ANALYSIS OF THE EFFECTIVE DEGREES OF FREEDOM IN GENETIC ALGORITHMS

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Abstract: An evolution equation for a population of strings evolving under the genetic operators: selection, mutation and crossover is derived. The corresponding equation describing the evolution of schematas is found by performing an exact coarse graining of this equation. In particular exact expressions for schemata reconstruction are derived which allows for a critical appraisal of the “building-block hypothesis” of genetic algorithms. A further coarse-graining is made by considering the contribution of all length-l schematas to the evolution of population observables such as fitness growth. As a test function for investigating the emergence of structure in the evolution the increase per generation of the in-schemata fitness averaged over all schematas of length \( l \), \( \Delta l \), is introduced. In finding solutions of the evolution equations we concentrate more on the effects of crossover, in particular we consider crossover in the context of Kauffman \( Nk \) models with \( k = 0, 2 \). For \( k = 0 \), with a random initial population, in the first step of evolution the contribution from schemata reconstruction is equal to that of schemata destruction leading to a scale invariant situation where the contribution to fitness of schematas of size \( l \) is independent of \( l \). This balance is broken in the next step of evolution leading to a situation where schematas that are either much larger or much smaller than half the string size dominate over those with \( l \approx N/2 \). The balance between block destruction and reconstruction is also broken in a \( k > 0 \) landscape. It is conjectured that the effective degrees of freedom for such landscapes are landscape connective trees that break down into effectively fit smaller blocks, and not the blocks themselves. Numerical simulations confirm this “connective tree hypothesis” by showing that correlations drop off with connective distance and not with intrachromosomal distance.
1. Introduction

One of the most important steps in developing a qualitative or quantitative model of a system is to gain an understanding of the nature of the effective degrees of freedom of the system. This is equally true if one is considering static, equilibrium properties or dynamics; in the context of “simple” systems or of complex systems. An important feature that distinguishes the effective degrees of freedom is that their mutual interactions are not very strong; that is to say that they must have a certain degree of integrity. In this sense, the aim of developing an effective model of a system is to arrive at a description of the system in terms of relevant (e.g., “macroscopic”) variables.

Identifying the correct effective degrees of freedom in complex systems is generally speaking a very difficult task. To begin with, more often than not the effective degrees of freedom are scale dependent, where what one means by “scale” depends on the particular problem under consideration. In the case of evolution theory and genetic algorithms, one expects to find different effective degrees of freedom at different time scales. Generically if a system is complex at the relevant scale then it will admit a simple effective dynamics only in terms of complex degrees of freedom: one trades the complicated dynamics that results from the non-linear interactions of the many “elementary” degrees of freedom for the simpler dynamics of more complicated effective degrees of freedom. What one gains in the trade is effective predictability; what one loses is detail.

It is well worth recalling in this context the example of spin glass models of neural networks [1, 2, 3]. In this case the effective degrees of freedom are the overlaps with a certain number of “patterns”, each of which is related to a local extremum of the energy landscape or Hamiltonian. Since a large number of uncorrelated patterns is involved in this effective representation it should be clear that the description of the effective degrees of freedom themselves requires a large amount of information: One gets a measure of the complexity of the system by the information in its effective degrees of freedom. Note that in this example the system’s dynamics is guided by large-scale attracting structures (the patterns), the effective degrees of freedom (overlaps) being the instruments which measure how structure emerges as the system condenses from a disordered phase.

Not all complex systems have a large-scale structure which can be described in terms of macroscopic variables with a “simple” effective dynamics. For example in a critical sandpile [4], the relevant macroscopic variable is the avalanche size, and nothing short of a detailed description of every grain of sand would allow one to predict the size of the next event. Some examples of structured complex systems besides the Hopfield models include the brain, gene expression in eukaryotic cells [5], and of course evolution theory and genetic algorithms, among many others. We know that these systems are structured because their behaviour is manifestly non-random; for instance neural dynamics must be structured if the brain is to be of any use! Yet in most cases we have no idea what the nature of this structure is, much less how to identify effective degrees of freedom.

In this paper we will begin to analyse the notion of effective degree of freedom in the context of genetic algorithms (GA’s) [6,7]. The claim that genetic algorithms are structured complex systems is central to their designer’s purpose, in that they yield intelligent solutions to complex optimization problems rather than a sophisticated sort of random search. We emphasize however that GA’s form only one area of interest where the results and conclusions of this paper are applicable, some others being statistical mechanics [8] and biology [5], the Kauffman Nk model [9], and evolution theory [10].

Trying to ascertain what effective degrees of freedom a GA is using in order to arrive at an optimal solution is in the strict sense a nonsensical question — roughly equivalent to asking “what are the effective degrees of freedom of a block of material?” Of course,
the answer depends on the type of material under consideration and its state, the effective
degrees of freedom of a superconductor being quite different to those of a spin-glass for
instance. However, it is not non-sensical to think of what are the effective degrees of
freedom in a generic type of fitness landscape. The fitness landscapes we choose to consider
as being representative of general classes of fitness landscapes are Kauffman’s \( Nk \) models
with \( k = 0 \) and \( k = 2 \).

As in the example of spin glasses, the dynamics of genetic algorithms can be viewed as
a condensation process in a rugged landscape. So again one expects the effective degrees of
freedom to represent the emergence of certain structures, or “patterns”, which are related
to local fitness optima. In GA theory one usually considers partly-specified patterns, called
“schematas”, and determines the fraction of all the individuals in the population which
include a particular schemata, this being a measure of order comparable to the “overlap”
of spin glass models. Since one does not know a priori which schematas lead to a useful
set of effective degrees of freedom some hypothesis must be made to this effect.

The standard conjecture about the effective degrees of freedom of genetic algorithms
is the “building block hypothesis” [6,7], the essence of which is that a GA arrives at an
optimal solution of a complex problem via the combination of short, fit schematas. In this
paper we will present both analytic and numerical evidence that generically this is not
the case. The argument for the block hypothesis is that large schematas are likely to be
“broken” by the crossover operator. Roughly speaking, the probability that a parent pass a
length-\( l \) schemata down to its offspring drops off like \( \frac{1}{N^l} \), where \( N \) is the size of the string.
However, this argument neglects the possibility that a schemata be repaired, if the other
parent has the part of the schemata that was broken by crossover; more importantly as it
turns out, it neglects the possibility that a schemata be reconstructed from two parents
that have incomplete parts of it.

It is clear that the validity of the block hypothesis will depend on the nature of the
fitness landscape. If there is a larger contribution to fitness from string bits that are
widely separated then clearly large schematas will be favoured irrespective of the effect
of crossover. On the contrary if the fitness landscape strongly favours smaller schemata
this would lend support to the block hypothesis. However, the intuition behind the block
hypothesis is firmly based on the action of crossover not with the pathologies of particular
landscapes. It is for this reason that we choose to consider the block hypothesis in the
context of Kauffman \( Nk \) models. In particular, the case \( k = 0 \) corresponds to the neutral
case where there are no bit-bit interactions to induce size dependence. In all cases, we will
assume that the fitness landscape is generic in the sense that there is no systematic bias
in the fitness function that would favour one part of the string over another.

The bulk of this paper is devoted to deriving an equation for the evolution of schematas,
and from there a coarse-grained equation which gives the average contribution of schematas
of size \( l \) to the improvement of fitness. We will show that under general assumptions the
coarse-grained variable is closely related to the spatial correlation function, so it provides
information about the size distribution of the effective degrees of freedom. We will apply
this equation to particular situations, to analyse the effect of crossover on the emergence
of correlations between distant bits in the strings. Both the theoretical analysis and the
numerical simulations lead to a new conjecture about the effective degrees of freedom of
direct-encoded genetic algorithms on an \( Nk \)-landscape, which we call the “connective tree
hypothesis”.

The format of the paper will be as follows: in section 2, as this paper is not intended for
a dedicated GA audience, we will give a brief overview of various elements of GA theory. In
section 3 we will derive an evolution equation for the development of a population of strings.
under the genetic operators of selection, mutation and simple crossover. We then “coarse
grain” this equation to derive an effective evolution equation for the evolution of schematas
of size $l$ and order $N^2$, thus arriving at a generalization of the fundamental theorem of
schematas [6]. In section 4 we consider a further coarse grain considering the effects of
schematas of size $l$ but of any order $N^2 \leq l$. We consider especially the increment in fitness
per generation from such schematas. In section 5 we consider asymptotic solutions of the
coarse grained evolution equation near a random initial population for a simple “neutral”
fitness landscape and also make some comments about what happens near the ordered
population limit. In section 6 we consider a more non-trivial landscape — a Kauffman $Nk$
model [9] with $k = 2$. Finally in section 7 we summarize our conclusions.

2. Genetic Algorithms and the Building Block Hypothesis

GA’s have become increasingly popular in the analysis of complex search and optimization
problems and in machine learning, one of their chief attributes being their robustness
(see [11] and references therein for a recent overview). One begins with a complex opti-
mization problem which depends on many variables. The variables and the rules that
govern them are subsequently coded in the form of a population of strings/“chromosomes”.
The latter consist of a set of symbols/“alleles”, each symbol taking values defined over an
alphabet. Here we will only consider binary codification though our general conclusions
apply also to alphabets of higher cardinality. We will denote by $A_s$ the space of possible
states of a string.

The population is evolved under the action of a set of genetic operators. Reproduction
can be implemented in many different ways, all have the effect of increasing the relative
numbers of “fit” strings between one generation and another; fitness being measured by a
fitness function, $f : A_s \rightarrow \mathbb{R}_+$. The role of most other genetic operators is to encourage
diversity in the population. In this paper we will restrict our attention to simple crossover
and mutation. The former is a type of recombination and involves the splitting of two
parents, $C_i, C_j \in A_s$, at a particular crossover point $k$, and the subsequent juxtaposition
and recombination of the left half of $C_i$ with the right half of $C_j$ and the right half of
$C_i$ with the left half of $C_j$, left and right being defined relative to the crossover point $k$.
As mentioned, the point of genetic operators such as crossover is to encourage population
diversity. Optimal strings that do not appear in the initial population cannot subsequently
appear through the effects of reproduction alone. Crossover is one method for generating
fit strings that weren’t originally in the population of a given generation. Mutation on the
other hand offers a form of insurance in that if a particular bit is lost it is irrecoverable
using only reproduction and crossover. Mutation offers a way to recover lost bits that
may subsequently be important in the construction of an optimum string. Speaking intu-
itively, we may say that relative to an optimum string, mutation produces “errors” whereas
crossover merely shuffles them around. We will find this distinction to be an important
one when we come to critique the building block hypothesis later. Using the language
of statistical mechanics the evolution of the GA is a competition between the “ordering”
tendency of reproduction and the “disordering” effects of crossover and mutation.

