An analysis of Punctuated Equilibria in Simple Genetic Algorithms

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Abstract. In the running of a genetic algorithm, the population is liable to be confined in the local optimum, that is the metastable state, making an equilibrium. It is known that, after a long time, the equilibrium is punctuated suddenly and the population transits into the better neighbor optimum. We adopt the formalization of Computational Ecosystems to show that the dynamics of the Simple Genetic Algorithm is represented by a differential equation focusing on the population mean of a phenotype. Referring to the studies of differential equations of this form, we show that the duration time of metastability is exponential in the population size and other parameters, on the one dimensional bistable fitness landscape which has one metastable and one stable state.

1 Introduction

Genetic Algorithms (GAs) are optimization methods modeled from some operations which are used during the natural reproduction and the natural selection [3]. Since the concepts of GAs are introduced by Holland [?], various GAs show practical successes in various fields. Among them, the Simple Genetic Algorithm (SGA) is the simplest genetic algorithm containing the essential operators: selection, mutation, and crossover.

Like the other optimization methods, SGAs have the problem of metastability that the population is liable to be trapped in a local optimum, making an equilibrium. If there is a better optimum state in the vicinity, the local optimum is the metastable state since the punctuated equilibrium appears [11]. The punctuated equilibrium is the phenomenon in which the system in a metastable state shows a sudden transition into the more stable neighbor state after a long time. Punctuated equilibria are analyzed in various fields including Computational Ecosystems (CEs) and neo-Darwinian evolution models [1, 8].

The analysis of CEs is based on the time derivative of the probability distribution P, where $P(\mathbf{r},t)$ is the probability that the system state is \mathbf{r} at time t in the ensemble of possible system states. They use dP/dt to find d < z > /dt where < z > is the ensemble mean of the interested system character z [5].

In the neo-Darwinian model, the population mean \bar{x} of a genetically determined character is governed by the equation $d\bar{x} = F'(\bar{x}) + \varepsilon dB$ where F is a landscape on x, B(t) is a standard Brownian process, and ε is a small constant. They use the theoretical results from diffusion processes [7] to show that

the punctuated equilibria appear in the natural evolution with the exponential duration time of metastability as ε decreases to zero [8].

In this paper, we adopt the formalization of Computational Ecosystems to show that the dynamics of the Simple Genetic Algorithm is represented by a differential equation like $d\bar{x} = F'(\bar{x}) + \varepsilon dB$ focusing on the population mean of a phenotype. Referring to the studies of differential equations of this form, we show that the duration time of metastability is exponential in the population size and other parameters, on the one dimensional bistable fitness landscape which has one metastable and one stable state.

In section 2, the CE and the equation from the diffusion process are described. We analyze the dynamics of the SGA adopting the methods of CEs in section 3. The bistable fitness landscape is introduced and the simulation results are shown in section 4. In section 5 we discuss the results obtained in previous sections focusing on the duration time of metastability. Conclusion and further work are covered in section 6.

2 Background

2.1 Computational Ecosystems

The CE is a very similar model to GAs. A population contains N agents, and each agent chooses one from R resources to get some payment which is determined by the payment function f. f is the function of the chosen resource and the population state which is represented by a vector $\mathbf{r} = (r_1, r_2, \dots, r_R)$ whose i-th element is the ratio of agents choosing the resource i. During a unit time, each agent has the α chances to change the resource to the new one according to ρ_i , which is the probability that resource i perceived to be the best choice and is the function of \mathbf{r} .

The possible population states at time t compose the ensemble represented by $P(\mathbf{r},t)$ which is the probability of the population state to be \mathbf{r} at t. Considering only one possible change of an agent's resource in a short time interval,

$$\frac{dP(\mathbf{n},t)}{\alpha dt} = -P(\mathbf{n},t) \sum_{i \neq j} n_j \rho_i + \sum_{i \neq j} P(\mathbf{n}^{[j,i]},t) (n_j + 1) \rho_i^{[j,i]}$$
(1)

where $\mathbf{n}^{[j,i]}$ is such that $n_j^{[j,i]} = n_j + 1$, $n_i^{[j,i]} = n_i - 1$ and all other elements are the same as \mathbf{n} . And ρ_i and $\rho_i^{[j,i]}$ are evaluated at \mathbf{n} and $\mathbf{n}^{[j,i]}$, respectively.

