Schemata Evolution and Building Blocks

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Abstract

In the light of a recently derived evolution equation for genetic algorithms we consider the schema theorem and the building block hypothesis. We derive a schema theorem based on the concept of *effective fitness* showing that schemata of higher than average effective fitness receive an exponentially increasing number of trials over time. The equation makes manifest the content of the building block hypothesis showing how fit schemata are constructed from fit sub-schemata. However, we show that generically there is no preference for short, low-order schemata. In the case where schema reconstruction is favored over schema destruction large schemata tend to be favored. As a corollary of the evolution equation we prove Geiringer's theorem.

Key Words: Schema Theorem, Building Block Hypothesis, Evolution equation, Effective fitness.

1 Introduction

One of the most commonly asked questions about genetic algorithms (GAs) is: under what circumstances do GAs work well? Obviously an answer to this question would help immeasurably in knowing to which problems one can apply a GA and expect a high level of performance. However, to answer this question one has to answer a more fundamental question: how do GAs work? For example, in a typical optimization problem how does the GA arrive at a good solution? It is clear that in very complex problems this is not

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achieved via a random search in the state space. The search is structured. However, the question remains as to what is the nature of this structure. To put this question another way, if we think of individual string bits as "degrees of freedom", the GA does not exhaustively search through the different combinations of individual bits, i.e. a search in the entire state space. Rather it searches through a restricted space spanned by different combinations of "effective degrees of freedom" (EDOF), which are combinations of the more fundamental "microscopic" bit degrees of freedom.

What exact form these EDOF take depends of course on the particular landscape under consideration. Hence, one might despair as to whether it was possible to say anything that applied to more than a specific case. However, it is not meaningless to try to understand if they exhibit generic properties, independent of the landscape, or at least properties that are common to a large class of possible landscapes. The building block hypothesis and the schema theorem [10], [6] attempt to identify such generic features and as such have played an important role in GA theory, if one accepts that one of the principal goals of a theory is to provide a framework within which one can gain a qualitative understanding of the behavior of a system. The basic gist of the building block hypothesis is that *short*, *low-order*, highly fit schemata play a preeminent role in the evolution of a GA; i.e. that the relevant EDOF for a GA are short, low-order, highly fit schemata. The schema theorem tries to lend a more quantitative aspect to the hypothesis by showing that such schemata are indeed favored. This fact is deduced via an analysis of the destructive effects of crossover. However, as is well known, the schema theorem is an inequality and is such because it does not say anything precise about schema reconstruction. To understand better the interplay between schema destruction, schema reconstruction and schema length one requires an evolution equation that is exact, and where schemata are the fundamental objects considered.

Various exact evolution equations have been derived previously: [7] wrote down exact equations for two-bit problems. Later these equations were extended to three and four-bit problems citewhitley. These equations allowed for an explicit analysis of string gains and losses. [25] also presented an algorithm for generating evolution equations for larger problems that was equivalent to an earlier equation of Bridges and Goldberg [3]. Although exact these equations are extremely unwieldy and it is difficult to infer general conclusions from their analysis. Another related approach is that of Vose and collaborators [21], [22], [11] that treats GA evolution as a Markov chain. One of the chief drawbacks of all the above, with respect to an analysis of the schema theorem and the block hypothesis, is that the former are evolution equations for strings whereas the latter refer to schemata. Evidently an evolution equation that is amenable to interpretation and analysis that treats schemata as fundamental objects would be preferable. Such an equation has been derived recently ¹ [17], [16] for the case of proportional selection and 1-point crossover. The chief aim of this paper is to analyze the schema theorem and the building block hypothesis in the light of this equation.

Crucially, we will be able to quantify the effect of schema reconstruction relative to

¹After the completion of this work we became aware of the related work of Altenberg [1].

that of schema destruction. Traditionally, crossover as a source of schema disruption has been emphasized [23], [13]. This idea is at the heart of the schema theorem and the building block hypothesis. There has been some work towards a more positive point of view of crossover vis a vis reconstruction [19], [15] but mainly in the light of the exploratory nature of crossover. Here, we will see exactly under what conditions schema reconstruction dominates destruction.

In analyzing the consequences of the evolution equation we will especially emphasize two ideas: effective fitness and EDOF. With respect to the former we will show that: if one thinks intuitively of fitness as representing the ability of a schema to propagate then effective fitness is a more relevant concept than the conventional idea of fitness. We will formulate a schema theorem in terms of the effective fitness showing that schemata with high effective fitness receive an exponentially increasing number of trials as a function of time. The second key idea, already mentioned, is that of EDOF. Generically one can think of a schema as an EDOF. However, schemata offer for every string a decomposition into 2^N different elements of a space with 3^N members. Not every decomposition will be useful. In fact, typically, only a small subset. So what do we mean by useful? EDOF, if they are to have any utility whatsoever, should not be very strongly coupled. This is a notion that is intimately associated with how epistasis is distributed in the problem. This type of thinking is common to many fields and generally is associated with the idea of finding a basis for a highly non-linear problem wherein it decomposes into a set of fairly independent sub-problems. An important feature of complex systems is that the EDOF are "scale" dependent. This scale dependence very often takes the form of a time dependence wherein the EDOF are different at different stages of evolution. This complicates life greatly in that if we find a useful decomposition of a problem at time t we have no guarantee that it will remain a useful decomposition indefinitely into the future.

2 Coarse Graining and Schemata

As is well known to any scientist or engineer a good model of a system is one that captures the relevant features and ignores irrelevant details. The deemphasis of irrelevant details we can think of as a "coarse graining". Of course, a great difficulty is that often what is relevant versus irrelevant depends on what one wants to say about the system, i.e. what level of description one requires. It also, more often than not, depends on time. One of the most obvious examples of this is evolution: the primitive constituents of life, amino acids, DNA, RNA etc, which represent the "microscopic" degrees of freedom, over time combined to form progressively more and more complicated EDOF such as cells, sponges, people etc. This evolution in time is intimately linked to an evolution in "scale" and a corresponding evolution in complexity.