The language used in GA theory obviously owes much to evolutionary biology, indeed
the whole point of GA’s was to try to adapt the methods used by adaptive systems in
nature in the context of artificial systems; selection, mutation and recombination being
extremely important elements in the search for “fit” organisms. In the discussion above,
for instance, a string could represent a protein chain of a certain size and the possible
values of a symbol the number of possible alleles at a particular site on the chain.

Theoretical analysis of how a GA seeks an optimum solution has focussed on the notion
of schematas. If we consider strings of \( N \) bits, a schemata is a subset, \( N_2 \leq N \), of bits defining a certain “word” constructed from the alphabet. In the \( N - N_2 \) positions not defined by the schemata one does not care about the value of the bit and this is taken into account by use of the metasymbol, or “wildcard”, \( \ast \). For an alphabet of size \( m \) there are \( \alpha_\xi = (m + 1)^N \) possible schematas for a particular string. The total number of possible schematas in the population is \( n_\xi \leq n(m + 1)^N \), the exact number depending on the population diversity. For a totally organised population \( n_\xi = \alpha_\xi \).

The essential idea behind the notion of schemata is that the GA arrives at an optimum solution through combining fit schematas. As each string is an example of \( \sim 2^N \) schematas it is clear that a very large number of them are being processed simultaneously by the GA, a phenomenon known as implicit parallelism [6]. Of course, not all these schematas survive crossover, which leads us to consider the size of a schemata, \( l \), which is defined as \( (l = j - i + 1) \), where \( i \) and \( j \) are the first and last of the \( N_2 \) defining elements of the schemata respectively. In terms of reproduction alone there is no preference for short versus long schematas, except as might be induced by the fitness function itself. Equally, mutation shows no favour for one or the other. However, if one considers the effects of crossover, purely in terms of the crossover point itself there is a higher probability to “break” a long schemata than a short one. This of course neglects the possibility of reconstructing a schemata even though it does not appear in either of the parents involved in the crossover process. This apparent disfavour for large schematas imposed by crossover has led to what is known as the “building block” hypothesis which claims that the joint effect of reproduction and crossover is to favour highly fit but short schematas which propagate from generation to generation exponentially. It is these highly fit, short schematas which are then considered to be the effective degrees of freedom in the system, the GA building a better solution through combining small sub-solutions.

3. String Evolution Equation

In this section we will derive an equation that describes the evolution of a GA induced by the effects of the three genetic operators: selection, crossover and mutation. In particular we will consider the change in number \( n(\xi, t) \) of strings that contain a particular schemata \( \xi \), of order \( N_2 \) and size \( l \geq N_2 \), as a function of time (generation) in a population of size \( n \). It is worth pointing out here that a schemata itself is already a coarse grained degree of freedom in the sense that to calculate any properties of a schemata, such as its fitness, one needs to take a population average.

We will first derive evolution equations for the “microscopic” degrees of freedom themselves — the strings. Considering first selection in the absence of mutation or crossover one has

\[
P(C_i, t + 1) = P'(C_i, t)
\]  

where \( P'(C_i, t) = (f(C_i, t)/\bar{f}(t))P(C_i, t) \), \( f(C_i, t) \) is the fitness of string \( C_i \) at time \( t \), \( P(C_i, t) = n(C_i, t)/n \) and \( \bar{f}(t) = \sum_i f(C_i, t)P(C_i, t) \) is the average string fitness. In (1) we are neglecting fluctuations in the numbers \( n(C_i, t) \), an approximation which should be reasonable as long as the population is not too “sparse”, we will return to this point later. Clearly, as previously mentioned, the effect of reproduction is to augment the number of fit strings, fit here meaning \( f(C_i, t) > \bar{f}(t) \), and to decrease the number of unfit strings, where by unfit we mean \( f(C_i, t) < \bar{f}(t) \). In terms of reproduction alone it is simple to prove that average fitness is a Lyapunov function, increasing monotonically as a function of time. As also discussed in the last section, the trouble with using selection as the sole genetic operator is that the search space for optima is restricted to that of the initial population.
where processes may be a more suitable framework in this regard [12].

Including in the effects of mutation but not crossover gives rise to the quasi-species model [13], with evolution equation

\[ P(C_i, t + 1) = P(c_i)P'(C_i, t) + \sum_{C_j \neq C_i} P(c_j \rightarrow c_i)P'(C_j, t) \]  \hspace{1cm} (2)

where \( P(c_i) = \prod_{k=1}^{N} (1 - p(k)) \) is the probability that string \( i \) remains unmutated, \( p(k) \) being the probability of mutation of bit \( k \) which we assume to be a constant, though the equations are essentially unchanged if we also include a dependence on time. \( P(c_j \rightarrow c_i) \) is the probability that string \( j \) is mutated into string \( i \),

\[ P(c_j \rightarrow c_i) = \prod_{k \in \{C_j - C_i\}} p(k) \prod_{k \in \{C_j - C_i\}_c} (1 - p(k)) \]  \hspace{1cm} (3)

where \( \{C_j - C_i\} \) 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 the mutation rate \( p \) is uniform, \( P(c_i) = (1 - p)^N \) and \( P(c_j \rightarrow c_i) = p^{d_H(i,j)} (1 - p)^{N-d_H(i,j)} \), where \( d_H(i,j) \) is the Hamming distance between the strings \( C_i \) and \( C_j \). The behaviour of the solutions of equation (2) has been much discussed in the literature (see for example [8] and references therein), although mainly in the context of a flat fitness landscape. One of the principal features of interest is the existence of an “error threshold” separating an “ordered” (selection dominated) phase from a “disordered” (mutation dominated) phase which manifests itself as a second order phase transition at a certain critical mutation rate.

We will now consider the effects of crossover without mutation. This is a much less studied case theoretically (though see [14]), but one that is very important from the point of view of effective degrees of freedom, since unlike mutations it is sensitive to the linear disposition of bits along the string. It is also plays a very important role in biology. With crossover the evolution equation can be written in the form

\[ P(C_i, t + 1) = P'(C_i, t) - \frac{p_c}{N-1} \sum_{C_j \neq C_i} \sum_{k=1}^{N-1} C_{C_iC_j}^{(1)}(k)P'(C_i, t)P'(C_j, t) \]

\[ + \frac{p_c}{N-1} \sum_{C_j \neq C_i} \sum_{C_l \neq C_i} \sum_{k=1}^{N-1} C_{C_jC_l}^{(2)}(k)P'(C_j, t)P'(C_l, t) \]  \hspace{1cm} (4)

where \( p_c \) is the probability to implement crossover in the first place,

\[ C_{C_iC_j}^{(1)}(k) = \theta(d_H^{R}(i,j))\theta(d_H^{L}(i,j)) \]  \hspace{1cm} (5)

and

\[ C_{C_jC_l}^{(2)}(k) = \frac{1}{2} \left( \delta(d_H^{L}(i,j))\delta(d_H^{R}(i,l)) + \delta(d_H^{R}(i,j))\delta(d_H^{L}(i,l)) \right) \]  \hspace{1cm} (6)

where \( d_H^{R}(i,j) \) is the Hamming distance between the right halves of the strings \( C_i \) and \( C_j \), “right” being defined relative to the crossover point \( k \). The other quantities are defined
analogously. $C_{c_i c_j}^{(1)}(k)$ is the probability that given that $c_i$ was one of the parents it is destroyed by the crossover process. $C_{c_j c_i}^{(2)}(k)$ is the probability that given that neither parent was $c_i$ it is created by the crossover process, so this represents a gain term. It is naturally much easier to destroy an individual string by crossover than create it hence $C_{c_j c_i}^{(2)}(k)$ is a very sparse matrix. $C_{c_j c_i}^{(2)}(k)$ represents a contact interaction term in Hamming space. Another important property of $C_{c_i c_j}^{(1)}(k)$ and $C_{c_j c_i}^{(2)}(k)$ is that they are completely population independent, depending only on string configurations and not string numbers.

In the case of mutations and selection without crossover the non-equilibrium evolution equation has been mapped into an equilibrium statistical mechanics problem using transfer matrix techniques [15], where the role of inverse temperature is played by

$$\beta = \frac{1}{2} \log(p/(1-p)).$$

One can also find an analogy for the crossover operator which can provide a more intuitive understanding of its effects. Imagine a “population” of $n$ one-dimensional Ising chains in a strong magnetic field $h$, where the effects of spin-spin couplings may be neglected. We denote spin up by 1 and spin down by 0. The “fitness” of string $i$ is simply $f(c_i) = h(n_1 - n_0)$. Clearly selection will favour strings with large values of $n_1$ relative to $n_0$. So what are the effects of crossover? Consider two selected chains of size $N = 7$: 1111000 and 0100111. One may think of the first chain as being composed of a domain of up spins of size 4 and a domain of down spins of size 3 separated by a domain wall or “kink”. Similarly, the second chain consists of two domains of up spins of sizes 1 and 3, and two of down spins of sizes 1 and 2. These domains are separated by two kinks and two anti-kinks. If the crossover occurs at $k = 5$ the resultant chains are 1111111 and 0100000. Chain number one is now “homogeneous”, containing no kinks or anti-kinks, whilst chain two contains a kink–anti-kink pair. Thus the action of crossover has been the annihilation of a kink–anti-kink pair. A crossover at $k = 3$ would have yielded: 1100111 and 0111000, each chain now having one kink–anti-kink pair. One can think of this as just a kink–kink scattering process that has conserved the total number of kinks and anti-kinks. Finally, a crossover at $k = 6$ would give 1111011 and 0100100 where now there are three kink–anti-kink pairs, one in the first chain and two in the second. In this case there has been kink–anti-kink creation. Thus we see here that crossover may be interpreted as creation, annihilation and scattering of kinks | domain walls, thought of as topological defects. Here, the fitness landscape is such as to favour spin chains without topological defects. This is because we are considering a “ferromagnetic” fitness landscape. If the fitness landscape were such as to favour 0’s in odd positions and 1’s in even positions then an optimum chain would be 0101010, i.e. an inhomogeneous state with a maximum number of kink–anti-kink pairs. Generically then, crossover may be thought of as inducing interactions between “domains”. Exactly what type of domain is favoured is of course a function of what is the particular fitness function of interest. It is also worth noting that in the population crossover without selection preserves the total number of 0’s and 1’s in any given bit position in the population. Thus for instance, if we consider a non-optimum string as having “errors” relative to an optimum string, pure crossover without selection cannot change the total number of errors in the population it can only shuffle them around.

Equation (4) is an extension of the “schema theorem”, or fundamental theorem of GA’s, [6,7] which states that for a schemata, $\xi$, of size $l$

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

(7)

to the case where the schemata of interest is the entire string (an analogous equation was derived in [16]). The evolution equation we have derived takes into account exactly, given
the approximation of a large population, the effects of destruction and reconstruction of
strings.

