

# Coarse-Graining in Genetic Algorithms: Some Issues and Examples

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**Abstract.** Following the work of Stephens and coworkers on the coarse-grained dynamics of genetic systems, we work towards a possible generalisation in the context of genetic algorithms, giving as examples schemata, genotype-phenotype mappings, and error classes in the Eigen model. We discuss how the dynamics transforms under a coarse-graining, comparing and contrasting different notions of invariance. We work out some examples in the two-bit case, to illustrate the ideas and issues. We then find a bound for the Selection Weighted Linkage Disequilibrium Coefficient for the two-bit onemax problem.

## 1 Introduction

To model the exact evolution of a genetic algorithm requires us, in general, to track what happens to each possible individual. For example, if the search space is binary strings of length  $\ell$ , we have evolution equations for each of the  $2^\ell$  possible strings. It may also be of interest to investigate what happens to certain subsets of individuals. There are three reasons for doing this. Firstly, it may be possible to reduce the number of degrees of freedom in the evolution equations and so make a more tractable model. This is particularly true when modelling the appropriate effective degrees of freedom for the dynamics. Secondly, one may be interested in the evolutionary history of one particular individual, and there may be only a limited number of subsets to which its ancestors could have belonged. Thirdly, of course, one may have some intrinsic interest in a certain subset (for example, it may be a subset of high quality individuals or represent some “kinship” or genetically related group such as the individuals associated with a “niche” or a species).

The idea of tracking subsets is the basis of Holland’s schemata [Holland, 1975], Radcliffe’s forma [Radcliffe, 1992] and Vose’s predicates [Vose, 1991]. More recently, Stephens [Stephens and Waelbroek, 1997] has formally studied evolution equations under this kind of coarse-graining using schemata and extended the analysis to other contexts than evolutionary computation in [Stephens, 2003] and

[Stadler and Stephens, 2003]. Van Nimwegen [van Nimwegen et al., 1997] has modelled the dynamics of GAs on royal-road, and other functions, using approximate coarse-grained models. Rowe [Rowe, 1998] has considered the use of unitation classes as a basis for a coarse-grained model of selection-mutation algorithms. We intend to extend this work by looking at possible generalisations and limitations in the context of genetic algorithms.

In [Stephens and Waelbroek, 1997] it was shown that the dynamical equations governing the evolution of a GA with proportional selection, mutation and one-point crossover was *form invariant* under a coarse graining to schemata. This was later extended [Stephens, 2001] to any selection, mutation and homologous crossover operators. This form invariance was later studied by Vose and Wright [Vose and Wright, 2001] who discussed a more restrictive form of the invariance using the notion of *compatibility* [Vose, 1999] between the coarse graining and the genetic operators.

In the following section, we formally define the idea of coarse-graining. We then consider how the dynamics looks after a coarse graining. The ideas and issues are then illustrated by a series of examples. Finally, we apply coarse-graining to help us estimate what happens to the linkage disequilibrium coefficient in the two-bit onemax problem.

## 2 Coarse-Grained Dynamics

Let  $\Omega = \{0, 1, 2, \dots, n-1\}$  be the search space. In the case of binary strings of length  $\ell$ , we identify each string with an integer under standard binary encoding, and  $n = 2^\ell$ . We represent a population by a vector  $p = (p_0, p_1, \dots, p_{n-1})$  in which  $p_k$  is the proportion of individual  $k$  in the population. Population vectors are elements of the *simplex*

$$\Lambda = \left\{ p \in \mathbb{R}^n : \sum_k p_k = 1, \text{ and } p_k \geq 0 \text{ for all } k \right\}$$

A coarse-graining of  $\Omega$  will be a collection of subsets of  $\Omega$ . Given a fitness function  $f : \Omega \rightarrow \mathbb{R}$  we wish to define the fitness of a given subset. Notice, that this will, in general, depend on the details of the population. One can think of this situation as being analogous to a *co-evolutionary* model, in which the fitness of an individual depends on the current population. Let  $\mathcal{P}(\Omega)$  denote the *power set* of  $\Omega$  (that is, the set of all subsets of  $\Omega$ ). Then, formally, we have a function

$$F : \Lambda \longrightarrow (\mathcal{P}(\Omega) \longrightarrow \mathbb{R})$$

defined as

$$F(p)(A) = \frac{\sum_{i \in A} p_i f(i)}{\sum_{i \in A} p_i}$$

That is, given a population  $p \in \Lambda$ ,  $F(p)$  is a “fitness function” which assigns fitnesses to subsets of  $\Omega$ . The fitness of a subset  $A$  is the average fitness of elements of  $A$  in population  $p$ .