The ensemble mean $\langle r_i \rangle$ of r_i satisfies

$$\frac{d < r_i >}{dt} = \alpha(< \rho_i > - < r_i >). \tag{2}$$

using equation (1) [5].

2.2 Diffusion processes

Consider the one dimensional diffusion process z(t) satisfying

$$dz(t) = F'(z) + \varepsilon dB(t) \tag{3}$$

where B(t) is the standard Brownian process and ε is a small constant. Let F satisfy the following conditions:

- F is a differentiable function defined on $-\infty < z < \infty$,
- there exists $z_1 < z_2 < z_3$ such that F is strictly increasing on $(-\infty, z_1] \cup [z_2, z_3]$ and strictly decreasing on $[z_1, z_2] \cup [z_3, \infty)$, and
- $F(z_1) < F(z_3).$

If $z(0) = z_1$, then the punctuated equilibrium appears and the duration time T of metastability satisfies

$$T \propto \exp\left(\frac{2(F(z_1) - F(z_2))}{\varepsilon^2}\right) \tag{4}$$

when $\varepsilon \ll 1$. And the transition is unidirectional in the sense that the system remains in the stable state permanently [7]. These results about the duration time can be expanded to the cases that F has more than two peaks or z is multidimensional [7, 2].

3 Analysis

The analysis of genetic algorithms in the genotype is somewhat complex since it considers vector values and matrix operations. We focus on the phenotype x_i of an individual where x_i corresponds to the genotype i.

3.1 Simple Genetic Algorithms

A SGA in this paper deals with a population which consists of N individuals. Each individual is a binary string of L bits, each bit has one of two values 0 and 1, and there are $R = 2^L$ genotypes. The phenotype for the genotype i is x_i and the fitness f is the function on the phenotype domain. The population state is represented by $\mathbf{n} = (n_1, n_2, \ldots, n_R)$ or $\mathbf{r} = (r_1, r_2, \ldots, r_R)$ where $n_i(t)$ is the number of individuals with the genotype i and $\mathbf{r} = \mathbf{n}/N$.

The population of the next generation is produced from the current one through some SGA operators: roulette wheel selection, 1-point crossover and simple mutation [3]. After two individuals are selected from the current population by the roulette wheel selections, the 1-point crossover and the simple mutation are applied to the pair. In the 1-point crossover, each individual is cut at the same point and divided into two substrings, and then the second substrings are exchanged. The cutting point is determined randomly among all the points between two bits. And then, the simple mutation toggles each bit of

individuals with the probability p_m . After the mutations, one of two children is chosen randomly and added into the next generation.

Repeating this process N times, the new generation with the generation gap 1 can be completely produced. For the simplicity, the crossover is not considered in the analysis and is mentioned in section 5.2. The parameters and the functions related to selection, crossover and mutation are superscripted with s , c and m respectively.

3.2 Brownian part

As it is defined in the CE, let $P(\mathbf{r}, t)$ be the probability that the population state is \mathbf{r} at time t. Then the ensemble mean and the population mean of z are represented, respectively as $\langle z \rangle = \sum_{\mathbf{r}} z P(\mathbf{r}, t)$ and $\bar{z} = \sum_{i} z r_{i}$.

Let α be the average number of generations per unit time. Then the SGA changes the population state $\alpha \Delta t$ times during Δt . When an individual is chosen after selection, crossover and mutation, the phenotype of the individual can be considered as a random variable X. Using the central limit theorem [10], the population mean \bar{X} of the phenotypes follows

$$\bar{x}(t + \Delta t) - \bar{x}(t) = \langle \bar{x}(t + \Delta t) \rangle - \bar{x}(t) + \alpha \Delta tG$$
 (5)

where G is a Gaussian random variable with mean 0 and variance $V(\bar{X})$.