Combining the effects of both crossover and mutation, where we assume that mutation
is carried out after crossover, we have the evolution equation
\[ P(C_i, t + 1) = \mathcal{P}(c_i) P_c(C_i, t) + \sum_{c_j \neq c_i} \mathcal{P}(c_j \rightarrow c_i) P_c(C_j, t) \]
where
\[ P_c(C_i, t) = P'(C_i, t) - \frac{pc}{N-1} \sum_{c_j \neq c_i} \sum_{k=1}^{N-1} C_{i,j}^{(1)}(k) P'(C_i, t) P'(C_j, t) \]
\[ + \frac{pc}{N-1} \sum_{c_j \neq c_i} \sum_{c_l \neq c_i} \sum_{k=1}^{N-1} C_{j,l}^{(2)}(k) P'(C_j, t) P'(C_l, t) \]

(8)

The various evolution equations exhibit different dynamical fixed points. In the “low
temperature limit” \( p \to 0 \), in a non-trivial fitness landscape, one has stable fixed points at
the local fitness extrema. If \( f(C_i, t) > f(C_j, t) \forall C_j : \mathcal{P}(c_i \rightarrow C_j) > 0 \), then
\[ n(C_i) = n, \quad n(C_j) = 0 \]

is a stable fixed point of (8). These evolution equations are exact only in the approximation
of an infinite population. For a finite population there are no stable fixed points (for \( p \neq 0 \))
due to the effect of fluctuations in the reproduction process. This can be seen in the simple
example of two types of string, A and B, with a population of size 10 and fitnesses \( f_A \)
and \( f_B \) (\( f_A > f_B \)). If we start with equal proportions of A and B the probability that
\( n_A \to 6 \) relative to the probability that \( n_A \to 4 \) is \( (f_A/f_B)^2 \). So the effect of fitness
is to increase the probability that we have more A’s in the population. Consider now if
the initial population is \( n_A = 1, \quad n_B = 9 \). The probability that A will disappear at the
first time step is \( S_A = (1 + (f_A/9f_B))^{-10} \). In a flat fitness landscape \( S_A = 0.35 \). For
\( f_A = 2f_B, \quad S_A = 0.13 \) and for \( f_A = 10f_B, \quad S_A = 0.01 \). We see then that unless the fitness
advantage of A over B is quite pronounced there is a non-trivial probability that the fitter
fixed point is not reached, whereas reaching the latter is an inevitable conclusion of the
evolution equation neglecting fluctuations. In general, the Neutral Theory predicts that
the selective coefficient must be greater than \( 1/n \) to ensure that selection dominates over
random drift.

We now turn our attention to the derivation of an evolution equation for schematas,
\( \xi \), of order \( N_2 \) and size \( l \). Before doing this it is convenient to return to equation (4) to see
that the notions of schemata and coarse graining appear very naturally when considering
crossover of strings. Considering the destruction term: the matrix (5) 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 \( d_L(i, j) = 0 \) and/or \( d_R(i, j) = 0 \). Similarly one may write the
reconstruction term as
\[ \frac{pc}{N-1} \sum_{k=1}^{N-1} \left( \sum_{c_j} \sum_{c_l} C_{i,j}^{(2)}(k) P'(C_j, t) P'(C_l, t) \right) \]
\[ -2 \sum_{c_j} C_{i,j}^{(2)}(k) P'(C_i, t) P'(C_j, t) - P'(C_i, t) P'(C_i, t) \]

(10)
The second and third terms cancel with corresponding expressions from the destruction term hence (10) can now be written as

$$\sum_{c_j > c_i^L} \sum_{c_i > c_i^R} P'(c_j, t)P'(c_i, t)$$

(11)

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

$$\bar{f}(c_i^L, t) = \frac{1}{n(c_i^L)} \sum_{c_j > c_i^L} P'(c_j, t)$$

(12)

where $n(c_i^L)$ is the total number of strings in the population that contain $c_i^L$. As $\bar{f}(c_i^L, t)$ is the average fitness of the substring $c_i^L$, one can think of this substring as a schemata, likewise for $c_i^R$. In terms of these “schematas” the final form of the string equation is

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

(13)

with

$$P'(c_i^L, t) = \sum_{c_j > c_i^L} P'(c_j, t)$$

(14)

and similarly for $P'(c_i^R, t)$.

One sees that crossover very naturally introduces the notion of coarse graining even though we are working in terms of the microscopic degrees of freedom — the strings. The reconstruction probability depends on the relative fitness of strings that contain the constituent elements of $c_i$, but given that there can be many strings that contain $c_i^L$ one must take an average over these strings. In this sense we are integrating out the “degrees of freedom” represented by the bits that are not contained in $c_i^L$ or $c_i^R$. Equation (13) shows that the effects of reconstruction will outweigh destruction if the parts of a string are more selected than the whole.

Before deriving a schemata evolution equation including crossover and mutation let us consider the effects of reproduction alone. The proportion of elements of the population, $P(\xi, t)$, that contain $\xi$ satisfies the evolution equation

$$P(\xi, t + 1) = P'(\xi, t)$$

(15)

where $P'(\xi, t) = \frac{\bar{f}(\xi, t)}{f(t)} P(\xi, t)$,

$$\bar{f}(\xi, t) = \frac{\sum_{c_i \ni \xi} f(c_i, t)n(c_i, t)}{n(\xi, t)}$$

(16)

the sum is over all strings $c_i$ that contain $\xi$, and $\bar{f}(t) = \sum_{\xi} \bar{f}(\xi, t)P(\xi, t)/\sum_{\xi} P(\xi, t)$ is the average fitness per string or per schemata of the population. Note that the sum over
strings that contain $\xi$ is a sum over the possible values of the bits that are not definite elements of $\xi$, i.e. the wildcards. In this sense, as above in (13), “degrees of freedom” have been integrated out of the problem and (15) represents an exact coarse-graining of the original string evolution equation.

Note that the sum over different binary words on the $N_2$ defining bits of the schemata is a partition of the identity, i.e.

$$\sum_{\text{words}} P(\xi, t) = 1$$

(17)

If we sum also over different possible schemata configurations we have

$$\sum_{\xi} 1 = \sum_{N_2=1}^{N} NC_{N_2} \sum_{\text{words}} 1 = 3^N - 1$$

(18)

which is just the total number of schematas (except for the order 0 schemata with no defining bits).

Considering mutation without crossover we “coarse grain” the microscopic equation (2) by summing over all $C_i \supset \xi$. One can write an effective evolution equation for schematas evolving under mutation

$$P(\xi, t + 1) = P(\xi)P'(\xi, t) + \sum_{\xi_i \supset \xi} P(\xi_i \rightarrow \xi)P'(\xi_i, t)$$

(19)

where the effective coefficients $P(\xi)$ and $P(\xi_i \rightarrow \xi)$ are

$$P(\xi) = \prod_{k=1}^{N_2} (1 - p(k))$$

(20)

and

$$P(\xi_i \rightarrow \xi) = \frac{\sum_{C_j \supset \xi_i} P'(C_j, t)P(c_i \rightarrow c_j)}{n(\xi, t)f(\xi, t)}$$

(21)

In the latter the sum is over strings $C_j$ that contain the schemata $\xi_i$, where $\xi_i$ differs in at least one bit from $\xi$ on the $N_2$ defining bits of the schemata.

As with strings the effect of recombination in the form of crossover is two fold: it potentially destroys schematas that were present in one parent but not the other; on the other hand it offers the possibility of reconstructing schematas even though they were not present in either parent. To derive an evolution equation for schematas, including in the effects of crossover, we return to equation (13) and sum over all strings $C_i \supset \xi$. One finds

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

(22)

We now break the sum over crossover points into those that cut the schemata itself and those that cut outside the schemata. In the reconstruction term if the cut is outside...
the schemata, to the right say, then the sum over \( C^R_i \) is one. Similarly if the cut is to the left with the sum over \( C^L_i \). The remaining sums yield \( P'(\xi, t) \) and this term cancels with an analogous expression originating in the destruction term. For the reconstruction contribution from cuts in the schemata we denote by \( \eta_L (\eta_R) \) the bits to the left (right) of the crossover point that are not in the schemata and note that

\[
\sum_{C_i \ni \xi} P'(C^L_i, t) P'(C^R_i, t) = \sum_{\eta_L} \sum_{\eta_R} P'(C^L_i, t) P'(C^R_i, t). \tag{23}
\]

We will denote by \( \xi_L \) and \( \xi_R \) the parts of the schemata to the left and right of the crossover point respectively. Now, \( \sum_{\eta_L} P'(C^L_i, t) = P'(\xi_L, t) \), where by definition \( P'(\xi_L, t) = (\bar{f}(\xi_L, t)/\bar{f}(t))P(\xi_L, t) \), \( \bar{f}(\xi_L, t) \) being the average fitness of the schemata \( \xi_L \). Analogous expressions hold for \( \xi_R \). With these results the final form of the schemata evolution equation including crossover is

\[
P(\xi, t+1) = P'(\xi, t) - \frac{p_c}{N-1} \sum_{k=1}^{l-1} (P'(\xi, t) - P'(\xi_L, t)P'(\xi_R, t)) \tag{24}
\]

where the sum is only over crossover points that cut the schemata.

The interpretation of this equation is very similar to that of (13). In the reconstruction term \( P'(\xi_L, t)P'(\xi_R, t) \) is the probability that one parent is selected that contains the left part of the schemata and the other contains the right part. A schemata will be augmented by the effects of crossover if, as in the string case, its constituent parts are selected more than the whole schemata. Compared with (13) a further coarse graining has been carried out by summing over all the states of bits outside of \( \xi \). Combining now the effects of selection, mutation and crossover the schemata evolution equation is

\[
P(\xi, t+1) = \mathcal{P}(\xi) P_c(\xi, t) + \sum_{\xi_i} \mathcal{P}(\xi_i \rightarrow \xi) P_c(\xi_i, t) \tag{25}
\]

where

\[
P_c(\xi, t) = P'(\xi, t) - \frac{p_c}{N-1} \sum_{k=1}^{l-1} (P'(\xi, t) - P'(\xi_L, t)P'(\xi_R, t)) \tag{26}
\]

This evolution equation is the fundamental equation governing the evolution of schematas and is written at a “semi-microscopic” level in that it is written in terms of individual schematas. It represents an exact coarse-graining of the corresponding string evolution equation after summing over all possible states of the non-schemata degrees of freedom.