**Definition 1.** Let  $\Gamma = \{\gamma_i\} \subseteq \mathcal{P}(\Omega)$  be a collection of subsets of the search space that covers the search space. That is,

$$\bigcup \gamma_i = \Omega$$

We call such a collection a coarse-graining of  $\Omega$ . For any population  $p \in \Lambda$  we can assign a fitness to each element of  $\Gamma$  using the function  $F(p)$ .

A coarse-graining is non-degenerate if  $\Gamma$  is a partition of the search space

$$i \neq j \implies \gamma_i \cap \gamma_j = \emptyset$$

Notice that the fitness of a subset in a coarse-graining depends on the current population and therefore on time, even if the underlying fitness function  $f$  is static.

## Examples

- 1) **Schemata.** We can associate a schema with the set of all strings which match it. The set of all schemata forms a highly degenerate cover of the search space, however given an arbitrary choice of string then all the schemata that contain the string forms a new basis of the same dimensionality as the original - the Building Block Basis [Stephens, 2003]. However, unless the fitness function is a constant for all strings matching a given schema, then the fitness of the schema itself will be a dynamic quantity (that is, it will depend on the details of the current population).
- 2) **Genotype-phenotype mappings.** Suppose we have a map  $\varphi : \Omega \rightarrow \Phi$  which maps genotypes to phenotypes, where  $\Phi$  is the space of phenotypes. Fitness is then assessed via an individual's phenotype. That is, there is a function  $g : \Phi \rightarrow \mathbb{R}$ . The fitness of a genotype is then  $f = g \circ \varphi$ . We can create a non-degenerate coarse-graining by considering subsets of  $\Omega$  which map to the same phenotype. That is, for each  $i \in \Phi$ , set

$$\gamma_i = \{a \in \Omega : \varphi(a) = i\}$$

The fitness of such a subset is constant:

$$\begin{aligned} F(p)(\gamma_i) &= \frac{\sum_{j \in \gamma_i} p_j f(j)}{\sum_{j \in \gamma_i} p_j} \\ &= \frac{\sum_{\varphi(j)=i} p_j g \circ \varphi(j)}{\sum_{j \in \gamma_i} p_j} \\ &= \frac{g(i) \sum_{\varphi(j)=i} p_j}{\sum_{j \in \gamma_i} p_j} \\ &= g(i) \end{aligned}$$

This coarse-graining is natural with respect to selection, as we only need to keep track of what happens to the subsets, without worrying about their detailed composition.

- 2.1 **Unitation.** A particular example of a genotype-phenotype mapping is when we have a function of unitation. That is, the search space is binary strings of length  $\ell$  and fitness only depends on the number of ones in a string. The phenotype set is

$$\Phi = \{0, 1, 2, \dots, \ell\}$$

**2.2 The Eigen Model (Needle-in-a-haystack).** A second example is that of the Eigen model [Eigen, 1971]. In this landscape all the strings have the same fitness except for a special string (the optimum) that has a relatively high fitness. - the so called “master sequence”. In this landscape, the genotype-phenotype coarse-graining creates only two equivalence classes, hence there is a reduction in degrees of freedom from  $N$  to one.

### 3 Exact and Approximate Invariance under a Coarse-Graining

Having motivated the idea of coarse graining and given some simple examples one needs to understand how the evolution equations for the GA look under the coarse graining. As mentioned, it was shown in [Stephens and Waelbroek, 1997] that the canonical GA is form invariant under a coarse graining to schemata, i.e. that the equations have exactly the same functional form after such a coarse graining. This is a highly non-trivial result, as a coarse graining in general will not preserve the functional form, as can be simply seen, for example, in the case of coarse graining from genotype to phenotype in the presence of mutation or crossover. Vose later showed [Vose, 1999] that schemata are the only coarse-grained variable that leave the dynamical equations for homologous crossover invariant and hence form a privileged set. However, Vose also introduced a more restrictive form of invariance under coarse graining - *compatibility* - wherein it was not sufficient that the equations be form invariant. Formally, if an operator  $\mathcal{M} : \Lambda \rightarrow \Lambda$  gives the effect of applying an operator to a population, then a coarse-graining ( $\Gamma$ ) is compatible with  $\mathcal{M}$  if and only if, for any two populations  $x, y \in \Lambda$

$$\sum_{j \in \gamma_i} x_j = \sum_{j \in \gamma_i} y_j \implies \sum_{j \in \gamma_i} \mathcal{M}(x)_j = \sum_{j \in \gamma_i} \mathcal{M}(y)_j$$

for all  $\gamma_i \in \Gamma$  (see chapter 16-17 of [Vose, 1999]). It is known, for example, that schemata are compatible with crossover (by masks) and that unication classes are compatible with mutation.