In a GA specifying all the bits of a string gives us the most fine grained, microscopic description possible. For strings of size N and a population of size n there are Nn degrees of freedom and, for a binary alphabet, $O(n2^N)$ possible population states. Consider the

different classes of fitness maps that may be defined: first, $f_G : G \longrightarrow R^+$, where G denotes the space of genotypes (string states) and f_G is the fitness function that assigns a number to a given genotype; second, $f_Q : Q \longrightarrow R^+$, where Q is the space of phenotypes. These mappings may be explicitly time dependent. In fact, this will normally be the case when the "environment" is time dependent. They may also be injective or not, although the map f_Q will usually be injective. If f_G is many-to-one then there exist "synonymous" genotypes, i.e. the mapping is degenerate. If we assume there exists a map $\phi: G \longrightarrow Q$ between genotype and phenotype then we have $f_G = f_Q \circ \phi$, i.e. the composite map induces a fitness function on G. A schema, ξ , consists of $N_2 \leq N$ defined bits. The defining length of the schema, l, is the distance between its two extremal defining bits. The space of all schemata, S, may be partitioned according to schema order; i.e. $S = \sum_{N_2} S_{N_2}$, where S_{N_2} is the space of schemata of order N_2 . The mapping $g : G \longrightarrow S$ between strings and schemata is many-to-one. The degree of degeneracy of the map, $g_{N_2} : G \longrightarrow S_{N_2}$, is 2^{N-N_2} . Except for the trivial case of a 0-schema, maximal degeneracy occurs when $N_2 = 1$ where half of S is mapped onto one schema. The fitness of a schema is the map $f_S: S \longrightarrow R^+$, which is related to f_G via the composite map $f_S \circ g = f_G$. Explicitly,

$$\bar{f}(\xi,t) = \frac{\sum\limits_{C_i \supset \xi} f(C_i,t) n(C_i,t)}{\sum\limits_{C_i \supset \xi} n(C_i,t)}$$
(1)

where $f(c_i, t)$ is the fitness of string c_i at time t, $n(c_i, t)$ is the expected number of strings of type c_i at time t and the sums are over all strings in the population that contain ξ .

As mentioned, the total number of schemata for a binary alphabet is 3^N . Why go to an even bigger space than the state space itself? One answer to this question is related to the idea of coarse graining. In defining a schema we *average* over all strings that contain the given schema. In such a sum we are summing over all possible values for the string bits $c_i - \xi$ present in the population. A schema thus represents a coarse grained degree of freedom because we are forfeiting explicit information about the out of schema string bits. Clearly the lower the order of the schema the higher the degree of coarse graining, the maximal coarse graining being associated with the maximally degenerate schema where $N_2 = 1$.

A schema of order N_2 has only N_2 degrees of freedom and 2^{N_2} possible states. Given that one of the fundamental characteristics of complex systems is the existence of a large number of degrees of freedom and an exponentially large state space any methodology that purports to reduce the number of EDOF will prove very useful. To see this in the context of an explicit example let us say that we wish to calculate the average fitness in a GA evolving according to proportional selection with strings of size N, where N is a multiple of 2. The evolution equation for the expected number of strings of type c_i , $n(C_i, t)$, is

$$n(c_i, t+1) = \frac{f(c_i, t)}{\bar{f}(t)} n(c_i, t).$$
(2)

The average population fitness, $\bar{f}(t)$, for the case of a non-time dependent landscape obeys the equation

$$\bar{f}(t+1) = \sum_{C_i} \frac{f^2(C_i)}{\bar{f}(t)} P(C_i, t)$$
(3)

where $P(c_i, t) = n(c_i, t)/n$, *n* being the population size which we regard as being constant. As proportional selection is a stochastic process, for small population sizes one will typically see large fluctuations, i.e. in any given experiment one may well see large deviations between the results of (2) and (3) and the corresponding experimental quantities. However, taking averages over repeated experiments the results converge to those of the above equations. In fact, in the infinite population limit $P(c_i, t)$ will converge to the probability of finding string c_i at time t. The string fitness maps every string state to R^+ . If the population is large then many strings will be represented and hence many terms in $\bar{f}(t)$ will be non-zero. Thus, to calculate the evolution of $\bar{f}(t)$ one needs to solve $\sim 2^N$ coupled equations. Let us instead take the following approach: we will average over odd string positions in the population leaving strings, c'_i , (or rather now schemata) of N/2 definite bits that satisfy

$$n(c'_{i}, t+1) = \frac{f(c'_{i}, t)}{\bar{f}(t)} n(c'_{i}, t)$$
(4)

where now the fitness of C'_i depends on time even if $f(c_i)$ didn't. To calculate $\bar{f}(t)$ one now only needs to solve $2^{N/2}$ coupled equations. One can repeat this process, each step of coarse graining reducing the number of EDOF by one half, until we reach the situation where a 1-schema has been reached. This cannot be further coarse grained of course, except by passing to the trivial situation wherein all string bits are summed over, i.e. a 0-schema. At this level the evolution equation for the effective string of size one (1-schema α) is

$$n(\alpha, t+1) = \frac{f(\alpha, t)}{\bar{f}(t)} n(\alpha, t)$$
(5)

Now, α can only take two values, 1 and 0 say, hence $\bar{f}(t) = [f(1,t)n(1,t)+f(0,t)n(0,t)]/n$. Thus, the problem of finding the average fitness has been reduced to that of solving a problem with one degree of freedom and two possible states!