Another useful concept we will introduce here is that of “effective fitness”, \( f_{\text{eff}}(\xi, t) \), which we define via the relation

\[
P(\xi, t+1) = \frac{f_{\text{eff}}(\xi, t)}{\bar{f}(t)} P(\xi, t) \tag{27}
\]
comparing with equation (25) one finds

\[
f_{\text{eff}}(\xi, t) = \mathcal{P}(\xi) \left(1 - p_c \left(\frac{l-1}{N-1}\right)\right) \bar{f}(\xi, t) + \sum_{\xi_i} \mathcal{P}(\xi_i \rightarrow \xi) \frac{\mathcal{P}'(\xi_i, t)}{\mathcal{P}(\xi, t)} \bar{f}(\xi_i, t)
\]

\[
+ p_c \left(\frac{l-1}{N-1}\right) \frac{\mathcal{P}(\xi)}{\mathcal{P}(\xi, t)} \bar{f}(t) \mathcal{P}'(\xi_{L}, t) \mathcal{P}'(\xi_{R}, t)
\]

\[
- \frac{p_c}{N-1} \sum_{\xi_i} \mathcal{P}(\xi_i \rightarrow \xi) \bar{f}(t) \sum_{k=1}^{N-1} \left( \frac{\mathcal{P}'(\xi_i, t) - \mathcal{P}'(\xi_{iL}, t) \mathcal{P}'(\xi_{iR}, t)}{\mathcal{P}(\xi, t)} \right)
\]

Thus we see that the effect of mutation and crossover is to “renormalize” the “bare” fitness \(\bar{f}(\xi, t)\). The destructive effects of crossover and mutation give a multiplicative type renormalization whilst the reconstruction terms give an additive type renormalization. In the low “temperature” limit where mutation and crossover go to zero \(f_{\text{eff}}(\xi, t) \rightarrow \bar{f}(\xi, t)\).

Another concept we will find useful is that of an effective selection coefficient \(s_{\text{eff}} = f_{\text{eff}}(\xi, t) / \bar{f}(t) - 1\). If we think of \(s_{\text{eff}}\) 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 schemata \(\xi\) at time \(t_0\).

4. Effective Degrees of Freedom and Coarse Graining

As mentioned in the introduction one of the most important steps in obtaining a qualitative and quantitative understanding of a system is deciding what are the relevant degrees of freedom of the system. This is often a quite difficult thing to do owing to the fact that they are “scale” dependent. In the case of evolution dynamics this means that the effective dynamics depends on the time scale considered. Trying to understand such time dependent behaviour quantitatively is very difficult as almost inevitably one will have to resort to an approximation technique, which invariably depends on focusing on the relevant effective degrees of freedom as in the methods of effective field theory. However, if they are time dependent then what starts as a good approximation focusing on a certain type at one time will usually break down as one approaches time scales where they are qualitatively quite different.

One feature that is very common, if one has found a reasonable set of effective degrees of freedom, is that their mutual interactions are not very strong, so that they have a certain degree of integrity. Calling something an effective degree of freedom is not a very useful thing to do if it is not readily identifiable as such. For instance, in low energy QCD gluons and quarks are not very useful concepts as they are so strongly coupled via highly non-linear interactions that they form baryons and mesons, bound states of the former. The latter have a much higher degree of integrity than the former at such energies.

So how is the above related to the present discussion of GA’s? GA’s, as algorithmic representations of complex systems, have many degrees of freedom. For instance, in the case where the state of a string of size \(N\) is defined as a binary word, for a population \(n\) the total number of possible states is \(\sim (2^N)^n\) in the case where strings are identifiable by a label other than the state of their bits, and \(\sim n 2^N\) in the case where permutations of identical strings are not counted separately. Both are exponentially large numbers.

Ideally, the search for optima proceeds in a smaller space, spanned by effective “coarse-grained” degrees of freedom. The traditional answer to the question: “What is the nature
of these degrees of freedom?” is, as mentioned previously, the “building block hypothesis”: that small segments of string have an activity that is relatively decoupled from the rest of a string — these “blocks” are assumed to be sufficiently compact that they have a high probability of being preserved by crossover. The GA supposedly uses these building blocks in order to arrive at a global solution.

We can get some idea of the dynamical behaviour of schemata due to crossover by restricting attention for the moment to a flat fitness landscape. In this case

\[ P(\xi, t + 1) = P(\xi, t) - \frac{p_c}{N - 1} \sum_{k=1}^{l-1} (P(\xi, t) - P(\xi_L, t)P(\xi_R, t)) \]  

(29)

For an uncorrelated population crossover is completely neutral and we have a scale invariant situation.

To solve the evolution equation (29) in the case of a correlated population one needs to solve the corresponding equations for \( \xi_L \) and \( \xi_R \); these will involve reconstruction terms that contain \( \xi_{LL} , \xi_{LR}, \xi_{RL} \) and \( \xi_{RR} \). The first two are the components of \( \xi_L \) and the latter two of \( \xi_R \). Naturally this process can be iterated relating fine grained degrees of freedom to more and more coarse grained degrees of freedom, where more and more bits \( (N - N_2) \) have been summed over. Obviously when one arrives at one schematas, the maximally coarse grained degrees of freedom, the process stops as one cannot split by crossover such schematas. We see then that crossover leads to an hierarchy of equations relating fine grained degrees of freedom to successively more and more coarse grained degrees of freedom.

Restricting attention to two schematas in the flat fitness landscape setting and considering the continuous time limit one arrives at the following differential equation

\[ \frac{dP(ij, t)}{dt} = -p_c \frac{l - 1}{N - 1} (P(ij, t) - P(i, t)P(j, t)) \]  

(30)

where \( i \) and \( j \) are the definite bits that define the two schemata and also the two one schematas respectively. As one cannot split a one schemata \( P(i, t) \) and \( P(j, t) \) are conserved quantities thus one finds

\[ P(ij, t) = P(ij, 0)e^{-p_c \frac{l - 1}{N - 1} t} + P(i, 0)P(j, 0) \left(1 - e^{-p_c \frac{l - 1}{N - 1} t}\right) \]  

(31)

Thus one sees that \( P(ij, t) \) approaches an uncorrelated fixed point \( P^*(ij) = P(i, 0)P(j, 0) \) exponentially rapidly. The sole effect of the size of the schemata is to govern the rate of approach to the fixed point, an exponentially small preference being given to smaller schematas.

The steady state solution for a schemata \( \xi \) of order \( N_2 \) is

\[ P^*(\xi) = \prod_{i=1}^{N_2} P(\xi(i), 0) \]  

(32)

where \( P(\xi(i), 0) \) is the probability of finding the one schemata corresponding to the i’th bit of \( \xi \) at \( t = 0 \). One can verify that this steady state solution also is a result purely of the effects of reconstruction. Without reconstruction there is no other fixed point other than zero! We see then that reconstruction is the driving force of crossover and will always
come to dominate. This is very much contrary to the standard block hypothesis point of view which treats schemata destruction as the dominant effect. We can also make another interesting observation associated with the effective fitness $f_{\text{eff}}(\xi, t)$ and crossover. Here the effect of crossover is to renormalize the fitness. The effective selection coefficient is

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

(33)

Thus schemata destruction gives a multiplicative renormalization that contributes negatively to the effective fitness advantage. However, schemata reconstruction leads to an additive renormalization of the effective fitness which exceeds the contribution of the destruction term if $i$ and $j$ are negatively correlated.

In general the fitness landscape itself induces correlations between $\xi_L$ and $\xi_R$. 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 $k=0$ landscape one has $1 + \frac{2N_2}{N} \delta f_\xi < (1 + \frac{2N_2}{N} \delta f_{\xi L})(1 + \frac{2N_2}{N} \delta f_{\xi R})$, so selection induces an anticorrelation when $\delta f_{\xi L}, \delta f_{\xi R} > 0$: 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 schemata to appear in the same individual.

We can analyze this effect in more detail taking once again the case of 2-schematas. Defining the correlation $C(i,j,t) \equiv (P(i,j,t)/P(i,t)P(j,t)) - 1$ then in terms of the selection coefficient, $s_\xi = \bar{f}(\xi, t)/\bar{f} - 1$, one finds

$$C(i,j,t+1) = \left(1 - p_c \frac{l-1}{N-1}\right) \left(\frac{1 + s_{ij}}{(1 + s_i)(1 + s_j)}C(i,j,t) - \frac{s_is_j + s_i + s_j}{(1 + s_i)(1 + s_j)}\right)$$

(34)

Note that the effect of crossover is to diminish correlations induced by the fitness landscape, however crossover cannot change the sign of the correlations. The larger the value of $l$ in this simple case the more the correlations are damped.

This is the effect which we saw previously in the context of a flat landscape. In the extreme case $l = N$, $p_c = 1$ the effect of crossover is to eliminate all correlation between $i$ and $j$. In the neutral ($k=0$) case, $s_{ij} = s_i + s_j$ and

$$C(i,j,t+1) = \left(1 - p_c \frac{l-1}{N-1}\right) \left(\frac{1 + s_i + s_j}{(1 + s_i)(1 + s_j)}C(i,j,t) - \frac{s_is_j}{(1 + s_i)(1 + s_j)}\right).$$

(35)

Thus the effect of crossover is to weaken but not cancel completely the anti-correlations induced by $k=0$ selection. In the remainder of this section we will consider this effect for general schematas.

In our search for the relevant effective degrees of freedom and in analysing the building block hypothesis we will consider schematas of length $l$ irrespective of their order or their overall position in a string. It should be clear that this is a further coarse graining relative to the evolution equations considered earlier. Unfortunately the evolution equation (25) by itself is not very useful for analysing schematas of size $l$, the reason being that any given string contains schematas of all sizes. However, consideration of just about any quantity in conjunction with (25) and a sum over schematas of a given length is meaningful. For instance, one could consider how $\bar{f}(\xi, t)$ changes in time and subsequently how its average,
$< f(\xi, t) >_l$, over all possible schematas of size $l$ changes. Our notation here is that for any function $A(\xi, t)$,

$$< A(t) >_l = \frac{\sum_{i=1}^{(N-l+1)} \sum_{N_2=2(N_2) \text{ words}} P(\xi, t) A(\xi, t)}{(N - l + 1)2^{l-2}}$$

(36)

where $l \geq 2$. The first sum is over the possible beginning point, $i$, of the schemata and the following two sums represent the different configuration s of any number $N_2 \leq l - 2$ specified bits chosen among the $l - 2$ available sites. The number of available sites is $l - 2$ because we fix the ends bits.

Using (25) one may derive a recursion relation for the expectation value of the observable $A$, from

$$< A(t + 1) >_l = \frac{\sum_{i=1}^{(N-l+1)} \sum_{N_2=2(N_2) \text{ words}} P(\xi, t + 1) A(\xi, t + 1)}{(N - l + 1)2^{l-2}}$$

(37)

We now encounter a difficulty: time dependence enters in the above equation not only in the changing probability distribution $P(\xi, t + 1)$, which can be substituted using (25), but also in $A(\xi, t + 1)$. This occurs even though many observables of interest are time-independent functions of the string states as the summing over degrees of freedom associated with passing to a more coarse grained description induces an implicit time dependence in the coarse grained observables. For example $\bar{f}(\xi, t)$ is a population-dependent observable even though $f(C_i)$ is not.