A simple example illustrates the difference between the two different notions of invariance and coarse graining. Consider selection only in a two-bit one-max model: The equation of motion for proportional selection is

$$P(h_1 h_2, t + 1) = (f(h_1 h_2) / \bar{f}(t)) P(h_1 h_2, t). \quad (1)$$

We pass to the schema  $h_1^*$  by coarse graining  $h_2$  to find

$$P(h_1^*, t + 1) = (f(h_1^*, t) / \bar{f}(t)) P(h_1^*, t) \quad (2)$$

where  $f(h_1^*, t) = (f(h_1 h_2) P(h_1 h_2, t) + f(h_1 \bar{h}_2) P(h_1 \bar{h}_2, t)) / (P(h_1 h_2, t) + P(h_1 \bar{h}_2, t))$  and  $\bar{h}_2$  is the bit complement of  $h_2$ . Clearly (1) and (2) have the same functional form. However, to satisfy compatibility  $f(h_1^*, t)$  would have to satisfy  $f(h_1^*, t) = f(h_1)$ , where  $f(h_1 = 1) = 1$  and  $f(h_1 = 0) = 0$ . Compatibility will only be valid when the problem exhibits an exact equivalence relation (“symmetry”) and the genetic operators respect this symmetry, such as is the case for the genotype-phenotype map and selection only, or with schemata and crossover only. The existence

of an exact symmetry usually allows for a reduction in the number of degrees of freedom by going to those effective degrees of freedom that are invariant under the symmetry.

However, the utility of coarse graining is not restricted to when it is compatible with the dynamics. For instance, in [Stephens, 2001] the form invariance of the equations of motion was used to prove a generalization of Geiringer’s theorem to the case of non-flat landscapes. Further, in the physical sciences, where coarse graining has played an essential role, its utility is precisely for those cases where symmetries are not present, but rather where the coarse-grained dynamics can provide an approximate description of the system. In this case the closer are the coarse-grained variables to the true effective degrees of freedom then the better the approximation. For instance, in a strong selection regime one would expect phenotypes to approximate well the true dynamics with mutation and/or crossover inducing a small “interaction” between different phenotypes. Similarly, in the case of strong crossover and weak selection one would expect one-schemata to approximate well the dynamics with selection inducing a small interaction between the different one-schemata.

## 4 Crossover and Schemata Coarse Graining

We can track the evolutionary history of the production of a string via crossover, by looking at its constituent schemata, i.e. by using the Building Block basis. Suppose that we only have one-point crossover and no selection or mutation. We adopt the following notation, given that  $\gamma$  is a schema:

- $D(\gamma)$  is the set of indices for which  $\gamma$  has defined bit values. For example

$$D(1 * * 1 1 *) = \{1, 4, 5\}$$

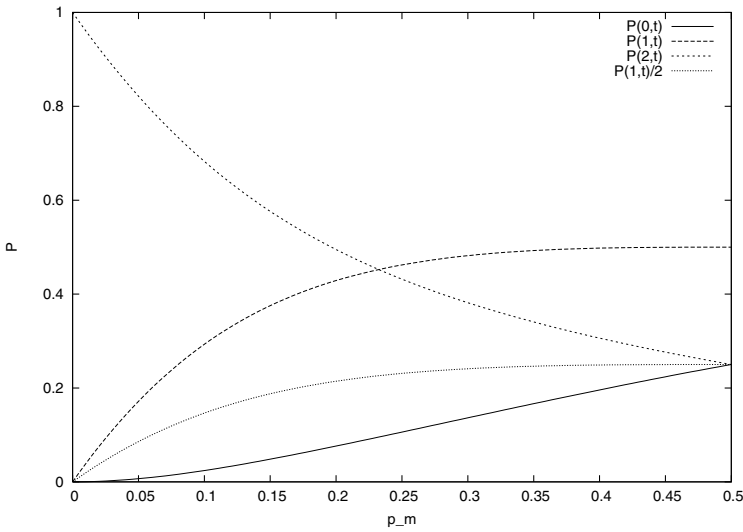
- $L_j(\gamma)$  is the schema which has the same defining bits as  $\gamma$  for all indices  $\leq j$ , and stars elsewhere. For example,  $L_4(1 * * 1 1 *) = 1 * * 1 * *$ .
- $R_j(\gamma)$  is the schema which has the same defining bits as  $\gamma$  for all indices  $> j$ , and stars elsewhere. For example,  $R_4(1 * * 1 1 *) = * * * * 1 *$ .
- If the population at time  $t$  is  $p \in \Lambda$ , we write  $P(\gamma, t) = \sum_{i \in \gamma} p_i$ .