So what's the catch? The principal, and more fundamental, problem is that the genetic operators, principally reproduction and crossover, are defined at the microscopic level. In other words, as can be seen in (1), to assign a fitness to a schema one has to sum

over the different strings in the population that contain it. Thus, to calculate quantities associated with the coarse grained degrees of freedom one must consider the microscopic degrees of freedom. One might be tempted therefore to think that even though there is an apparent reduction in the number of EDOF the net gain is canceled out by the fact that one has to return to the microscopic degrees of freedom in order to calculate their evolution under the genetic operators. If one wished to calculate the dynamics exactly then the above would be true. However, returning to the idea of emphasizing the relevant degrees of freedom it may well be that in the averaging process certain ones are more important than others, therefore allowing one to neglect, or treat as a perturbation, the effect of the irrelevant ones. In particular, near a fixed point of the dynamics one might well expect to see a simplification.

A second problem is that if we wish to ask a question about a particular string and we only have access to schemata of order $N_2 < N$ then the question will be impossible to answer. In other words, if we are going to accept a coarse grained description then we can only ask questions about coarse grained variables. This in no way will affect the calculation of population variables such as average population fitness, standard deviation about the average fitness etc. Neither should it affect the ability of the GA to find an optimum as a fixed point of the dynamics as this can be represented in terms of optimal schemata.

In the above we discussed a particular coarse graining which led to a certain, definite set of schemata of order N/2, N/4, ..., 1 associated with averaging over the odd bits of each successive coarse grained string. Generally there are very many different coarse grainings possible, $3^N - 1$ for a given string. Which are useful and which aren't? This depends on the fitness landscape under consideration. What one wishes to do is to choose a coarse graining that gives rise to EDOF that are relatively weakly coupled. Finding such a coarse graining may well of course be very difficult. The coarse graining by factors of 2 above is a proposal for an algorithm to calculate GA evolution. Whether this particular coarse graining would be useful, as mentioned, depends on the fitness landscape. Although the method might seem somewhat artificial it is important to emphasize that such methods, based on the idea of the renormalization group (see for example Goldenfeld (1989) for a review) have proved to be extremely effective in many areas of physics and applied mathematics and have yielded very good results on canonical optimization problems such as the Traveling Salesman problem.

Later we will emphasize that 1-schemata are very useful coarse grained variables, as being of size 1 they are immune to the effects of crossover. In terms of 1-schemata the average fitness in the population is

$$\bar{f}(t) = \sum_{i=\alpha}^{N} f(\alpha, t) P(\alpha, t)$$
(6)

where the sum is over the N possible 1-schemata, $f(\alpha, t)$ is the fitness of the 1-schemata α at time t and $P(\alpha, t) = n(\alpha, t)/n$ is the expected proportion of strings present in the population that contain the 1-schemata α .

3 Schema Equation

In this section we will review the derivation of the schema evolution equation of [17], [16]. Given that the microscopic degrees of freedom are strings however, we will first derive an equation for strings evolving under the effects of the three genetic operators: proportional selection, crossover and mutation. We will throughout only consider simple one-point crossover. The analysis can be repeated, with analogous results, for the case of n-point crossover.

We will consider the change in the expected number, $n(\xi, t)$, of strings that contain a particular schema ξ , of order N_2 and length $l \ge N_2$, as a function of time (generation). If mutation is carried out after crossover one finds that the expected relative proportion of c_i in the population, $P(c_i, t) = n(c_i, t)/n$, satisfies

$$P(c_i, t+1) = \mathcal{P}(c_i \to c_i) P_c(c_i, t) + \sum_{C_j \neq C_i} \mathcal{P}(c_j \to c_i) P_c(c_j, t)$$
(7)

where the effective mutation coefficients are: $\mathcal{P}(c_i \to c_i) = \prod_{k=1}^{N} (1 - p_m(k))$, which is the probability that string *i* remains unmutated, and $\mathcal{P}(c_j \to c_i)$, the probability that string *j* is mutated into string *i* given by

$$\mathcal{P}(_{C_j \to C_i}) = \prod_{k \in \{C_j - C_i\}} p_m(k) \prod_{k \in \{C_j - C_i\}_c} (1 - p_m(k))$$
(8)

where $p_m(k)$ is the mutation probability of bit k. For simplicity we assume it to be constant, though the equations are essentially unchanged if we also include a dependence on time. $\{C_j-C_i\}$ is the set of bits that differ between C_j and C_i and $\{C_j-C_i\}_c$, the complement of this set, is the set of bits that are the same. In the limit where p_m is uniform, $\mathcal{P}(c_i \rightarrow c_i) = (1 - p_m)^N$ and $\mathcal{P}(c_j \rightarrow c_i) = p_m^{d^H(i,j)}(1 - p_m)^{N-d^H(i,j)}$, where $d^H(i,j)$ is the Hamming distance between the strings C_i and C_j . The quantity $P_c(C_i, t)$ is the expected proportion of strings of type C_i in the population after selection and crossover. Explicitly

$$P_{c}(c_{i},t) = P'(c_{i},t) - \frac{p_{c}}{N-1} \sum_{C_{j} \neq C_{i}} \sum_{k=1}^{N-1} \mathcal{C}_{C_{i}C_{j}}^{(1)}(k) P'(c_{i},t) P'(c_{j},t) + \frac{p_{c}}{N-1} \sum_{C_{j} \neq C_{i}} \sum_{C_{l} \neq C_{i}} \sum_{k=1}^{N-1} \mathcal{C}_{C_{j}C_{l}}^{(2)}(k) P'(c_{j},t) P'(c_{l},t)$$

$$(9)$$

where p_c is the crossover probability, k is the crossover point, and the coefficients $\mathcal{C}_{C_i C_j}^{(1)}(k)$ and $\mathcal{C}_{C_j C_l}^{(2)}(k)$, represent the probabilities that, given that c_i was one of the parents, it is destroyed by the crossover process, and the probability that given that neither parent was c_i it is created by the crossover process. Explicitly

