\xi, t + 1) = \frac{f'_{\text{eff}}(\xi, t)}{f(t)} P(\xi, t) + j(t) \quad (15)$$

where

$$f'_{\text{eff}}(\xi, t) = (1 - p_c) \frac{(l - 1)}{N - 1} \frac{\bar{f}(\xi, t)}{f(t)} \quad \text{and} \quad j(t) = \frac{p_c}{N - 1} \sum_{k=1}^{l-1} P'(\xi_L(k), t) P'(\xi_R(k), t)$$

with the sum being over all crossover points within the schema ξ , l being the defining length of ξ . The corresponding effective selection coefficient is $s'_{\text{eff}} = ((1 - p_c) \frac{(l-1)}{N-1} \frac{\bar{f}(\xi, t)}{f(t)} - 1)$. In the limit of a continuous time evolution (15) may be formally integrated to yield

$$P(\xi, t) = e^{\int_0^t s'_{\text{eff}}(t') dt'} P(\xi, 0) + e^{\int_0^t s'_{\text{eff}}(t') dt'} \int_0^t j(t') e^{-\int_0^{t'} s'_{\text{eff}}(t'') dt''} dt' \quad (16)$$

This effective fitness is intuitively more similar to that of [12, 13, 14, 15] in that it takes into account only the destructive effect of crossover. Nevertheless, it captures a rather natural division into terms that lead to a multiplicative renormalization of reproductive fitness (destruction terms) and those that lead to an additive renormalization (creation terms). In this decomposition formal results such as Geiringer’s theorem follow in a most straightforward fashion [18].

The key element behind effective fitness, irrespective of its mathematical definition, is that population flows in the presence of operators other than pure reproductive selection are much more readily understood in terms of it. In fact, to go further, even in the case of pure reproductive selection, if one performs any sort of coarse graining and considers schemata rather than strings, then population flow is more readily understood in terms of an effective landscape rather than the reproductive one. As an example, for the evolution of a particular order 1 schema in a population of N -bit strings it is more natural to consider the *time dependent* one-dimensional landscape associated with the schema than the collective dynamics of the $2^{(N-1)}$ string types that go up to make the 1-schema. The job of evolution at the end of the day is to produce fit offspring which in their turn produce fit offspring which in their turn ... It is no use having an individual with high reproductive fitness that is associated with a high probability to mutate to a very low fitness individual.

5 Conclusions

In EC, as in biology, it is obviously of crucial importance to know what generic properties the effective degrees of freedom exploited by a genetic system possess. Of particular concern is what constitutes a “fit” string and what are the implications of the idea for population flows on the corresponding “fitness” landscapes. One of the main goals of this paper was to show that in general there is a strong difference between reproductive fitness and effective fitness and that it is the latter that really determines reproductive success. Another goal was to provide an algorithm for its computation in the context of GA evolution with proportional selection, one-point crossover and mutation. It is a simple matter to extend the results to other forms of crossover. The equations have also recently been extended to GP [21]. Effective fitness landscapes may serve as a conceptual tool, even without a quantitative method for computing it, in the same way as standard reproductive fitness landscapes have served an important purpose even though they can very rarely be computed. The further ability to compute the landscape adds an extra dimension to the theoretical framework.

One may of course ask why do we need another type of landscape? Isn’t the present one good enough? After all, the notion of an adaptive landscape has turned out to be one of the most powerful concepts in evolution theory. One of the strongest motivations for the fitness landscape concept is that it allows one to intuitively understand population flows as hill climbing processes, thus offering a compelling paradigm for how evolution works. However, as we have demonstrated the hill climbing analogy is intimately linked to a certain type of

dynamics associated with pure reproductive selection. In the presence of other genetic operators hill climbing is the exception rather than the rule and so the idea of a reproductive fitness landscape loses some of its appeal.

Another possible criticism is that effective fitness is intrinsically time-dependent. Doesn't this lead to an extra level of complication relative to that of a static landscape? As we have argued there are several motivations for thinking of a time dependent landscape as being more fundamental than a static one. First of all, it is more biologically realistic, as environmental effects that affect fitness are almost inevitably time dependent. Secondly, even if a landscape is static in terms of the microscopic degrees of freedom it will be time dependent in terms of any coarse grained degrees of freedom.

One might also argue that the definition is tautological — survival of the survivors. Such circularity is not very different to that which appears in other sciences such as physics where one can level the same sort of criticism at an equation such as Newton's Second Law. Such circularity is usually a hallmark of a truly fundamental concept and its definition. Additionally, and importantly, in the present context we have a way to, at least in principle, explicitly compute it in terms of the parameters associated with the various genetic operators. This has been explicitly carried out in this paper for some simple analytic models in the context of a GA with one-point crossover and mutation.

Another advantage of the effective fitness concept is that it allows one to quantitatively understand the different mechanisms by which order may arise in evolution, i.e. that order may arise due to the effect of genetic operators other than selection. In particular it provides a framework within which neutral evolution and natural selection can be understood as different sides of the same coin, and in particular under what circumstances neutral mutations may lead to adaptive changes. In this sense the phenomenon of orthogenesis, i.e. genetic drives in the presence of random mutations, is nothing more than the appearance of an effective fitness gradient in the case where there was no original reproductive fitness gradient. In the same vein it offers a quantitative measure of the degree of symmetry breaking by other genetic operators when the genotype-phenotype map is degenerate. This offers the possibility to understand quantitatively phenomena such as self-adaptation, bloat and robustness as all these phenomena are intimately associated with an induced symmetry breaking of the genotype-phenotype map. These matters will be discussed at much greater length in the second paper of this series.

The GA and GP exact schema equations provide a quantitative framework within which effective fitness may be further examined and refined. It will be of great interest to first build simple, tractable models within which bloat and self-adaptation could be understood. For instance, bloat could be first examined in the context of a variable length genome GA where several different length strings are all of equal reproductive fitness. It is intuitive to think that longer length solutions will be more stable to mutational disruption if the number of introns grows as the string size grows (without introns the well known complexity catastrophe of the Eigen model would tend to set in). One then must ask why strings shouldn't just grow without bound. This certainly doesn't happen in

nature as there is a cost to building longer strings. In EC the cost would be associated with having to do more function evaluations. Presumably these costs would lead to an equilibrium situation wherein strings of a given cost-dependent maximum size would be preferred. These strings would be of maximum effective fitness.

In paper II of this series we will consider some simple analytic models that exhibit behavior that can be very naturally understood in terms of an effective fitness landscape but that looks quite odd when viewed in terms of a reproductive fitness landscape. We show, in particular, using both simple analytic models and simulations of much more non-trivial evolving systems, that effective fitness is a perfect framework within which to understand and quantify the phenomenon of induced symmetry breaking of the genotype-phenotype map. We believe effective fitness will also be very useful as a formalism within which many interesting phenomena in molecular biology could be better understood. For example, understanding how large phenotypic changes can come about due to exploration of the “neutral net” [27] or how synonym-symmetry breaking in the HIV virus can be understood [28]. Clearly, much more work needs to be done in understanding the effective fitness concept and developing an intuition for landscape analysis based on it rather than the traditional idea of fitness landscape.

Acknowledgments

This work was partially supported through DGAPA-UNAM grant number IN105197. CRS is grateful to Riccardo Poli, Wolfgang Banzhaf, Bill Langdon and Alden Wright for useful discussions and also to Riccardo Poli for much encouragement both spoken and unspoken.

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