One can derive a function on schematas, such as schemata fitness, via a population average with the string probability $P(C_i, t + 1)$, for which one has the microscopic evolution equation, but this clearly leads to a very complicated calculation. To simplify matters, to search for structure in the population we define a time-independent function on schematas. The particular function we choose is the average selective advantage that in-schemata bits would enjoy if the schemata were immersed in a random population,

$$\delta f_\xi = \left( \frac{N}{N_2} \right) \left( \frac{1}{2^{N-N_2}} \right) \sum_{\eta \text{- words}} f(\xi, \eta) - \frac{1}{2}$$

(38)

where $\eta$ represents the out-of-schemata bits and the average fitness in a random population has been normalized to $1/2$. Note that here, and in the rest of the paper, we are looking at the fitness deviation per schemata bit as opposed to section 3 where the total fitness of a schemata was being considered. This observable corresponds to the effective fitness of in-schemata bits either if the population is in fact random, or if the landscape assigns an independent fitness contribution to each bit in the chromosome ($k = 0$ in the terminology of the Kauffman $Nk$-model). In general, it is a useful test function with which one can probe for the emergence of structure during the first steps of evolution away from a random initial population. We will refer to this observable below as the in-schemata fitness.

We will make use below of the following simplified averages: if $A(\xi)$ is independent of the initial defining point of the schemata, or if the landscape is “generic”, then we can sum over this point to find

$$< A(t) >_l = \frac{1}{2^{l-2}} \sum_{N_2=2}^{l} \sum_{(N_2) \text{ words}} P(\xi, t) A(\xi)$$

(39)
By “generic” we mean that within the class of landscapes we are considering, such as an $Nk$-model for a particular value of $k$, there is no systematic bias in the fitness function for a particular part of the string, i.e. the sums over words, configurations and $N_2$ leads to an average which is effectively translation invariant, i.e. the system is effectively self-averaging. Similarly, if $A(\xi)$ depends only on the order of the schemata, $N_2$, one has
\[
<A(t)>_l = \frac{1}{2^{l-2}} \sum_{N_2=2}^{l} l^{-2} C_{N_2-2} P(\xi,t) A(\xi)
\] (40)

We will also use the notation $<< A >>_l$ to represent the average over schematas and over crossover points, namely
\[
<< A >>_l = \frac{1}{l-1} \sum_{i=1}^{l-1} < A >_l
\] (41)

Considering the expectation value of the in-schemata fitness, the equation which gives the improvement of $< \delta f_\xi >_l$ from generation $t$ to generation $t+1$ is
\[
\Delta_l = << \frac{\delta f_\xi}{f(t)} - \overline{f}(t) >>_l
\] (42)

where $\delta f_\xi(\xi,t) = f_{\text{eff}}(\xi,t) - \overline{f}(t)$. More explicitly, using the evolution equation for schematas, one finds
\[
\Delta_l = << \frac{\delta f_\xi}{f(t)} \frac{\delta f_{\text{eff}}(\xi,t)}{f(t)} >>_l - p_c \left(\frac{l-1}{N-1}\right) << \frac{\delta f_\xi}{P(\xi,t)} \left(P'(\xi,t) - P'(\xi_{L},t)P'(\xi_{R},t)\right) >>_l,
\] (43)

where $\delta f(\xi,t) = \overline{f}(\xi,t) - \overline{f}(t)$. The first term is independent of $l$ in a random population if the fitness landscape itself is $l$ independent. All the $l$ dependence lies in the crossover terms. If the parts of a schemata are selected more than the whole it is clear that the net contribution from crossover will be positive.

It worth pausing here to consider the meaning of the quantity $\Delta_l$. As we defined it, $\Delta_l$ measures the average improvement of the in-schemata fitness over one step of evolution. How does this improvement come about? First of all, schematas with $\delta f(\xi,t) > 0$ will be more frequent in the parent population, thanks to the selection factor $(1+s)$, where
\[
s = \frac{\delta f(\xi,t)}{f(t)} = \frac{2N_2}{N} \delta f_\xi.
\] (44)

where the latter equality is only true for a random initial population or $k = 0$ model. The next step is to consider the action of the crossover operator. On the one hand selected parents with $\xi$ may not pass it on to their offspring if crossover “breaks” the schemata. However, there is a possibility that $\xi$ be reconstructed from parents that have parts of $\xi$ but not all of it. This reconstruction term gives a positive contribution because if $\xi$ has a selective advantage then subsets of $\xi$ will, for an average type of landscape, be more likely than not to have some selective advantage as well, so the parts of $\xi$ that are needed for reconstruction are available in the parent population with an enhanced probability. The key question is, of the destruction and the reconstruction terms which is larger for a
particular value of \( l \)? Before we turn to answering this question in particular cases, let us consider the relation between \( \Delta_l \) and the spatial correlation function.

If the population is uncorrelated, in other words if \( P(\xi, t) = \prod_i P(\xi_i, t) \), where \( \xi_i \) is the \( i \)'th bit of \( \xi \), then the expectation value of \( \delta f_\xi \) is independent of \( l \), as \( N_2 \delta f_\xi = \sum_i \delta f_{\xi_i} \), and

\[
\langle \sum_i \delta f_{\xi_i} \rangle > l \tag{45}
\]
is just the uncorrelated sum of contributions from 1-schemas. The fact that the existence of correlations in \( P(\xi, t + 1) \) implies an \( l \) dependence can be demonstrated explicitly. One writes

\[
f_{eff}(\xi, t) \approx \frac{1}{N_2} \sum_{i=1}^{N_2} f_1(\xi_i) + \frac{1}{N_2(N_2 - 1)} \sum_{i=1}^{N_2} \sum_{j \neq i} \left( f_2(\xi_i \xi_j) - \frac{1}{2}(f_1(\xi_i) + f_1(\xi_j)) \right), \tag{46}
\]

where

\[
f_1(\xi_i) = \frac{1}{2N_2-1} \sum_{\{\xi_k, k \neq i\}} f_{eff}(\xi, t)(\{\xi_k\}) \tag{47}
\]

\[
f_2(\xi_i \xi_j) = \frac{1}{2N_2-2} \sum_{\{\xi_k, k \neq i, j\}} f_{eff}(\xi, t)(\{\xi_k\}) \tag{48}
\]

and we are considering only up to two-point correlations. Defining \( \delta s_\xi = \delta f_{eff}(\xi, t) - \delta f_\xi \), which is a measure of the selective advantage over and above the in-schemata fitness, one finds

\[
\delta s_\xi \approx \frac{1}{N_2} \sum_{i=1}^{N_2} f_1(\xi_i) + \frac{1}{N_2(N_2 - 1)} \sum_{i=1}^{N_2} \sum_{j \neq i} \left( f_2(\xi_i \xi_j) - \frac{1}{2}(f_1(\xi_i) + f_1(\xi_j)) \right) - \bar{f}(t) - \delta f_\xi. \tag{49}
\]

For a \( k = 0 \) landscape,

\[
\delta s_\xi \approx \frac{1}{N_2(N_2 - 1)} \sum_{i=1}^{N_2} \sum_{j \neq i} \left( f_2(\xi_i \xi_j) - \frac{1}{2}(f_1(\xi_i) + f_1(\xi_j)) \right) \tag{50}
\]

So, in this case we see that the existence of a selective advantage is due to the existence of correlations in the effective fitness. Defining a selective coefficient \( s_l \) which represents the selective advantage for a schemata to be of size \( l \) one finds

\[
\Delta_l = \langle \langle \delta f_\xi^2 \rangle \rangle_l (1 + s_l) \tag{51}
\]

where

\[
s_l = \frac{\langle \langle \delta f_\xi^2 \delta s_\xi \rangle \rangle_l}{\langle \langle \delta f_\xi^2 \rangle \rangle_l}. \tag{52}
\]

In this expression for \( \Delta_l \), \( \langle \langle \delta f_\xi^2 \rangle \rangle_l \) is independent of \( l \) for a random initial population. Thus we see that any \( l \) dependence can be attributed to the existence of spatial correlations.
If the reconstruction term from crossover exceeds the destruction term for some \( l \), then from the above one concludes that the fitness improvement attributed to a particular bit in the string depends on it being part of selected schematas of this size. The maximum value of \( \Delta_l \) is attained when the contribution of an individual bit is most enhanced by the fact that this bit belongs to strings that include other specified bits at a distance at most equal to \( l \), namely those strings which include a selected schemata of size \( l \). That the conditioning information on the existence of other specified bits should be useful is a direct consequence of the correlations between the different bits in the string. The reason why we emphasize the relation between \( \Delta_l \) and the correlation function is that correlations are intimately linked to the emergence of effective degrees of freedom. In this sense, the function \( \Delta_l \) is related to the expected size distribution of the effective degrees of freedom.

5. Asymptotic Solutions

In this section we consider some asymptotic solutions of the evolution equation for \( \Delta_l \) derived in section 4. In particular we will consider two limiting cases: the evolution of schematas starting from a completely random initial state; and a random perturbation around a completely ordered state. As one of our principal considerations is in investigating the validity of the building block hypothesis we will set the mutation rate to zero as the effects of the latter do not depend on schemata size. We will derive expressions for \( \Delta_l(t+1) \) and \( \Delta_l(t+2) \) starting out from an initial random population at time \( t \).

For a random initial population at time \( t \),

\[
\Delta_l(t+2) = \langle\langle \delta f_\xi(t+2) \rangle\rangle_l - \Delta_l(t+1)
\]

Even though \( \delta f_\xi \) is time independent we use the above notation to indicate that its expectation value is with respect to the probability distribution at time \( t + 2 \).

In the initial random population, the effective schemata fitness is the in-schemata fitness \( \delta f_\xi \) and

\[
\delta f_\xi(t) = \frac{N_2}{N} \delta f_\xi,
\]

\[
P_\xi(t) = \frac{1}{2^{N_2}}.
\]

Thus one finds

\[
\Delta_l(t+1) = \left(1 - p_c \left(\frac{l - 1}{N - 1}\right)\right) << \alpha >>_l + \nonumber
\]

\[
p_c \left(\frac{l - 1}{N - 1}\right) << \frac{N_L}{N_2} \beta_L + \frac{N_R}{N_2} \beta_R + \frac{4N_LN_R}{N^2} \delta f_\xi \delta f_\xi_L \delta f_\xi_R >>_l
\]

where we have introduced the notation for the quadratic terms

\[
\alpha = \frac{1}{2^{N_2}} \sum_{\text{words}} \frac{2N_2}{N} \delta f_\xi^2,
\]

\[
\beta_L = \frac{1}{2^{N_2}} \sum_{\text{words}} \frac{2N_2}{N} \delta f_\xi \delta f_\xi_L,
\]
with an analogous expression for $\beta_R$.