$$\mathcal{C}_{C_i C_j}^{(1)}(k) = \theta(d_L^H(i,j))\theta(d_R^H(i,j)) \tag{10}$$

and

$$\mathcal{C}_{C_j C_l}^{(2)}(k) = \frac{1}{2} [\delta(d_L^H(i,j)) \delta(d_R^H(i,l)) + \delta(d_R^H(i,j)) \delta(d_L^H(i,l))]$$
(11)

where $d_R^H(i, j)$ is the Hamming distance between the right halves of the strings c_i and c_j , "right" being defined relative to the crossover point, with the other quantities in (10) and (11) being similarly defined. $\theta(x) = 1$ for x > 0 and is 0 for x = 0, whilst $\delta(x) = 0 \quad \forall x \neq 0$ and $\delta(0) = 1$. Finally, $P'(c_i, t) = (f(c_i, t)/\bar{f}(t))P(c_i, t)$ gives the expected proportion of strings c_i after the selection step. Note that $C_{C_iC_j}^{(1)}(k)$ and $C_{C_jC_i}^{(2)}(k)$ are properties of the crossover process itself and therefore population independent. The equation (7) yields an exact expression for the expectation values, $n(c_i, t)$, and in the limit $n \to \infty$ yields the correct probability distribution governing the GA evolution.

The evolution equation we have derived takes into account exactly the effects of destruction and reconstruction of strings and, at least at the formal level, has the same content as other exact formulations of GA dynamics [21]. It should also be formally equivalent to the equation of Bridges and Goldberg [3]. Before passing to the case of schemata it is interesting to put the equation into a simpler form. To see this, consider first the destruction term. The matrix (10) restricts the sum to those C_j that differ from C_i in at least one bit both to the left and to the right of the crossover point. One can convert the sum over C_j into an unrestricted sum by subtracting off those C_j that have $d_L^H(i, j) = 0$ and/or $d_R^H(i, j) = 0$. Similarly one may write the reconstruction term as

$$\sum_{C_j \supset C_i^L} \sum_{C_l \supset C_i^R} P'(C_j, t) P'(C_l, t)$$
(12)

where c_i^L is the part of c_i to the left of the crossover point and correspondingly for c_i^R . However, by definition

$$\bar{f}(C_i^L, t) = \frac{\sum_{C_j \supset C_i^L} f(C_j, t) n(C_j, t)}{\sum_{C_j \supset C_i^L} n(C_j, t)}$$
(13)

where $\sum_{C_j \supset C_i^L} n(c_j, t)$ is the total number of strings in the population that contain c_i^L . The final form of the string equation without mutation thus becomes

$$P(c_i, t+1) = P'(c_i, t) - \frac{p_c}{N-1} \sum_{k=1}^{N-1} (P'(c_i, t) - P'(c_i^L, t)P'(c_i^R, t))$$
(14)

with

$$P'(C_i^L, t) = \sum_{C_j \supset C_i^L} P'(C_j, t)$$
(15)

and similarly for $P'(C_i^R, t)$. It is important to note here that in this form the evolution equation shows that crossover explicitly introduces the idea of a schema and the consequent notion of a coarse graining. C_i^L and C_i^R are schemata of order and length k and N-k respectively.

The analogous equation for schema evolution can be found by summing equation (7) over all strings that contain the schema of interest ξ . The result is

$$P(\xi, t+1) = \mathcal{P}(\xi \to \xi) P_c(\xi, t) + \sum_{\boldsymbol{\xi}_i} \mathcal{P}(\boldsymbol{\xi}_i \to \xi) P_c(\boldsymbol{\xi}_i, t)$$
(16)

where

$$P_c(\xi,t) = P'(\xi,t) - \frac{p_c}{N-1} \sum_{k=1}^{l-1} \left(P'(\xi,t) - P'(\xi_L,t) P'(\xi_R,t) \right)$$
(17)

and the sum in (16) 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 . All other quantities are the schema analogs of quantities defined in (7). The effective mutation coefficients $\mathcal{P}(\xi \to \xi)$ and $\mathcal{P}(\xi_i \to \xi)$ are

$$\mathcal{P}(\xi \to \xi) = (1 - p_m)^{N_2}$$
 and $\mathcal{P}(\xi_i \to \xi) = p_m^{d^H(\xi, \xi_i)} (1 - p_m)^{N_2 - d^H(\xi, \xi_i)}$ (18)

where $d^{H}(\xi, \xi_{i})$ is the Hamming distance between the schemata ξ and ξ_{i} .

A very interesting feature of the evolution equations we have presented is their form invariance under a coarse graining. Starting with the string equation any coarse graining to schemata of order $N_2 < N$ yields an equation identical in form to that of its predecessor.

4 Effective Fitness

Having derived the schema evolution equation, before turning to an analysis of its many features, we wish to digress on the notion of fitness. The main intuitive idea behind fitness is that fitter parents have more offspring. In equation (16), neglecting for the moment mutation and crossover, taking the limit of a continuous time evolution one finds

$$P(\xi, t) = P(\xi, 0) e^{\int_0^t s_\xi dt'}$$
(19)

where $s_{\xi} = \frac{\bar{f}(\xi,t)}{f(t)} - 1$ is the selective advantage of the schema ξ . If $s_{\xi} > 0$ the expected number of ξ grows, whilst if $s_{\xi} < 0$ it decreases. However, consider the following two simple cases. First, consider the effect of mutation without crossover in the context of a model that consists of 2-schemata, 11, 01, 10, 00, where each schema can mutate to the two adjacent ones when the states 11, 10, 00, 01 are placed clockwise on a circle. For example, 11 can mutate to 10 or 01 but not to 00. This is evidently the limit where two-bit mutations are completely negligible compared to one-bit mutations. We assume a simple degenerate fitness landscape: f(11) = f(01) = f(10) = 2, f(00) = 1. In a random population, $P(11) = \ldots = P(00) = \frac{1}{4}$. If there is uniform probability p_m for each schema to mutate to an adjacent one then the evolution equation that describes this system is

$$P(i,t+1) = (1-2p_m)P'(i,t) + p_m(P'(i-1,t) + P'(i+1,t))$$
(20)