Since the dispersion of the ensemble starts from the instantiated state with $\bar{x}(t)$, $\langle \bar{x}(t) \rangle = \bar{x}(t)$. The accumulation of Gaussian random variables, each of which has the variance 1, makes the standard Brownian process. Then, since $V(\bar{X}) = V(X)/N$ by the central limit theorem,

$$d\bar{x}(t) = d < \bar{x}(t) > +\alpha \sqrt{\frac{V(X)}{N}} dB(t). \tag{6}$$

Ignoring the crossover, the random variable X of phenotype is composed of X^s and X^m ,

$$X = X^s + X^m \tag{7}$$

where X^s is the result of the selection and X^m is the change due to the mutation. The effects of the mutation is dependent on how the genotype is decoded into the phenotype, and then into the fitness. To obtain a general feature of the simple mutation, we define the phenotype as $x_i = l_i/L$, where l_i is the number of bits with the value 1 in the genotype i. In case of L = 1, X^m has the probability distribution with mean $(1 - 2l(t)/L)p_m$ and variance $p_m - (1 - 2l(t)/L)^2p_m^2$. Thus, in general, X^m has the Gaussian distribution with

$$E(X^m) = (1 - 2l(t)/L)p_m$$
 and
 $V(X^m) = [p_m - (1 - 2l(t)/L)^2 p_m^2]/L \simeq p_m/L$ (8)

by the central limit theorem.

Considering only the selection, the variance of the phenotype seems to be dependent on $f^{(1)}/\bar{f}$, where $f^{(m)}$ is the m-th derivative of f(x). Even when the

fitness landscape is flat, the selection makes the variance decrease by the factor of 1/N [9], and then

$$0 < V_{steepest} \le V(X) \le V_{flat} = \frac{Np_m}{L} \tag{9}$$

where $V_{steepest}$ and V_{flat} are variances when $|f^{(1)}/\bar{f}|$ is maximum and zero, respectively. That is, V(X) is finite within the range of equation (9).

3.3 Ensemble mean part

Consider the case of the generation gap 1/N, in which a child is produced from the SGA operators, a victim is chosen randomly from the current generation and then it is replaced by the child, producing the next generation. When genotypes of the child and the victim are i and j respectively, this random event corresponds with the resource changing from j to i for an agent in CEs. That is, the SGA with the generation gap 1/N is the special case of the CE, when ρ_i is interpreted as the probability that the child with the genotype i would be produced by the SGA operations.

However, if the generation gap is 1, equation (1) can not be used by the SGA since it is the result of considering maximally one change of an agent in a given time interval. Thus we focus on the macroscopic equation (2) whose right hand side is interpreted as $N\alpha$ generations per unit time multiplied by the effect of one generation, $(<\rho_i>-< r_i>)/N$ on condition that the generation gap is 1/N. If one generation contains N changes of individuals and they are all relatively independent, the effect of one generation is enlarged to be $(<\rho_i>-< r_i>)$. Strictly speaking, the changes of individuals in one generation of the SGA is not independent since the victim is selected in round robin. But it makes the same effect to the independent case since the round robin guarantees that each individual has the same probability to be selected as a victim. Modifying the definition of α as the average number of generations per unit time, equation (2) can also be used for the SGA with the generation gap 1.

From equation (2), we can obtain

$$\frac{d \langle \bar{x}(t) \rangle}{dt} = \alpha \sum_{i=1}^{R} x_i (\rho_i(t) - r_i(t)). \tag{10}$$

Considering only the selection,

$$\sum_{i=1}^{R} x_i \left(\frac{f(x_i)r_i}{\bar{f}} - r_i \right) = \frac{\overline{(x - \bar{x})f}}{\bar{f}} = \frac{1}{\bar{f}} \sum_{m=0}^{\infty} \frac{f^{(m)}(\bar{x})}{m!} \overline{(x - \bar{x})^{m+1}}.$$
 (11)

On condition that

$$f(x) \simeq f(\bar{x}) + (x - \bar{x})f^{(1)}(\bar{x})$$
 (12)

for each individual in the population, equation (11) becomes

$$\sum_{i=1}^{R} x_i \left(\frac{f(x_i)r_i}{\bar{f}} - r_i\right) = s_X^2 \frac{\partial \log f(\bar{x})}{\partial \bar{x}} \tag{13}$$

where $s_X^2 = \overline{(x - \bar{x})^2}$, the population variance.