Then, following [Stephens and Waelbroek, 1997] we have

$$P(\gamma, t + 1) = \sum_{j \in D(\gamma)} P(L_j(\gamma), t) P(R_j(\gamma), t)$$

Notice that this equation also applies to strings, by associating a string with the schema having all the corresponding bits defined.

We can use this equation to see how a given string can be created by crossover over several generations. For example, the string 1 1 1 can be created from the pairs 1 \* \*, \* 1 1 and 1 1 \*, \* \* 1. In the previous generation the schema \* 1 1 may have been created from the pair \* 1 \*, \* \* 1. We see that there are several different possible “family trees” that can be constructed, the leaves of which are the order-one schemata which match the string at the root. All of the elements of the trees however are elements of the Building Block basis associated with the string of interest.



**Fig. 1.** Asymptotic string proportions in a onemax landscape with mutation rate  $p_m$  and no crossover.  $P(2)$  decreases as we increase the probability of mutation, while  $P(1)$  and  $P(0)$  increase with  $p_m$ , and when  $p_m$  reaches  $1/2$ , all the strings are equally represented.

### 5 Mutation and the Genotype-Phenotype Coarse-Graining

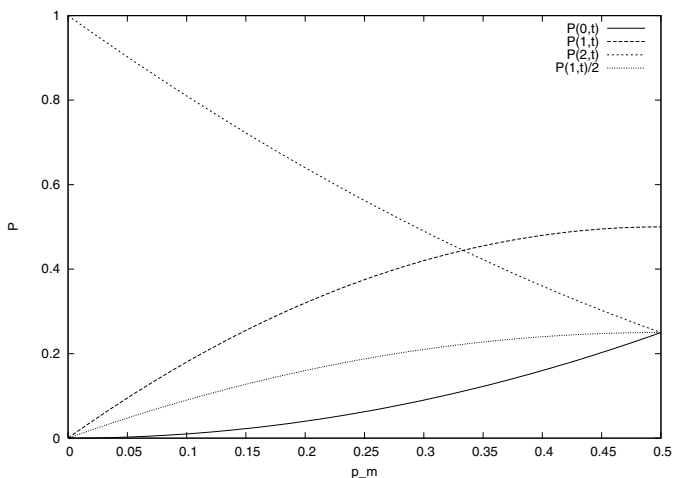
The unitation coarse graining is a particular case of the genotype-phenotype coarse-graining in which the fitness of a string is its Hamming weight (or the Hamming distance to the 0 string,  $f(i) = w(i) = d(i, 0)$ ). Now we can write the equivalence classes like  $\gamma_j = \{i \in \Omega | w(i) = j\}$ . In this particular case the reduction of the search space is huge, going from  $2^\ell$  degrees of freedom to only  $\ell + 1$  effective degrees of freedom.

As an example of the coarse-graining technique in this scenario, consider a GA with probability of crossover zero, probability of mutation  $\mu$  and  $\ell = 2$ , with the onemax fitness function. The set of equations describing the evolution of the system are as follows

$$\begin{pmatrix} p_{00}(t+1) \\ p_{01}(t+1) \\ p_{10}(t+1) \\ p_{11}(t+1) \end{pmatrix} = \begin{pmatrix} (1-\mu)^2 & (1-\mu)\mu & (1-\mu)\mu & \mu^2 \\ (1-\mu)\mu & (1-\mu)^2 & \mu^2 & (1-\mu)\mu \\ (1-\mu)\mu & \mu^2 & (1-\mu)^2 & (1-\mu)\mu \\ \mu^2 & (1-\mu)\mu & (1-\mu)\mu & (1-\mu)^2 \end{pmatrix} \begin{pmatrix} p_{00}(t) \\ p_{01}(t) \\ p_{10}(t) \\ p_{11}(t) \end{pmatrix} \tag{3}$$

$$\times \frac{1}{p_{01}(t) + p_{10}(t) + 2p_{11}(t)} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} p_{00}(t) \\ p_{01}(t) \\ p_{10}(t) \\ p_{11}(t) \end{pmatrix}$$