For $p_m = 0$ the steady state population is P(11) = P(01) = P(10) = 1/3, P(00) = 0. Thus we see the synonym symmetry of the landscape associated with the degeneracy of the states 11, 10 and 01 is unbroken. However, for $p_m > 0$, the schemata distribution at t = 1, starting from a random distribution at t = 0, is P(11) = 2/7, P(01) = P(10) = $(2 - p_m)/7$, $P(00) = (1 + 2p_m)/7$. Thus, we see that there is an induced breaking of the landscape synonym symmetry due to the effects of mutation. In other words the population is induced to flow along what in the fitness landscape is a flat direction.

As a second example consider the 2-schemata problem now with crossover but neglecting mutation, and with a fitness landscape where f(01) = f(10) = 0 and f(11) = f(00) = 1. The steady state solution of the schema evolution equation is

$$P(11) = P(00) = \frac{1}{2} \left(1 - \frac{p_c}{2} \frac{(l-1)}{(N-1)} \right) \qquad P(01) = P(10) = \frac{p_c}{4} \frac{(l-1)}{(N-1)} \tag{21}$$

For l = N and $p_c = 1$ we see that half the steady state population is composed of strings that have zero fitness!

Although the above examples are artificial they serve to make the point that the genetic operators can radically change the "effective" landscape in which the population evolves. The actual "bare" landscape associated purely with selection in the above offers very little intuition as to the true population evolution. Real populations can flow rapidly along flat directions and strings may be present even if they have zero fitness. To take this into account we propose using an "effective" fitness function [17], [16] defined via

$$P(\xi, t+1) = \frac{f_{\text{eff}}(\xi, t)}{\bar{f}(t)} P(\xi, t)$$
(22)

comparing with equation (16) one finds

$$f_{\rm eff}(\xi,t) = \mathcal{P}(\xi \to \xi) \bar{f}(\xi,t) + \sum_{\xi_i} \mathcal{P}(\xi_i \to \xi) \frac{P(\xi_i,t)}{P(\xi,t)} \bar{f}(\xi_i,t) - \frac{p_c}{N-1} \mathcal{P}(\xi \to \xi) \bar{f}(t) \sum_{k=1}^{N-1} \left(\frac{P'(\xi,t) - P'(\xi_L,t)P'(\xi_R,t)}{P(\xi,t)} \right) \frac{p_c}{N-1} \sum_{\xi_i} \mathcal{P}(\xi_i \to \xi) \bar{f}(t) \sum_{k=1}^{N-1} \left(\frac{P'(\xi_i,t) - P'(\xi_{i_L},t)P'(\xi_{i_R},t)}{P(\xi,t)} \right)$$
(23)

In the limit $p_m \to 0$, $p_c \to 0$ we see that $f_{\text{eff}}(\xi, t) \to \bar{f}(\xi, t)$. The above also leads to the idea of an effective selection coefficient, $s_{\text{eff}} = f_{\text{eff}}(\xi, t)/\bar{f}(t) - 1$, that measures directly

selective 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 (22) is

$$P(\xi, t) = P(\xi, 0) e^{\int_0^t s_{\text{eff}} dt'}$$
(24)

In the case of the toy examples above: for mutations without crossover

$$f_{\text{eff}}(i,t) = f_i + \frac{p_m}{P(i,t)} (f_{i-1}P(i-1,t) + f_{i+1}P(i+1,t) - 2f_iP(i,t))$$
(25)

At t = 0, $f_{\text{eff}}(11, 0) = 2$, $f_{\text{eff}}(01, 0) = f_{\text{eff}}(10, 0) = 2 - p_m$ and $f_{\text{eff}}(00, 0) = 1 + 2p_m$. Thus we see that the effective fitness function provides a selective pressure by selecting among the degenerate schemata those that have a higher probability to produce fit descendents.

Of course, the definition of effective fitness is not unique. Another natural definition 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 selection and crossover we have

$$P(\xi, t+1) = \frac{f'_{\text{eff}}(\xi, t)}{\bar{f}(t)} P(\xi, t) + j(t)$$
(26)

where $f'_{\text{eff}}(\xi,t) = (1 - p_c \frac{(l-1)}{N-1}) \frac{\bar{f}(\xi,t)}{f(t)}$ and $j(t) = \frac{p_c}{N-1} \sum_{k=1}^{l-1} P'(\xi_L,t) P'(\xi_R,t)$. 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 (26) may be formally integrated to yield

$$P(\xi, t) = e^{\int_0^t s'_{\text{eff}}(t')dt'} P(\xi, 0) + e^{\int_0^t s'_{\text{eff}}(t')dt'} \int_0^t j(t') e^{-\int_0^{t'} s'_{\text{eff}}(t'')dt''} dt'$$
(27)

5 Schema Theorem and Building Blocks

We now turn to a discussion of the schema theorem and the building block hypothesis. The standard "schema theorem" [10, 6], or fundamental theorem of GAs, states that for a schema, ξ , of length l evolving according to proportional selection and 1-point crossover

$$P(\xi, t+1) \ge P'(\xi, t) \left(1 - p_c \left(\frac{l-1}{N-1}\right) - N_2 p\right),$$
 (28)

and has the interpretation that schemata of higher than average fitness will be allocated exponentially more trials over time. The conventional schema theorem only provides us with a lower bound for the expected number of schemata due to the fact that it does not explicitly account for schema reconstruction. Equation (16), however, exactly takes into account the effect of schema reconstruction due to both mutation and crossover. Together with the definition of effective fitness in equation (23) of the previous section it allows one to state a new schema theorem:

Schema Theorem

$$P(\xi, t+1) = \frac{f_{\text{eff}}(\xi, t)}{\bar{f}(t)} P(\xi, t)$$
(29)

The interpretation of this equation is clear and analogous to the old schema theorem: schemata of higher than average *effective fitness* will be allocated an "exponentially" increasing number of trials over time. We put the word exponentially in quotes as the real exponent, $\int^t s_{\text{eff}} dt'$, is not, except for very simple cases such as a flat fitness landscape, of the form αt , where α is a constant. The illustrative examples of the last section show that there is potentially a strong difference between the standard selection based fitness and effective fitness as the latter takes into account the effect of all genetic operators. The fact that strings with zero selective fitness can receive an exponentially increasing number of trials shows quite clearly that effective fitness is a more relevant concept. In this sense our schema theorem does not just state the obvious — that fit schemata that are preserved by the crossover operator will prosper. Once again this emphasizes the role of the destructive effect of crossover. The novel element here is seeing exactly how important is schema reconstruction. In fact generically it is the dominant contribution.

The schema evolution equation we have derived possesses many interesting features one of the most interesting being the way that it relates evolution in time to different levels of coarse graining. To see this we first return to the string evolution equation (7). Up to this point we have presented our results in almost the most general way possible — for any type of landscape and taking into account both crossover and mutation. Throughout the rest of the paper we will concentrate more on the effect of crossover and thus neglect mutation. The reason for this is that we will mainly be concerned with the importance of schema length vis a vis the building block hypothesis. Mutation being a strictly local operator will not play a major role in this discussion. Note that this equation is written entirely in terms of the fundamental degrees of freedom — the strings. In passing to the form (14) we have performed a coarse graining by summing over all strings that contain C_i^L irrespective of what lies to the right of the crossover point, and similarly for strings containing C_i^R . The implication is that the very nature of crossover imposes on us the idea of coarse graining, and more specifically the idea of a schema, given that c_i^L and c_i^R define schemata of order and size k and N-k respectively. In order to solve the equation (14) we need to know $P(C_i^L, t)$ and $P(C_i^R, t)$. However, these in turn obey evolution equations of the form

$$P(c_i^L, t+1) = P'(c_i^L, t) - \frac{p_c}{N-1} \sum_{m=1}^{k-1} (P'(c_i^L, t) - P'(c_i^{LL}, t)P'(c_i^{LR}, t))$$
(30)

where c_i^{LL} and c_i^{LR} are the left and right parts of c_i^L , left and right being defined relative to the crossover point m, where m < k. Now, c_i^{LL} and c_i^{LR} as schemata are more coarse grained than c_i^L , i.e. they are of lower order. Clearly this pattern of behavior continues, i.e. in order to calculate $P(c_i, t+1)$ one requires $P(c_i^L, t)$ and $P(c_i^R, t)$ which in their turn require $P(c_i^{LL}, t-1)$, $P(c_i^{LR}, t-1)$, $P(c_i^{RL}, t-1)$ and $P(c_i^{RR}, t-1)$ etc. For each step back in time we pass to more coarse grained degrees of freedom. c_i thought of as a schema is of higher order than c_i^L or c_i^R , which in their turn are of higher order than c_i^{LL} , c_i^{LR} , c_i^{RL} and c_i^{RR} . So where does this process stop? The maximally coarse grained EDOF are 1-schemata. It is not possible to cut a 1-schemata and hence crossover is explicitly neutral, i.e. 1-schemata obey the equation

$$P(i, t+1) = P'(i, t)$$
(31)

l

As a simple example consider a 4-bit string ijkl. The hierarchical structure of one possible ancestral tree can be written as

 $ijk,l \qquad ij,kl \qquad i,jkl$

$$t+1$$
 $ijkl$

t

t-1
$$ij, k \quad i, jk \quad i, j \quad k, l \quad jk, l \quad j, kl$$

t-2
$$i, j = j, k = j, k = k$$

This tree shows only the effect of the reconstruction term in the schema equation over the space of 3 generations. Of course there are many other processes that contribute to the appearance of ijkl at time t + 1 that involve various combinations of schemata destruction and reconstruction. As far as pure schemata reconstruction is concerned however we see that 1-schemata play a privileged role as they represent the ultimate building blocks. For an N-bit string the maximum number of time steps before all ancestors are 1-schemata is N - 1.

All the above equally applies to a generic schema, ξ , composed of schemata, ξ_L and ξ_R which in their turn are composed of the schemata ξ_{LL} , ξ_{RL} , ξ_{LR} and ξ_{RR} etc. It should be clear that the idea of building blocks is manifest in the very structure of our evolution equations. ξ_{LL} , ξ_{RL} , ξ_{LR} and ξ_{RR} are building blocks for ξ_L and ξ_R which in their turn are building blocks for ξ . The ultimate building blocks are of course the 1-schemata. In the above example of a 4-bit string or schema the four building blocks of order one, i, j, k and l combine to form building blocks of order two ij and kl which in turn combine with the building blocks of order three combine with the blocks of order one and the blocks of order two combine together to give blocks of order four, and so the process continues.