The change due to the mutation is, from equation (8),

$$\left[\frac{d \langle \bar{x}(t) \rangle}{\alpha dt}\right]^m = p_m (1 - 2\bar{x}^s) \simeq p_m (1 - 2\bar{x}). \tag{14}$$

3.4 Dynamics due to selection and mutation

Let V^s be the some constant representing the selection term of V(X) within the range of equation (9). If we assume that s_X^2 is independent of \bar{x} for the simplicity then the global fitness function F can be defined by

$$F(\bar{x}) = s_X^2 \log f(\bar{x}) + p_m(\bar{x} - \bar{x}^2). \tag{15}$$

This assumption will be mentioned again in section 5.3. Finally, from equations (6), (8), (13) and (14), we can summarize the dynamics of the SGA as

$$\frac{d\bar{x}(t)}{\alpha dt} = \frac{\partial F(\bar{x})}{\partial \bar{x}} + \sqrt{\frac{V^s + p_m/L}{N}} \frac{dB(t)}{dt}$$
(16)

considering selections and mutations except the crossover.

4 Simulation

4.1 Bistable landscape

Punctuated equilibria appear if F has the landscape as is shown in section 2.2. In this simulation, we restrict f to have three features. First, F satisfies the conditions in section 2.2 except that F is not differentiable at finite number of points. Secondly, the selection pressures from the barrier are the same for the metastable and stable attractors. And lastly, the condition of equation (12) is satisfied for each individual. Strictly speaking, the third is not always true since there are some generations in which some individuals are in the right side of the barrier and the others remain in the left side. But this dispersion is condensed into a population in one side very quickly and hence we ignore the effect. The phenotype x is defined by $x_i = l_i/L$ as in the case of mutation analysis.

The typical f and F are shown in figure 1, where d = f(0) - f(1/3) is the barrier depth in f landscape. Other fitness function like the generalized deceptive functions [12] could also be used if it has the deceptiveness and the multistep trajectory from the local optimum to the global optimum state, but are not covered in this paper.

Figure 2 shows typical punctuated equilibria appeared in the running of the SGA. The population starts from the state $\bar{x}=0$, converges quickly into the metastable state, and shows perturbations around it. After a long duration, \bar{x} transits the fitness barrier to the stable state suddenly.

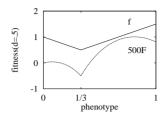


Fig. 1. A fitness function with barrier depth d

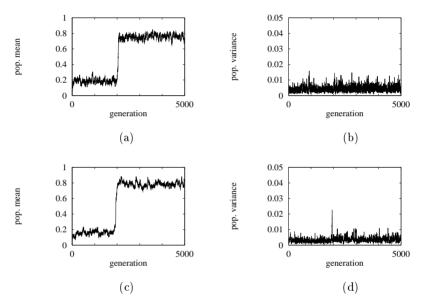


Fig. 2. The punctuated equilibria are shown on the graph of \bar{x} as generations are succeeded. (a) and (b) are \bar{x} and s_X^2 respectively, where N=20, $p_c=1.0$, $p_m=0.012$ and d=0.5. (c) and (d) are \bar{x} and s_X^2 respectively, where N=30, $p_c=0.0$, $p_m=0.008$ and d=0.5.

4.2 The time of metastability

Beginning with the population state with $\bar{x}=0$, we record the duration T of metastability varying some parameters, where T is defined as the number of generations till the transition to the stable state occurs. The time required for the transition is so short relative to T that it is ignored. Considered parameters are the population size N, the barrier depth d in f landscape, and the mutation probability p_m .

Figure 3 is the simulation results when $p_c = 0$. Figure 3(a) and 3(b) shows that T is a rapidly increasing function of N and d. And figure 3(c) shows that

T is a rapidly decreasing function of p_m .

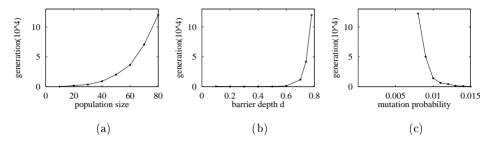


Fig. 3. The duration T of metastability versus some parameters. Each point is an average of 30 runs. Default parameter values are L = 30, N = 40, $p_c = 0$, $p_m = 0.01$ and d = 0.7.