While in the coarse-grained basis the equations are:



**Fig. 2.** Asymptotic string proportions in a Eigen model landscape with mutation rate  $p_m$  and no crossover.

$$\begin{aligned}
 \begin{pmatrix} p(\gamma_0, t + 1) \\ p(\gamma_1, t + 1) \\ p(\gamma_2, t + 1) \end{pmatrix} &= \begin{pmatrix} (1 - \mu)^2 & (1 - \mu)\mu & \mu^2 \\ 2(1 - \mu)\mu & (1 - \mu)^2 + \mu^2 & 2(1 - \mu)\mu \\ \mu^2 & (1 - \mu)\mu & (1 - \mu)^2 \end{pmatrix} \\
 &\times \frac{1}{p(\gamma_1, t) + 2p(\gamma_2, t)} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} p(\gamma_0, t) \\ p(\gamma_1, t) \\ p(\gamma_2, t) \end{pmatrix} \tag{4}
 \end{aligned}$$

We can solve this system using a similarity transformation for the state-transition matrix, finding the eigenvectors and replacing the original matrix with a diagonal similar matrix (see, for example, chapter 6 of [Reeves and Rowe, 2001]). The results are shown in figure 1, where we can see the fixed points as a function of the probability of mutation irrespective of the initial conditions of the population.

The unitation coarse-graining allow us to eliminate a redundant variable. Of course, it proves to be more useful as we increase the dimension of the search space [Rowe, 1998].

In contrast, for the Eigen model the genotype-phenotype coarse-graining is not compatible with mutation. Instead, we divide the space into Hamming distance classes from the master sequence. That is  $\gamma_j = \{i \in \Omega | d(i, c_{ms}) = j\}$ , where  $c_{ms}$  is the master sequence. In the case where  $c_{ms} = 0$ , this gives us the unitation coarse-graining.

Now we can solve the system using the same method as before, considering  $f(c_{ms}) \gg f(j), \forall j \neq c_{ms}$ . The results in the long-time limit for the two-bit problem are shown in figure 2. Note that qualitatively we obtain a very similar behaviour to the onemax landscape. This means that in spite of the fact that all the strings different to the master sequence have the same low fitness, evolution favours those close to the master sequence as we can see in figure 2. This phenomenon is known in the literature as the formation of a quasi-species.

## 6 Linkage-Disequilibrium

Let  $ij$  be any string of 2 bits,  $i, j \in \{0, 1\}$ , then the dynamics of the system under proportional selection (with the onemax landscape) and one-point crossover is given by the equations:

$$\begin{aligned} P(ij, t+1) &= (1-p_c)P'(ij, t) + p_c P'(ij, t) [P'(ij, t) + P'(i \bar{j}, t) + P'(\bar{i}j, t)] \\ &\quad + p_c P'(i \bar{j}, t) P'(\bar{i}j, t) \\ &= (1-p_c)P'(ij) + p_c P'(ij, t) [1 - P'(\bar{i} \bar{j}, t)] + p_c P'(i \bar{j}, t) P'(\bar{i}j, t) \\ &= P'(ij) + p_c [P'(i \bar{j}, t) P'(\bar{i}j, t) - P'(ij, t) P'(\bar{i} \bar{j}, t)] \end{aligned}$$

where  $P'$  is the proportion after selection,  $p_c$  is the probability of crossover and  $\bar{i}$  is the complement base 2 of  $i$ .