As one of our principle purposes here is to examine the block hypothesis in light of the evolution equation we have derived, and the associated notions of coarse graining and effective degrees of freedom, we will try to derive explicit results in some concrete cases based on generic fitness landscapes. The Kauffman $N_k$-models provide such a set of landscapes. Here we will specialize to the case $k = 0$ which is neutral in the sense that it neither favours nor disfavours correlations between bits. We will discuss how our results generalize to a $k = 2$ landscape in the next section. In the $k = 0$ landscape,

$$\delta f_\xi = \frac{N_L}{N^2} \delta f_{\xi_L} + \frac{N_R}{N^2} \delta f_{\xi_R}.$$  \hfill (59)

We also have that $\langle\langle \delta f_\xi \delta f_{\xi_L} \delta f_{\xi_R} \rangle\rangle_l = 0$ which results in the complete cancellation of the destruction and reconstruction crossover terms the final result being

$$\Delta_l(t+1) = \langle\langle \alpha \rangle\rangle_l.$$  \hfill (60)

The above expression is for an arbitrary $k = 0$ landscape. In order to find a more explicit solution we must consider a more explicit landscape. We will consider two: a binary landscape where the fitness of a bit may only take two values, 1 and 0; and a landscape where the fitness of a bit is selected uniformly at random from the interval $[0, 1]$. Both landscapes conform with the requirement that the average fitness per bit in a random population is $1/2$. Let $x_i$ denote the deviation from the mean fitness of bit number $i$, i.e. $x_i = f_i - 1/2$. We find

$$N_2 \delta f_\xi = \sum_{i=1}^{N_2} (2\xi_{n_i} - 1) x_{n_i},$$

where the indices $n_i$ denote the specified bits of the schemata ($i = 1, \cdots, N_2$). Squaring this expression and using $\sum_{i \neq j} <(2\xi_{n_i} - 1)(2\xi_{n_j} - 1)> = 0$ one finds

$$<N_2 \delta f_\xi^2> = \frac{1}{N_2} \sum_{i=1}^{N_2} x_{n_i}^2 >.$$

The averaging over configurations then gives, for $l \geq 3$,

$$\langle\langle \alpha \rangle\rangle_l = \frac{2}{N(N - l + 1)l(l - 1)(l - 2)} \sum_{i=1}^{N} m_i x_i^2,$$

where

$$m_i = l(l - 1)(l - 2) \quad (l \leq i \leq N - l + 1),$$

$$m_i = (l^2 - 3l) + i(l^2 - 5l + 8) + \frac{l - 2i}{2l - 2} \quad (i < l),$$

and symmetrically for $i > N - l$.

For the case of a binary landscape the final answer is

$$\langle\langle \alpha \rangle\rangle_l = \frac{1}{2N}.$$  \hfill (61)
In the random landscape for large $N$ we can assume that the average over the $N$ bits (weighted by $n_i$) can be replaced by an average over the distribution of $x_i$ used to generate the landscape. Then,

$$\langle \langle \alpha \rangle \rangle_t = \frac{1}{6N}.$$ (62)

Thus one sees that crossover acts in a scale invariant way at the first time step of evolution from a random initial population: there is no preference whatsoever for small blocks at the expense of large blocks.

We will now consider what happens at time $t+2$. The extra ingredient we need relative to the above calculation is $\langle \langle \delta f_\xi (t+2) \rangle \rangle_t$. To calculate this we in turn need to calculate $P'(\xi, t+1)$, $P'(\xi_L, t+1)$ and $P'(\xi_R, t+1)$ i.e. the selection probabilities at time $t+1$, calculation of which requires knowledge of $\bar{f}(\xi, t+1)$, $\bar{f}(\xi_L, t+1)$ $\bar{f}(\xi_R, t+1)$ and $\bar{f}(t+1)$. Specializing once again to a $k=0$ landscape, one finds

$$P(\xi, t+1) = \frac{1}{2N_2} \left( 1 + \frac{2N_2}{N} \delta f_\xi + \frac{p_c}{N-1} \sum_{k=1}^{N-1} \frac{4N_LN_R}{N^2} \delta f_\xi \delta f_{\xi_L} \delta f_{\xi_R} \right),$$ (63)

and

$$\bar{f}(t+1) = (1 + 2\alpha_s)\bar{f}(t)$$ (64)

and

$$P'(\xi, t+1) = \frac{1}{2N^2(1+2\alpha_s)} \left[ \left( 1 + \frac{2N_2}{N} \delta f_\xi \right)^2 + 2 \frac{(N-N_2)}{N} \alpha_{(N-N_2)} \right. \right.$$

$$+ \frac{p_c}{N-1} \left( 1 + \frac{2N_2}{N} \delta f_\xi \right) \sum_{k=1}^{l-1} \frac{4N_LN_R}{N^2} \delta f_\xi \delta f_{\xi_L} \delta f_{\xi_R} \right. \right.$$

$$+ \frac{4p_c}{N(N-1)} \left( \sum_{k=1}^{l-1} (N_R \delta f_{\xi_R} \beta_{(k-N_L)}) + N_L \delta f_{\xi_L} \beta_{(N-k-N_R)} + N_2 \delta f_\xi \left( \sum_{k<\xi} \beta_k + \sum_{k>\xi} \beta_{(N-k)} \right) \right).$$ (65)

where

$$\alpha_{(N-N_2)} = \frac{1}{2N-N_2} \sum_{\eta-words} \frac{2(N-N_2)}{N} \delta f_{\eta}^2.$$ (66)

$$\beta_{(k-N_L)} = \frac{1}{2k-N_L} \left( \frac{2(k-N_L)}{N} \right)^2 \sum_{\eta_L-words} \delta f_{\eta_L}^2.$$ (67)

$$\beta_k = \frac{1}{2k} \left( \frac{2k}{N} \right)^2 \sum_{L-words} \delta f_{L}^2.$$ (68)

In (68) the sum is over words associated with bits to the left of the crossover point given that all the schemata $\xi$ lies to the right of the crossover point. The expression for $\beta_{(N-k)}$ is analogous but with the sum over words being associated with bits to the right of the crossover point given that the schemata lies to the left. Equation (67) is associated with a sum over words for the bits to the left of the crossover point but excluding bits that are in the schemata. Likewise the expression $\beta_{(N-k-N_R)}$ contains a sum over words associated
with bits that are out of schemata to the right of the crossover point. Finally, \( \alpha_s = 1 + (2N_2/N)\alpha + (2(N - N_2)/N)\alpha_{(N-N_2)} \).

If one considers \( \xi_L \) and \( \xi_R \) as schematas on exactly the same footing as \( \xi \) then the expressions for \( P'(\xi_L, t + 1) \) and \( P'(\xi_R, t + 1) \) are completely analogous to those above except that one is now considering the bits of \( \xi_L \) and \( \xi_R \) which lie to the left and the right of the crossover point. Combining these expressions with equations (65-68) after some lengthy but straightforward calculations one finds

\[
\Delta_l(t + 2) = \left( \frac{1 - 2\alpha_s}{1 + 2\alpha_s} \right) <\alpha>>>_l + \frac{p_c}{(1 + 2\alpha_s)(N - 1)} <\frac{2N}{N_2}(\beta_R\beta_k + \beta_L\beta_{(N-k)})>>>_l + \frac{2p_c}{(1 + 2\alpha_s)(N - 1)} <\alpha\sum_{k<\xi}\beta_k + \alpha\sum_{k>\xi}\beta_{(N-k)}>>>_l.
\]

(69)

The first term in the right hand side of (69) is the result of selection at \( t + 1 \) on the population that was the result of selection at \( t \). It is crossover independent as is manifest in the fact that \( p_c \) does not appear. The last two terms are associated with the effects of selection on the population at time \( t + 1 \) which has incorporated non-trivial contributions from crossover at time \( t \). More precisely, the picture is the following: \( k = 0 \) selection on a random population induces anti-correlations in \( P'(\xi_L, \xi_R, t) \) when both \( \delta f_{\xi_L} \) and \( \delta f_{\xi_R} \) are positive due to the quadratic term \( \sim \delta f_{\xi_L}\delta f_{\xi_R} \). Crossover reduces these anticorrelations, thereby enhancing the whole schemata \( \xi = \xi_L + \xi_R \) relative to its parts. Selection at \( t + 1 \) reinforces this effect of crossover to enhance \( \xi \), leading to the net positive contribution to \( \Delta_l(t + 2) \).

As above, we will consider the binary landscape and a landscape where the fitness of a bit is selected uniformly at random from the interval \([0,1]\]. Similar calculations to the ones given above for \( <\alpha>>>_l \) lead to the following expressions for \( <\frac{2N}{N_2}(\beta_R\beta_k + \beta_L\beta_{(N-k)})>>>_l \) and \( <\alpha\sum_{k<\xi}\beta_k + \alpha\sum_{k>\xi}\beta_{(N-k)}>>>_l \), for \( l \geq 4 \):

\[
<\frac{2N}{N_2}(\beta_R\beta_k + \beta_L\beta_{(N-k)})>>>_l = \frac{c}{108N^3}(N - l)(N - l - 2)
\]

(70)

\[
<\alpha\sum_{k<\xi}\beta_k + \alpha\sum_{k>\xi}\beta_{(N-k)}>>>_l = \frac{c(l - 1)}{72N^3} - \frac{c(l^2 - 5l + 8)}{216N^3} + \frac{c}{27N^4l}
\]

(71)

where \( c = 3 \) for the binary landscape and \( c = 1 \) for the random landscape. Putting these terms together we arrive at the final expression for \( \Delta_l(t + 2) \),

\[
\Delta_l(t + 2) = \left( \frac{3N - c}{3N + c} \right) \frac{c}{6N} + p_c \left( \frac{2N^2 - Nl + l^2 + N + l - 8 - (8/2^l)}{144(3N + c)N^2(N - 1)} \right)
\]

(72)

From this expression one can readily see that the effects of crossover are always positive, i.e. the effects of schemata reconstruction outweigh those of schemata destruction. A graph of \( \Delta_l(t + 2) \) versus \( l \) can be seen in figure 1.

We now turn our attention briefly to the limiting case of an almost organised population. In this limit, one can consider that the strings differ from the population-consensus at most at one site; we will refer to the differing site as a “defect”. There are \( N \) possible
defects each with an effective negative fitness differential over the consensus string. The evolution equation implies an equation for the growth or decay of defects, where one immediately sees that the effect of crossover is strictly neutral: there is no net creation or destruction of defects by pure crossover without selection. In other words the geometrical effect of crossover is zero. The role of crossover in this limit is only to mix the defects in the population. So in this limit $\Delta t$ is once again strictly independent of $l$. The possibility of multiple defects in a single string raises the possibility of correlations in the distribution of defects along the string, which would induce mirroring correlations in the schematas, so $\Delta l$ may acquire a non-trivial $l$-dependence as a second order effect in the mean density of defects, which is the perturbative expansion parameter near the ordered limit.