In case of $p_c = 1$, figure 4 is the counterpart of figure 3. This shows that the crossover makes the duration be longer for any parameter set in this simulation environment.

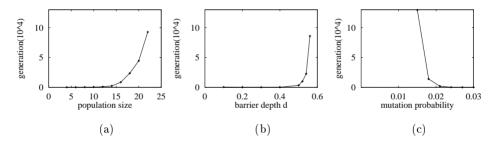


Fig. 4. The duration T of metastability versus some parameters. Each point is an average of 30 runs. Default parameter values are L=30, N=40, $p_c=1$, $p_m=0.01$ and d=0.7.

5 Discussion

5.1 Effects of selection and mutation

Since equation (16) has the form of equation (3), the duration T of metastability satisfies

$$T \propto e^{\frac{2DN}{V^s + p_m/L}} \tag{17}$$

by equation (4), where D is the barrier depth in F landscape.

The mean population phenotype $\bar{x}(t)$ oscillates around the equilibrium value x_e which is determined from the non-Brownian part of equation (16), $\partial F(\bar{x})/\partial \bar{x} = 0$. Given p_m and d, the relation between s_X^2 and x_e can be obtained from this equation and is approximately consistent with the graphs of figure 2.

Among the SGA runs in the simulation, there is not any case that the population returns to the metastable state once the punctuated equilibrium occurs, provided that $p_m \ll 1$. This means that the transition is unidirectional.

Figure 3(a) qualitatively confirms that T is exponential in the population size N. But figure 3(b) needs an explanation since the barrier depth d is the quantity of f landscape. Let x_e be the root of $\partial F(\bar{x})/\partial \bar{x} = 0$ in the metastable area. Then, from equation (17),

$$T \propto e^{K[\log f(x_e) - \log(1 - d)]} = \left[\frac{f(x_e)}{1 - d}\right]^K \tag{18}$$

where K is a constant. That is, the shape of the graph of T is that of 1/(1-d) rather than that of e^d . Figure 3(c) shows that why the condition of $p_m \ll 1$ is needed for the punctuated equilibria to be appeared, and is consistent to equation (17).

5.2 Effects of crossovers

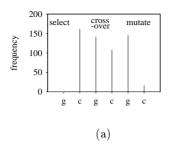
In a bistable problem, individuals can be divided into two types according to which basin of attractor they belong to : A-type and B-type, respectively in metastable and stable area. Let r_B and f_B be the ratio and the average fitness of B-type individuals, respectively.

For most generations, $r_B = 0$, and r_B becomes positive at long intervals by crossovers or mutations. When this event occurred at τ -th generation,

$$r_B(\tau + 1) \simeq [r_B^s(\tau)]^2 + \beta r_A^s(\tau) r_B^s(\tau)$$
 (19)

since the term of $[r_A^s(\tau)]^2$ and the effect of mutation can be ignored. The parameter β is the rate that B-type children are produced from the crossover of one A-type and one B-type parents.

When the phenotype is defined as x=l/L, the crossover has the tendency that the x's of two parents are averaged. If one A-type and one B-type parents crossover then the children would be around the barrier terminating the appearance of the B-type, and hence $\beta \ll 1$. That is, the crossover not only enhances the appearance of B-type individual, but also would eliminate it. Figure 5 shows that the crossover interrupts the appearance of the B-type as a whole if the genotype is decoded into the fitness as is done in section 4. On condition that β is larger than a particular criterion, this interrupt would be replaced by the enhancement. But the crossover is highly dependent on the definitions of x and f, and the generalization is not considered in this paper.



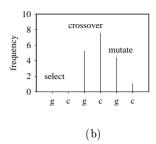


Fig. 5. The individual with the maximal phenotype in the population is traced. It sometimes goes and comes across the particular phenotype criterion value after each SGA operation. The criterion is 1/3 for (a), and 14/30 for (b). For the parameters in this simulation, the individuals in $1/3 \le x \le 14/30$ disappear by the selections. Hence we focus on (b) to elucidate the contributions of GA operations to the transition into the stable state. The number of goings or comings in a run is counted until the transition occurs, and then averaged over 100 runs. g and c represent 'going' and 'coming', respectively. Paremeter values are L = 30, N = 20, $p_m = 0.012$ and d = 0.5.