$\Delta'(t) = p_c [P'(i \bar{j}, t) P'(\bar{i}j, t) - P'(ij, t) P'(\bar{i} \bar{j}, t)]$  is the Selection Weighted Linkage Disequilibrium Coefficient (SWLDC) explicitly introduced in [Stephens, 2001] (and implicit in earlier work) in analogy with the original Linkage Disequilibrium Coefficient (LDC), well known in population biology, that measures how far is the current population from Robbins proportions (in which the bits are distributed independently — Geiringer's Theorem tells us that this is the limit of repeatedly applying crossover [Geiringer, 1944]). We can write

$$w(t+1) = \frac{p_c x(t)y(t)}{\bar{f}^2(t)} \quad (5)$$

$$x(t+1) = \frac{x(t)}{\bar{f}(t)} - \frac{p_c x(t)y(t)}{\bar{f}^2(t)} \quad (6)$$

$$y(t+1) = \frac{y(t)}{\bar{f}(t)} - \frac{p_c x(t)y(t)}{\bar{f}^2(t)} \quad (7)$$

$$z(t+1) = \frac{2z(t)}{\bar{f}(t)} + \frac{p_c x(t)y(t)}{\bar{f}^2(t)} \quad (8)$$

where  $w(t) = P(00, t)$ ,  $x(t) = P(01, t)$ ,  $y(t) = P(10, t)$ ,  $z(t) = P(11, t)$ , notice that  $P(00, t) = \Delta'(t) \forall t > 0$

Substituting the value of  $x(t)$  from (6) and  $y(t)$  from (7) in (5)

$$w(t+1) = \frac{p_c}{\bar{f}^2(t)} \left[ \frac{x(t-1)}{\bar{f}(t-1)} - \frac{p_c x(t-1)y(t-1)}{\bar{f}^2(t-1)} \right] \left[ \frac{y(t-1)}{\bar{f}(t-1)} - \frac{p_c x(t-1)y(t-1)}{\bar{f}^2(t-1)} \right] \quad (9)$$

which we can rewrite as:

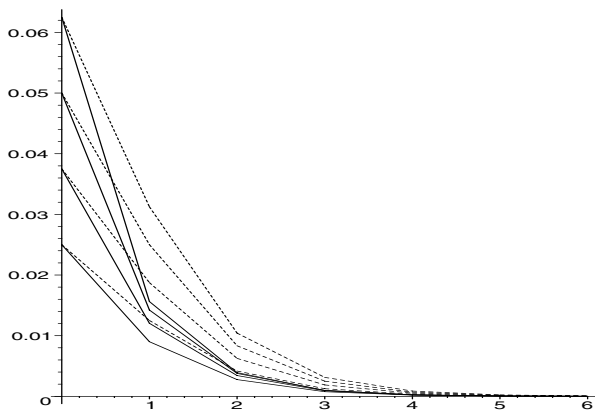
$$w(t+1) = \frac{1}{\bar{f}^2(t)} \left[ w(t) - p_c w(t) \left( \frac{x(t-1) + y(t-1)}{\bar{f}(t-1)} \right) + p_c w^2(t) \right] \quad (10)$$

As there are four genotypes and three phenotypes we now coarse-grain using the genotype-phenotype map, considering the phenotypic variable  $b(t) = x(t) + y(t)$ , adding (6) and (7) at time  $t$  to find

$$\frac{b(t-1)}{\bar{f}(t-1)} = b(t) + 2w(t) \quad (11)$$

which can then be substituted into (10) to obtain





**Fig. 3.** Linkage Disequilibrium Coefficient  $w(t)$  (continuous line) and the bound  $w^*(t)$  (dotted line) in a typical run with a random initial population. The initial values correspond to different values of  $p_c = \frac{j+2}{5}, j \in \{0, 1, 2, 3\}$

$$w(t + 1) = \frac{w(t)}{\bar{f}^2(t)} [1 - p_c(w(t) + b(t))] \tag{12}$$

with  $\bar{f}(t) = b(t) + 2z(t)$ . Now if we assume  $p_c = 1$  we can simplify (12) to

$$w(t + 1) = \frac{w(t)}{2z(t) + b(t)} \left[ \frac{z(t)}{2z(t) + b(t)} \right] \tag{13}$$

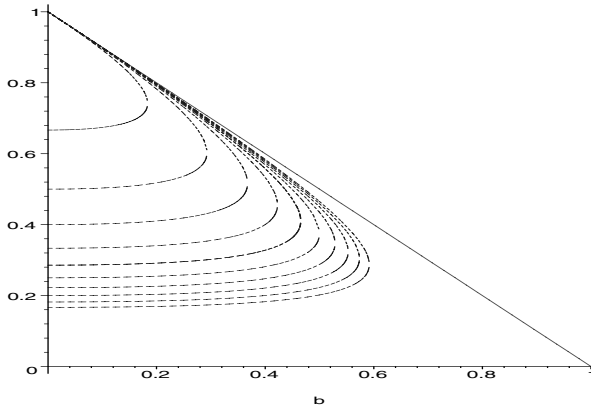
Note that this equation, because of the substitution (11), is only valid for  $w(t) = 0$ , as the latter is a fixed point of (13) but not of (5) (unless  $x(t) = y(t) = 0$  as well), and also for  $p_c > 0$ .