Taking once again the $k = 0$ landscape, the fitness penalty per bit for two defects is given by $2\delta f_{ij} = \delta f_i + \delta f_j$, so

$$
\frac{P'(ij,t)}{P'(i,t)P'(j,t)} \sim \frac{1 + \frac{2\delta f_{ij}}{j^N}}{(1 + \frac{\delta f_i}{j^N})(1 + \frac{\delta f_j}{j^N})} = \left(1 + \frac{\delta f_i \delta f_j}{j^2 N^2}\right)^{-1}.
$$

Since $\delta f_i \delta f_j > 0$, $P'(ij,t) < P'(i,t)P'(j,t)$: selection induces an anticorrelation between the defects. Now, crossover enhances $P(ij,t+1)$ to bring it closer to $P(i,t+1)P(j,t+1)$. Since the schemata $(ij)$ is more strongly damped than $i$ or $j$ separately, the selection at the next time step will destroy more defects than without crossover. So here again as near the random limit crossover has a beneficial effect due to the enhancement of whole schematas relative to its parts. Near the random limit this was beneficial because the whole schemata was picked up by selection, here it is beneficial because the whole schemata is more strongly damped by negative selection so defects die out more rapidly.

One can think of the initial random population as being the high temperature fixed point of the model, given that every point in configuration space is equally occupied; in this limit the correlation length is zero. The ordered limit would then naturally be interpreted as the low temperature limit. Our results from this section can be summarised by saying that crossover is a net positive contributor to fitness growth at second order near both temperature limits, $T \rightarrow 0$ and $T \rightarrow \infty$.

6. Effective degrees of freedom in the $N^2$ landscape

The $k = 0$ landscape discussed in the last section has the virtue of being “neutral” from the point of view of the block hypothesis, however it is not a realistic example of landscapes usually encountered in complex optimization problems: It is strongly correlated, has a single optimum and does not present frustration we will therefore turn our attention now to Kauffman’s $Nk$ model with $k = 2$. There are two mechanisms by which connected landscapes can induce correlations: On the one hand, schematas that contain landscape-related bits have a sharper selective coefficient because there are fewer unspecified bits involved in their fitness contribution. On the other hand, the balance between the schemata destruction and reconstruction terms from crossover is broken to first order. For example if the effective fitness of a whole schemata is less than the sum of the effective fitnesses of its parts, the growth of a schemata can be magnified by breaking it down into parts, growing the parts and then reconstructing the schemata. We will analyse both of these correlating effects below.

The $Nk$ model can be described as follows: the fitness function is specified by giving, for each bit of the string, $k$ connections to as many other bits and a table of $2^k + 1$ random
numbers uniformly distributed in the unit interval. To compute the fitness contribution of one bit of a string one forms a \((k + 1)\)-word from this bit and its connected partners and translates it into an integer \(n \in \{1, 2, \ldots, 2^{k+1}\}\). The fitness is then given by the entry number \(n\) in the table of random numbers. Note that the \(k\) connections and the table of random numbers are chosen independently for each bit in the string. For \(k = 0\) the fitness contribution from each bit is independent of the others and takes one of two possible values. The resulting landscape gives rise to a unique extremum (barring accidental degeneracies). At the other extreme, \(k = N\), the fitness of every string is an independent random number (random landscape). The ruggedness of the landscape increases with \(k\), which allows one to use \(k\) as a free parameter in order to be able to model real landscapes of arbitrary ruggedness. Here we will consider only the representative case \(k = 2\).

Let us first restrict our attention to schematas of two definite bits \((N_2 = 2)\). There are three possible situations for a 2-schemata. Either the two bits are not connected by the fitness landscape, one bit is the connected partner of the other, or the bits are connected both ways. This last situation is improbable for \(N \gg 1\), so we will focus on the first two cases. If one has two unrelated bits in an otherwise random initial population, the effective fitness of each bit in this schemata is equal to an average of four of the eight random numbers in the fitness table at that site, because one of the three bits is fixed and the other two are picked at random. If, on the other hand, one of the bits is connected to the other then its fitness contribution is given by averaging over the two possible values that the other connected partner can take. This is an average of two out of the eight random numbers in the fitness table. The key point is that the average of two random numbers typically differs from \(1/2\) more than the average of four. Therefore, schematas which include landscape-related bits will have a stronger selective coefficient, in absolute value. This leads to a bias for the condensation of schematas that recognize the structure of the fitness landscape.

In order to make this argument more precise, we need to compute the expectation value of the best of \(m_1\) averages of \(m_2\) random numbers, where each random number is uniformly distributed in the unit interval. The probability distribution of the best of \(m_1\) averages of \(m_2\) random numbers is equal to the derivative of the probability that \(z\) is larger than all \(m_1\) averages. If we call \(P(x_1, \ldots, x_{m_1})\) the distribution of the averages, the probability that \(z\) is greater than all of the averages is

\[
p(z > \sup(m_i)) = \int_0^1 \cdots \int_0^1 P(x_1, \ldots, x_{m_1}) \prod_{i=1}^{m_1} \theta(z - x_i).
\] (73)

Since the \(m_1\) averages are statistically independent in this case, this expression reduces to

\[
p(z) = \left(\int_0^1 dx P(x)\theta(z - x)\right)^{m_1}.
\] (74)

The expectation value of the best of the \(m_1\) averages is

\[
< z_{\text{max}} > = \int z p'(z) dz
\] (75)

For our purposes it is sufficient to consider the cases where \(m_1, m_2 \in \{2, 4\}\). For \(m_2 = 2\) the distribution of the average of two uniformly distributed random numbers is given by

\[
P(x) = 4x \quad \text{for} \quad x < 1/2
\]
and the symmetry condition $P(1/2 + x) = P(1/2 - x)$. The expectation values for the best of $m_1$ such averages are: for $m_1 = 2$, $m_2 = 2$, $<z_{\text{max}}>= 0.6167$; while for $m_1 = 4$, $m_2 = 2$, $<z_{\text{max}}>= 0.7300$. For $m_2 = 4$ (averages of four uniformly distributed variables), one has

$$P(x) = \frac{128}{3} x^3 \quad \text{for} \quad x < 1/4,$$

$$P(x) = \frac{128}{3} x^3 - \frac{2}{3} \quad \text{for} \quad 1/4 < x < 1/2,$$

and the symmetry condition given above. One finds the following result: for $m_1 = 2$, $m_2 = 4$, $<z_{\text{max}}>= 0.5673$. Finally, the expectation value of the best of $m_1$ uniformly distributed random variables is

$$<z_{\text{max}}>= \frac{m_1}{m_1 + 1}. \quad (78)$$

Here we will need only the best of eight, which is equal to $8/9 = 0.8889$.

As mentioned previously, we will consider only schematas with two definite bits. If the two bits are not related by a landscape connection the effective fitness of any one of these bits in a random population is given by the average of four random numbers from the fitness table, where the averaging is over the values of the two connected partners which determine the fitness contribution of this bit. Thus, the best schemata can be expected to have a selective advantage

$$s_1 = \frac{\bar{f}_\xi}{\bar{f}} - 1 = \frac{4}{N}(0.567 - 0.5). \quad (79)$$

Now, if there is a landscape connection between the two bits of the schemata, the contribution of one of these bits to the string fitness is given by an average of two random numbers, since we only need to average over the other connected partner which is not in the schemata. The best schemata in this case will have a selective advantage

$$s_2 = \frac{4}{N} \left(\frac{0.567 + 0.73}{2} - 0.5\right). \quad (80)$$

In the case $N = 40$ analyzed in the previous section, the ratio of the growth rates of a 2-schemata which recognizes a landscape connection to that of one that doesn’t is

$$r = \frac{1 + s_2}{1 + s_1} = 1.0081. \quad (81)$$

This result should be compared to the effect of crossover which we computed in the $k = 0$ landscape at the second time step: $1 + s_1$ was found to fluctuate between 1.0025 at $l = N/2$ and 1.0029 at $l = 2, l = N - 1$. Clearly, the conclusion is that landscape correlations should be taken into account in a proper analysis of the condensation of “schematas”.

In our discussion we neglected the possible existence of frustration and assumed that the fitness contribution of the two bits of the schemata could be optimized independently without affecting the mean fitness contribution of the other bits in the string. A more careful analysis including frustration would be much more complicated; however one expects that at least for small $N_2$ frustration should be marginal and that our conclusions should
hold qualitatively. Of course, there are fewer 2-schematas that recognize a landscape connection than not, so the overall contribution of such schematas to the condensation of effective degrees of freedom is diluted by a phase space factor $2/N$, relative to 2-schematas of landscape-related bits. Thus, one expects that the first stage of divergence from a random population will be dominated by schematas which do not understand the fitness landscape. The landscape-related schematas, which grow at a faster rate, will eventually overcome the contrary phase space factor and become more important in the condensation process.

Returning to the fundamental equation (24) for the growth of in-schemata fitness we can evaluate the effect of crossover in a $k = 2$ landscape by calculating $\Delta_l$ in the first step away from a random population:

$$\Delta^{(n)}_{N_2=2} = \langle \frac{4}{N} \delta f_{\xi}^2 \rangle^{(n)} - \frac{4p_c}{N(N-1)} < l - 1 >^{(n)} < \delta f_{\xi} \left( \delta f_{\xi} - \frac{N_L}{N_2} \delta f_{\xi L} - \frac{N_R}{N_2} \delta f_{\xi R} \right) >^{(n)},$$

where we have used the identity, valid in a random population, $\sum_{\text{words}} \delta f_{\xi L} \delta f_{\xi R} \delta f_{\xi} = 0$, and the average $<\rangle^{(n)}$ runs over the set of all schematas with $N_2 = 2$ definite bits with $n = 0, 1, 2$ landscape connections between schemata bits. We are also assuming that there is no explicit $l$ dependence in the fitness landscape itself.

The evaluation of $\delta f_{\xi}$ depends on the number of in-schemata connections. One must evaluate the contribution of each of the two bits in the schemata. If there are no in-schemata connections then the averaging over unspecified bits leads to a contribution to $\delta f_{\xi}$ equal to the average of four of the eight random numbers in the fitness table. If one of the bits is connected to the other, then in evaluating its fitness contribution one has only one unspecified bit and the contribution to $\delta f_{\xi}$ turns out to be the average of two of the eight random numbers. The values of $\delta f_{\xi L}$ and $\delta f_{\xi R}$ are always given by the average of four random numbers.