5.3 Variance of phenotype

Since the population variance s_X^2 is the sample variance corresponding to the ensemble variance V(X), the sampling of s_X^2 has the distribution with mean $E(s_X^2) = V(X)$ and variance $V(s_X^2) = 2(V(X))^2/(N-1)$, in which $V(s_X^2)$ represents the sampling perturbation [10].

The selection makes V(X) decrease according to the relative gradient of f, $(\partial f/\partial x)/\bar{f}$. As the relative gradient of f decreases, the selection force decreases and V(X) increases. However the increment is small relative to the change of $\log f$ as shown in figure 6 and this supports the assumption for equation (15).

As the population size N increases, the diversity of genotypes within the population increases but it does not directly mean that the phenotype variance increases. Instead, figure 7 shows two things that, as N increases, the increment of V(X) is negligibly small compared with the linear increment, and the amplitude of sampling perturbations of s_X^2 decreases as predicted above. The first supports the assumption that V^s is approximately independent of N. The second means that, as N increases, the effect of increasing V(X) could be dominated by that of decreasing $V(s_X^2)$ in the small range of N.

6 Conclusion and future work

In this paper, we have analyzed the dynamics of the SGA to get a differential equation about the population mean of phenotype values. It is divided into the Brownian part and non-Brownian part by the central limit theorem, as shown in equation (6). Detailing the equation, we have considered selections and mutations except the crossover for the simplicity, and the result is equation (16).

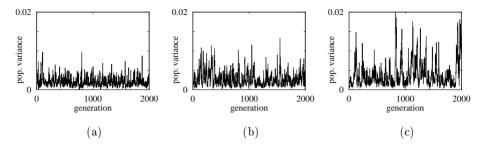


Fig. 6. The population variance s_X^2 of phenotype at each generation. Parameter values are N=20, $p_c=0$ and $p_m=0.01$ except that d=0 and d=0.5 for (a) and (b) respectively. The fitness function of (c) is the same as that of (b) except that the gradient is increased to 1500 on x>1/3. The population goes into the stable area after several generations in these cases, where the gradients are 0, 1.5 and 1500 for (a), (b) and (c), respectively.

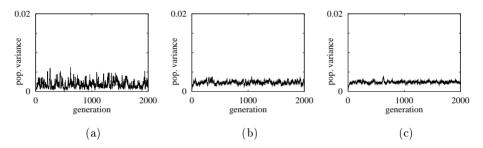


Fig. 7. The population variance s_X^2 of phenotype at each generation. Parameter values are $p_c = 0$, $p_m = 0.005$ and d = 0.5, except that N = 40, N = 400, and N = 1600 for (a), (b) and (c), respectively.

The non-Brownian part is the dynamics of the ensemble mean of phenotype values and has been analyzed adopting the method of the CE. The effect of roulette wheel selections is proportional to the population variance and the logarithm of the fitness function in condition of equation (12). The effects of mutations and crossovers are dependent on how the genotype is decoded into the phenotype, and then into the fitness. When the phenotype is defined as x = l/L, the effect of simple mutations is proportional to the mutation probability and $(1/2 - \bar{x})$.

For the equation (16) has the typical form which has been analyzed in diffusion processes, we can adopt the theoretical results from them. That is, running the SGA on the bistable global fitness landscape F which is defined as equation (15), (i) the punctuated equilibrium appears, (ii) the duration time of metastability is exponential as shown in equation (17), and (iii) the transition is unidirectional. These theoretical results are qualitatively confirmed by the simulation

results.

These results about the duration time could be expanded to the cases that F has more than two peaks or x is multidimensional [7, 2].

Though this paper shows some interesting results, it has some defects to be supplemented. The major one is that the effect of crossovers is just roughly analyzed. When the phenotype is defined as x = l/L, 1-point crossovers make the duration of metastability be longer. The next one is that, we have regarded the variance of the phenotype V(X) to be constant, on a basis of simulation results. For the more accurate analysis, the relation between V(X) and GA parameters such as the population size and the gradient of the fitness landscape should be examined.

Since GAs have direct relations with CEs, the results obtained from the studies of CEs could be applied to GAs. These include the issues about time delay, cooperation, competition, chaos, and so on [6, 4]

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