Let  $g(t) = \left[ \frac{z(t)}{2z(t)+b(t)} \right]$ , iterating we find the following solution

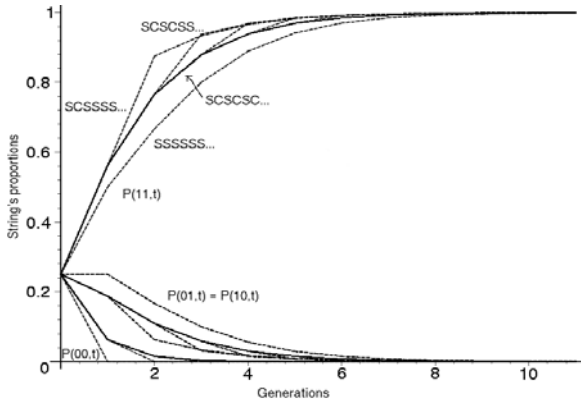
$$w(t) = \frac{w(0) \prod_{i=0}^{t-1} g(i)}{2^t z(0) + b(0) + \delta_{t \geq 3} w(0) \sum_{i=1}^{t-2} 2^i \prod_{j=0}^{t-2-i} g(j)} \tag{14}$$

where  $\delta_C = 1$  if  $C$  is true and 0 otherwise. It is easy to see that  $g(t) \leq \frac{1}{2} \forall t$ , so we can write

$$\begin{aligned} w(t) &\leq \frac{\left(\frac{1}{2}\right)^t w(0)}{2^t z(0) + b(0) + \delta_{t \geq 3} w(0) \left(\sum_{i=1}^{t-2} 2^i \left(\frac{1}{2}\right)^{t-i-1}\right)} \\ &= \frac{\left(\frac{1}{2}\right)^t w(0)}{2^t z(0) + b(0) + \delta_{t \geq 3} \frac{w(0)}{3} (2^{t-1} - 2^{3-t})} \\ &\leq \frac{\left(\frac{1}{2}\right)^t w(0)}{2^t z(0) + b(0)} = w^*(t) \end{aligned} \tag{15}$$



**Fig. 4.** The dotted lines represent zones with similar SLDC in the simplex as a function of  $x(t) + y(t)$ . The continuous line is the limit of the simplex.



**Fig. 5.** The dotted lines represent the SCSSSS and the continuous SCSCSCSC

A comparison of the bound and the actual results are shown in fig. 3. Note that we would expect the bound to be better when  $b(t) \ll z(t)$ , however, for  $3b(0) = 2z(0)$  so it is interesting to see that the bound gives reasonable results. Of course, strictly speaking the derived bound is for  $p_c = 1$ . The weaker the selective difference between 11 and 10 or 01 then the worse the bound. On the contrary, when the selective advantage of 11 over the other strings is large we expect the bound to become better and better. A further simplification lead us to

$$w^*(t) = \frac{\left(\frac{1}{2}\right)^t w(0)}{2^t z(0) + b(0)} \leq \left(\frac{1}{4}\right)^t \frac{w(0)}{z(0)} \tag{16}$$

where we can appreciate more clearly the exponential decay of the SWLDC.

By the definition of  $w(t)$  in (5) and its value in (12) when  $p_c = 1$  we can conclude that in every generation before selection we have  $w(t)z(t) - x(t)y(t) = 0$  i.e. the population is in linkage (in the usual sense). This means that the population follows a path (in the simplex) always in linkage equilibrium, i.e. on the Geiringer manifold, towards a selective linkage equilibrium. Clearly, the latter is of more relevance than the former for the dynamical evolution.

In figure (4) we can see the different “contours” with the same SWLDC as a function of the coarse-grained variable  $b(t)$ . Notice  $b(t) = P(1, t)$  plays an important role in the solution of the equations suggesting again a possible effective degree of freedom.