In terms of the effective fitness, $f'_{\text{eff}}(\xi, t)$ introduced previously

$$P(\xi,t) = e^{\int_0^t s'_{\text{eff}}(t')dt'} P(\xi,0) + \frac{p_c e^{\int_0^t s'_{\text{eff}}(t')dt'}}{N-1} \sum_{k=1}^{N-1} \int_0^t P'(\xi_L,t') P'(\xi_R,t') e^{-\int_0^{t'} s'_{\text{eff}}(t'')dt''} dt' (32)$$

Up to now we have been able to analyze a general landscape. To arrive at more explicit, analytic formulae in an arbitrary landscape is prohibitively difficult. We will therefore temporarily restrict our attention to some more restrictive but simpler cases. We start with the case of a flat fitness landscape. In this case $s_{\text{eff}} = -p_c(l-1)/(N-1)$, hence

$$P(\xi,t) = e^{-p_c \frac{(l-1)}{(N-1)}t} P(\xi,0) + e^{-p_c \frac{(l-1)}{(N-1)}t} \frac{p_c}{N-1} \sum_{k=1}^{N-1} \int_0^t P'(\xi_L,t') P'(\xi_R,t') e^{p_c \frac{(l-1)}{(N-1)}t'} dt'$$
(33)

Notice that dependence on the initial condition, $P(\xi, 0)$, is exponentially damped unless ξ happens to be a 1-schema, the solution of the 1-schemata equation being

$$P(i,t) = P(i,0) \tag{34}$$

An immediate consequence is that when considering the source term describing reconstruction the only non-zero terms that need to be taken into account are those which arise from 1-schemata, as any higher order term will always have an accompanying exponential damping factor. Thus we see that the fixed point distribution for a GA with crossover evolving in a flat fitness landscape is

$$P^{*}(\xi) = Lt_{t \to \infty} P(\xi, t) = \prod_{i=1}^{N_{2}} P(i, 0)$$
(35)

which is basically Geiringer's Theorem [5] in the context of schema distributions and simple crossover. We see here that the theorem appears in an extremely simple way as a consequence of the solution of the evolution equation.

Note that this fixed point distribution arises purely from the effects of reconstruction, the absence of which leads to a pure exponential damping and the unphysical behavior $P(\xi) \to 0$. We can also see from the above that a version of Geiringer's theorem will also hold in a more general non-flat landscape where selection is only very weak, where what we mean by weak is that $\frac{\bar{f}(\xi,t)}{f(t)} \sim (1+\epsilon)$ and $\epsilon < \frac{p_c (l-1)}{(N-1)}$ $\forall l > 1$. Under such circumstances once again anything other than a 1-schema will be associated with an exponential damping factor. A distinction between the two cases however is that for a flat fitness landscape the fixed point is fixed by the initial proportions of the various 1-schemata as there is no competition between them. Here, however, due to the non-trivial landscape would be $f_i = 1 + \alpha_i$ where $\sum_i |\alpha_i| \leq \frac{\epsilon}{(2+\epsilon)}$ and f_i is the fitness of the ith bit. Note there is no need to restrict to a linear fitness function here, arbitrary epistasis is allowed as long as it does not lead to large fitness deviations away from the mean. In this case $\frac{\bar{f}(\xi,t)}{f(t)} < 1 + \epsilon$.

So what is the analog of the building block hypothesis here? Our schema theorem states that schemata of above average *effective* fitness will be allocated "exponentially" more trials over time. In the way the evolution equation is structured we see that the effective fitness in terms of the effects of crossover consists of a destruction term and a reconstruction term. Inherent in the structure of the reconstruction term is a form of the building block hypothesis — that higher order schemata are built from fit, shorter, lower order schemata. If $P'(\xi, t) > P'(\xi_L, t)P'(\xi_R, t)$ then the effects of destruction will outweigh those of reconstruction, whilst if $P'(\xi, t) < P'(\xi_L, t)P'(\xi_R, t)$ reconstruction will dominate. The content of this inequality is that reconstruction will dominate destruction if the probability to select the parts of a schema is greater than the probability to select the whole schema. Once again this is a general conclusion valid for any landscape. To give a more analytic slant we restrict to the case of two-schemata in a flat fitness landscape wherein one finds

$$s_{\rm eff} = -p_c \left(\frac{l-1}{N-1}\right) + p_c \left(\frac{l-1}{N-1}\right) \frac{P(i,0)P(j,0)}{P(ij,t)}$$
(36)

Thus we see that the effect of reconstruction is greater than that of destruction if i and j are negatively correlated. Notice that if reconstruction is more important then the contribution from the latter is maximized by maximizing the schema length, l. In other words large, rather than small, schemata are favored!

In general the fitness landscape itself induces correlations between ξ_L and ξ_R . In this case there is a competition between the (anti-) correlating effect of the landscape and the mixing effect of crossover. Selection itself more often than not induces an *anti*correlation between fit schemata parts, rather than a positive correlation. Indeed, in the neutral case of a non-epistatic landscape one has $1 + \frac{2N_2}{N} \delta f_{\xi} < (1 + \frac{2N_L}{N} \delta f_{\xi_L})(1 + \frac{2N_R}{N} \delta f_{\xi_R})$ where δf_{ξ} , δf_{ξ_L} and δf_{ξ_R} are the fitness deviations of the schemata ξ , ξ_L and ξ_R from an average fitness which we have normalized to one half. Thus we see that selection induces an anti-correlation when δf_{ξ_L} , $\delta f_{\xi_R} > 0$ and hence in an uncorrelated initial population, $P'(\xi, t) < P'(\xi_L, t)P'(\xi_R, t)$. This means that crossover plays an important role in allowing both parts of a successful schema to appear in the same individual. The effect of crossover is to weaken but not cancel completely the anti-correlations induced by selection and thus make it easier to find the whole schema. Indeed, it is possible to show that for a non-epistatic landscape that the contribution to population fitness from all schemata of length l, starting with a random initial population at time t, is independent of l at time t + 1 and is an increasing function of l for large l at time t + 2[17].