Thus, if there are no in-schemata connections then $\delta f_{\xi} = \frac{N_L}{N_2} \delta f_{\xi L} + \frac{N_R}{N_2} \delta f_{\xi R}$ and the contribution of the crossover term vanishes as in the $k = 0$ case. If we denote by $\sigma^2$ the variance of the random number distribution used to generate the tables of eight possible fitness contributions for each bit, the averaging over schematas with $n = 0$ landscape connections gives

$$\Delta^{(0)}_{N_2=2} = \langle \frac{4}{N} \delta f_{\xi}^2 \rangle^{(0)} = \frac{\sigma^2}{2N}.$$

On the other hand, if there is one in-schemata connection then $< \delta f_{\xi}^2 >^{(0)}$ is the variance of the average of two random numbers plus the variance of an average of four, while one of the terms $< \delta f_{\xi} \delta f_{\xi L} >^{(0)}$ or $< \delta f_{\xi} \delta f_{\xi R} >^{(0)}$ is equal to half the variance of two random numbers, the other being the variance of an average of four. Using $< l - 1 > = (N + 1)/3$, one finds

$$\Delta^{(1)}_{N_2=2} = \left( \frac{3}{4} - \frac{p_c(N + 1)}{12(N - 1)} \right) \frac{\sigma^2}{N} = \Delta^{(0)}_{N_2=2} + \Delta^{(0)}_{N_2=2} \left( \frac{1}{2} - \frac{p_c(N + 1)}{6(N - 1)} \right).$$

Similarly, for $n = 2$ in-schemata connections,

$$\Delta^{(2)}_{N_2=2} - \Delta^{(0)}_{N_2=2} = \Delta^{(0)}_{N_2=2} \left( 1 - \frac{p_c(N + 1)}{3(N - 1)} \right).$$

25
In these expressions, the $p_c$-independent correction is the result of the selective advantage of schematas that recognise landscape connections, which we discussed previously. These numbers appear somewhat magnified relative to $r$. This is only because here we are examining the in schemata fitness per bit whereas $r$ was associated with the growth rate of the entire string. The crossover contribution reduces this correlating effect of the landscape but only by a factor of $2/3$ in the limit $p_c \to 1$, $N \to \infty$. In conclusion, schematas which reflect the landscape connections contribute more (per bit) to the growth of fitness than schematas involving unrelated bits.

A similar conclusion can be expected to hold if one considers larger schematas with $N_2 > 2$. Extending the argument to general schematas one is led to consider fitness trees: the fitness tree of a bit is the set which consists of the bit itself, its connected partners, the connected partners of the these connected partners, and so on. We can define an order $n$ truncated fitness tree by truncating this procedure after $n$ steps. The dominant value of $n$ depends on the degree of order in the system, which is a function of the mutation rate. For a high mutation rate one expects the gene pool to be highly disordered and effective degrees of freedom are mostly single bits ($n = 0$) or truncated fitness trees with small values of $n$. As the mutation rate decreases larger trees can condense and the dominant value of $n$ increases. This leads us to propose the following conjecture on the nature of the effective degrees of freedom, which we shall call the “fitness tree hypothesis”.

- The effective degrees of freedom of genetic algorithms with $Nk$ fitness landscapes are the truncated order $n$ fitness trees. The effective value of $n$ increases as the condensation process allows for an increasingly structured gene pool.

In order to test this hypothesis we designed a numerical simulation with a population of 1000 individuals in an $Nk$ landscape, with $N = 40$ and $k = 2$. The crossover probability was taken to be equal to one. The spatial correlation function measures the correlation of bits at distance $d$ along the string and tests the block hypothesis directly. A second correlation function measures this correlation as a function of the connective distance between bits, defined as the smallest number of landscape connections from one bit to the other. The results are shown in [Figures 2 a-c]. At generation 15 ([Fig. 2a]) the spatial correlation function reflects the preference for small schematas, as suggested by the block hypothesis. After 100 generations ([Fig. 2b]) the spatial correlation function has become weak and roughly independent of the distance; on the other hand the correlation of landscape-related bits becomes significant at connective distance one. By generation number 150 one finds statistically significant correlations up to connective distance four, which are progressively reinforced. In [Figure 2c] we show the correlation functions at generation 200. Since the mutation rate is equal to zero in these simulations, population diversity eventually decreases and becomes insufficient to derive statistically relevant correlation coefficients. At generation 350 the strings are totally condensed up to connective distance two (the first two correlation coefficients are equal to one); the gene pool is completely organized at the 500’th generation.

Throughout this article, with the exception of the numerical experiments finite size effects were neglected. If one considers their contribution the failure of the block hypothesis only becomes more apparent. Here we will mention only briefly two arguments to this effect.

In a finite population the difficulty of finding a good schemata must be considered, since not all schematas are present in the initial population. Since the number of schematas with fixed $N_2$ grows with $l$ as $l^{-2}C_{N_2-2}$, one expects it to be easier to discover good large schematas than small ones. Another important finite size effect is the effective non-linearity of selection emphasised in the Neutral Theory of Molecular Evolution [17]: Schematas
with only weak selective coefficients are not necessarily selected, as the neutral drift due
to fluctuations in the selection of parents dominates over selection unless $|s_{eff}| > 1/P$, $P$
being the effective breeding population. This leads to an effective non-linearity of selection
due to the existence of a threshold in favour of schematas with a selective coefficient above
this value. Since the selective coefficient of a schemata grows in proportion to $N_2$, this
effect favours schematas with large $N_2$. Combining this result with the previous comment
on the probability to find good schematas being proportional to $l^{-2}C_{N_2-2}$, we find that
schematas with small values of $l$ are strongly disfavoured by the finite size effects.
7. Conclusions

The bulk of this paper has been devoted to deriving equations that describe the evolution of string populations in genetic algorithms, and in particular how effective degrees of freedom may emerge during this evolution. We started with an equation that governed the evolution of the strings themselves under the joint action of selection, mutation and crossover. We found that this equation could be elegantly expressed in terms of the evolution of a string $C_i$ and its subcomponents relative to the crossover point, $C_i^L$ and $C_i^R$. This naturally introduced the notion of a coarse graining relative to a description in terms of the strings themselves, the coarse graining being associated with sums over strings that contained a part of $C_i$. Subsequently we derived an analogous equation for the evolution of schematas, this time in terms of a schemata and its constituent parts. Schemata evolution is coarse grained relative to string evolution because of the summing over the $N - N_2$ non-schemata bits. The evolution of a schemata of $O(N_2)$ is described in terms of its constituent parts which are schemata are of order less than $N_2$. Thus the action of crossover invokes a natural hierarchy of coarse grainings. Such a hierarchy is reminiscent of a renormalization group transformation where there is a coarse graining over a subset of degrees of freedom, such as in the one-dimensional Ising model where one may sum over every other spin in the partition function for instance. In the genetic algorithm case this coarse graining stops naturally when one arrives at the evolution of 1-schematas as these are not decomposable into even more coarse grained degrees of freedom.

In one sense it is remarkable that one may solve analytically a genetic algorithm albeit for a simple fitness landscape and over a short time interval, however, what is lacking is a reasonable approximation scheme with which one may attack the evolution equations. Just as solving an exact renormalization group equation is almost impossible so with genetic algorithms finding exact solutions is probably hopeless. However, implementing renormalization group transformations approximately has had remarkable success in explaining many physical phenomena. We hope that finding analogous techniques in the study of genetic algorithms might lead to similar success.

Starting from the evolution equation for schematas, a further coarse-graining was performed to arrive at an expression for the average contribution of all schematas of size $l$ to the improvement of fitness. Applying this equation to the particular case of a $k = 0$ landscape, where each bit contributes independently to fitness, we showed that the net effect of crossover on fitness growth is slightly positive for all $l$: the effect of schemata reconstruction always exceeds that of destruction! Schematas that are either much smaller or much larger than half the string size are most enhanced.

A different situation arises if one considers a $k > 0$ landscape. In this case the sum of the effective selective advantages of the parts of a schemata is not necessarily equal to the effective selective advantage of the entire schemata. Only when the parts of a selected schemata are less selected than the whole (the deceptive case), crossover leads to a net destructive force as schematas are broken down into pieces which are then lost due to their low selectivity. The schematas that are selected over a long time scale are those that break down into useful parts, independently of their size.

Finite size effects break the apparent symmetry of the geometrical effect of crossover about $l = N/2$: The existence of a selection threshold favours highly fit schematas with a large number of specified bits $N_2$, and these can be found with a reasonable probability only if their length $l$ is large. Combining this argument with the $l$-dependence of in-schema fitness growth $\Delta_1$ one concludes that the effective degrees of freedom will be schematas with large $N_2$ and $l > N/2$.

This conclusion has important and surprising consequences for the designer of Genetic
Algorithms. It is often thought that GA designers should strive to find a coding such that bits that “cooperate” are placed near each other on the chromosome, so as to resist the destructive effect of crossover. This is generally speaking a very difficult task, since the structure of the optimisation problem usually does not match the linear topology of the strings. Our results show that this task is pointless: if anything one should try to place cooperating bits as far from each other as possible. Of course this is the most probable outcome if no attention is placed to the linear disposition of the bits, so this is not a problem one should worry about.

We should stress that the above comment by no means implies that the choice of coding is irrelevant. The choice of a genetic interpreter is crucial to generate a high density of states near desired fitness extrema and perhaps also to guide the emergence of an algorithmic language [18] which facilitates the search for new highly fit schematas. These issues however lie beyond the scope of the present paper.

With the results of this paper in mind it is interesting to recall the analogy between GA’s and spin glass dynamics discussed in the introduction. In both cases one is describing a condensation process in a rugged landscape, guided by the emergence of overlaps with certain structures or “patterns”. One of the chief reasons why in GA’s the overlaps with schematas is considered rather than with entire strings ($N_2 = N$ schematas) is that genetic populations are generally too disordered for such a rigid structure as a completely-specified string to be of much relevance. Of course the same can be said of spin glasses far from equilibrium. This suggests that the notion of “schemata” may find some usage to study the condensation of spin glasses from an initial disordered phase. One can carry the analogy between GA’s and spin glasses one step further and suggest that, in the case of sparsely-connected neural networks, the truncated connective trees may form a privileged class of schematas for the purpose of developing an effective theory of neural dynamics.

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FIGURE CAPTIONS

Figure 1. The multiplicative renormalization of the effective fitness due to crossover, \((1 + s_l)\), is represented as a function of the schemata length \(l\). The crossover term gives a positive contribution to fitness growth for all values of \(l\), which is greater for schemata sizes that are either much smaller or much larger than half the chromosome size.

Figure 2. The average absolute correlations between bits in the chromosome are given in terms of \((B)\) the linear distance which separates the bits on the chromosome, and \((C)\) the connective distance defined as the smallest number of landscape connections to go from one bit to the other. Very early on one notes a slight preference for correlations between bits that are near each other on the chromosome, i.e. with \(l << N\) \((2a)\). By \(t = 100\) the correlations between landscape-related bits become important \((2b)\), and they come to dominate at \(t = 200\) \((2c)\). At this point the population is highly organised and correlations on the basis of linear chromosome distance are no longer significant.