As the effects of crossover decay in time, as  $b(t)$  gets smaller, we might think about approximating the usual iteration sequence SCSCSC... with the sequence SCSSSS... Where S denotes selection and C crossover. The effects can be seen in Figure 5. Note how the approximation to SCSCSC... uniformly improves in a “perturbative” fashion as we include more Cs in the sequence, four Cs giving a very good approximation.

## 7 Conclusion

We have discussed the notion of coarse graining in GAs, giving a formal definition and some representative examples such as genotype-phenotype mappings, schemata, error classes. We discussed how the dynamical equations for a GA transform under a coarse graining comparing and contrasting the notions of form invariance and compatibility and discussed some practical issues and potential problems that arise when applying arbitrary coarse-grainings. However, the evolution equations of certain GAs can be simplified with an appropriate choice of subsets. Schemata are natural subsets to consider as the dynamics is form invariant under a schema coarse graining for selection, mutation and crossover, whereas only mutation and crossover are compatible with the dynamics. Unitation classes were also seen to be natural in the case of selection and bitwise mutation. Genotype-phenotype coarse-grainings are natural in the case of selection, since they give rise to constant (that is, static) fitness values for the subsets. We have illustrated these ideas and problems with some simple examples. Finally, we have shown how a genotype-phenotype coarse-graining can help calculate an estimate for the selective linkage disequilibrium coefficient in the two-bit case.

## References

- [Eigen, 1971] Eigen, M. (1971). Self-organization of matter and the evolution of biological macromolecules. *Naturwissenschaften*, 58:465.
- [Geiringer, 1944] Geiringer, H. (1944). On the probability theory of linkage in Mendelian heredity. *Annals of Mathematical Statistics*, 15(1):25–57.
- [Holland, 1975] Holland, J. (1975). *Adaptation in Natural and Artificial Systems*. University of Michigan Press, Ann Arbor, Michigan.
- [Radcliffe, 1992] Radcliffe, N. J. (1992). The algebra of genetic algorithms. *Annals of Mathematics and Artificial Intelligence*, 10:339–384.
- [Reeves and Rowe, 2001] Reeves, C. R. and Rowe, J. E. (2001). *Genetic Algorithms — Principles and Perspectives*, chapter 6, The Dynamical Systems Model. Kluwer Academic Publishers.

- [Rowe, 1998] Rowe, J. (1998). Population fixed-points for functions of unitation. In Banzhaf, W. and Reeves, C., editors, *Foundations of Genetic Algorithms*, pages 69–84. Morgan Kaufmann.
- [Stadler and Stephens, 2003] Stadler, P. F. and Stephens, C. R. (2003). Landscapes and effective fitness. *Comm. Theor. Biol.* Accepted for publication.
- [Stephens, 2001] Stephens, C. R. (2001). Some exact results from a coarse grained formulation of genetic dynamics. In Spector, L., Goodman, E. D., Wu, A., Langdon, W. B., Voigt, H.-M., Gen, M., Sen, S., Dorigo, M., Pezeshk, S., Garzon, M. H., and Burke, E., editors, *Proceedings of the Genetic and Evolutionary Computation Conference (GECCO-2001)*, pages 631–638, San Francisco, California, USA. Morgan Kaufmann.
- [Stephens, 2003] Stephens, C. R. (2003). The renormalization group and the dynamics of genetic systems. *Acta Phys. Slov.*, 52:515–524.
- [Stephens and Waelbroek, 1997] Stephens, C. R. and Waelbroek, H. (1997). Effective degrees of freedom in genetic algorithms and the block hypothesis. In Bäck, T., editor, *Proceedings of the Seventh International Conference on Genetic Algorithms*, pages 34–41. Morgan Kauffman.
- [van Nimwegen et al., 1997] van Nimwegen, E., Crutchfield, J. P., and Mitchell, M. (1997). Finite populations induce metastability in evolutionary search. *Physics Letters A*, 229:144–150.
- [Vose, 1991] Vose, M. D. (1991). Generalizing the notion of a schema in genetic algorithms. *Artificial Intelligence*, 50:385–396.
- [Vose, 1999] Vose, M. D. (1999). *The Simple Genetic Algorithm: Foundations and Theory*. MIT Press, Cambridge, MA.
- [Vose and Wright, 2001] Vose, M. D. and Wright, A. H. (2001). Form invariance and implicit parallelism. *Evolutionary Computation*, 9(3):355–370.