More complicated landscapes one has to examine on a case by case basis. Of course, it is always possible to invent a landscape where there is a fitness advantage associated with bits that are close together. However, it is equally easy to find one where there is a fitness advantage for bits that are widely separated. The non-epsitatic landscapes above are neutral in this respect and therefore any results about the nature of schemata and building blocks are a reflection of the geometric effect of crossover and not associated with bit-bit correlations induced by the landscape itself. We now have ample experimental evidence that this is the case as well for "generic" landscapes with epistasis such as the Kaufmann Nk models. This evidence will be published elsewhere. A particularly interesting example of epistasis is deception as it has played an important role in the theory of GAs [7]. The very nature of deception is such that the bits of a schema are less selected than the whole and hence we can see from the schema equation that in this circumstance destruction will outweigh reconstruction. However, this will only be totally deceptive if all possible schema reconstruction channels $\xi_L + \xi_R \rightarrow \xi$ are deceptive. For a schema of order N_2 there are $N_2 - 1$ such channels. Thus, for N_2 large it will typically be quite unlikely that all channels will be deceptive. If there exist non-deceptive channels then it is probable that the population will evolve in those directions. In fact, as the example of a two-schema shows, for every deceptive channel there is a non-deceptive one. One may explicitly see this from

$$P(11, t+1) = P'(11, t) - p_c \left(\frac{l-1}{N-1}\right) \left(P'(11, t)P'(00, t) - P'(01, t)P'(10, t)\right)$$
$$P(01, t+1) = P'(01, t) - p_c \left(\frac{l-1}{N-1}\right) \left(P'(01, t)P'(10, t) - P'(11, t)P'(00, t)\right)$$
(37)

Here 11-channel deception, i.e. P'(11,t)P'(00,t) > P'(01,t)P'(10,t), implies that the 01-channel is non-deceptive. However, this is not much consolation if the 11-schemata happens to be the optimum. If we start with a random population then 11-channel deception is equivalent to the statement $f_{\text{eff}}(11) < f(11)$. For something as simple as the two-schemata problem there is only a single 11-channel. For the 4-bit schemata ijkl we see that there are six reconstruction channels in total. There are various ways to end at a totally deceptive problem. For instance, the three channels $ijk + l \rightarrow ijkl$, $ij+kl \rightarrow ijkl$ and $i+jkl \rightarrow ijkl$ might all be deceptive. Alternatively all the 1-schemata \rightarrow 2-schemata channels might be deceptive. Generically the deviation of the effective fitness from the selective fitness will offer a reasonable measure of deception.

6 Conclusions

In this paper we have analyzed the Schema Theorem and the Building Block Hypothesis based on an exact evolution equation for GAs. At the level of the microscopic degrees of freedom, the strings, we established that the action of crossover by its very nature introduces the notion of a schema, the probability to reconstruct a given string being dependent on the probabilities for finding the right and left parts of the string relative to the crossover point in the two parents. These probabilities involve a coarse graining, i.e. an averaging over all strings that contain the constituent parts of the string, and hence represent schema probabilities. We saw that the same equation, after a suitable coarse graining, also described the evolution of any arbitrary schema.

One might enquire as to what advantages a formulation based on schemata, as has been presented here, has over other existing formulations, such as the Vose Markov chain model. Indeed, the value of schemata and the Schema theorem in understanding GA evolution has been seriously questioned [9, 20, 14, 12] There are many possible answers to this question: first a pragmatic one — that all "things" are made out of "building blocks", whether they be tables, giraffes or computer programmes. Having an exact, amenable description of complex systems from the microscopic point of view is a vain hope. Complex systems and complex behaviour can much better be understood in terms of EDOF. EDOF, almost by definition, are much fewer in number than the microscopic degrees of freedom and hence, in principle, would offer a computationally simpler picture. However, the number of ways of combining the microscopic degrees of freedom into EDOF is very large, hence one might think that such a description is even more costly than one based on the microscopic degrees of freedom such as the Vose model. This would be true if in analysing the GA one had to search through all the possible "coarse grainings" available. For a given landscape, however, a preferred coarse graining will often suggest itself. Secondly, we believe strongly that approximation schemes for solving GA evolution equations will be much more forthcoming via a formulation in terms of schemata wherein one may appeal to all the intuition and machinery of the renormalization group.

We introduced the notion of effective fitness showing through explicit examples that it was a more relevant concept than pure selective fitness in governing the reproductive success of a schema. Based on this concept of effective fitness and our evolution equation we introduced a new schema theorem that showed that schemata of high effective fitness received an exponentially increasing number of trials as a function of time. We then went on to discuss the building block hypothesis. One of the more remarkable features of our equation is that it implicitly contains a version of the latter in that the structure of the reconstruction term relates in an ancestral tree the relation between a given schema and its more coarse grained ancestors as a function of time. This ancestral tree terminates at 1-schemata, which are in some sense the ultimate building blocks as they cannot be destroyed by crossover. We also showed that generically there is no preference for short, low-order schemata. In fact if schema reconstruction dominates the opposite is true, typically large schemata will be favored. Only in deceptive problems does it generally seem that short schemata will be favored, and then only in totally deceptive problems as the system will tend to seek out the non-deceptive channels if they exist.

There are many points of departure from the present work to future research. On the theoretical side it will be very interesting to see if other exact results besides Geiringer's theorem follow very simply from our evolution equation. A fundamental issue is trying to find approximation schemes within which the equations can be solved, as for a general landscape an exact solution will be impossible. In this respect, as mentioned, techniques familiar from statistical mechanics such as the renormalization group might well prove very useful. In fact the very structure of our evolution equation is very similar to that of a renormalization group equation, a theme we shall return to in a future publication. It is of course necessary to verify the equations numerically. Some work in this direction has already been done [17] and further work has confirmed its qualitative conclusions [18]. In this respect one has to tread carefully, as the interplay between selection and crossover can be very subtle as the work on Royal Road functions [4] has shown. Although very simple we favor preliminary analytic analyses based on non-epistatic landscapes where one knows that there is no intrinsic inter-bit linkage due to the fitness landscape

and therefore one can study the geometric effects of crossover in a more uncluttered environment.

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