

Application of Eigen's Evolution Model to Infinite Population Genetic Algorithms with Selection and Mutation

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Abstract. Eigen's model for the molecular evolution of self-replicating macromolecules is used to develop a method for predicting the distribution of alleles in the framework of infinite population genetic algorithms (GAs) with selection and mutation. A set of ordinary differential equations which take into account selection and mutation is derived and applied to GAs. By calculating the spectrum of a matrix appearing in the equations, the method makes it possible to obtain the distribution of alleles. It is shown that eigenvectors of the matrix which includes only mutation are Walsh monomials. Some approximate expressions for the asymptotic behavior of GAs with small mutation rates are also presented.

1. Introduction

Genetic algorithms (GAs) are a class of algorithms based on biological evolution. In recent years, they are becoming more and more important in machine learning and nonlinear optimization. However, in spite of the fact that mathematical properties of GAs have long been investigated since the pioneering work of Holland [1], the mechanisms of evolution in GAs are still not well understood.

In this paper, we present a mathematical model for describing the time rate of changes of relative frequencies of strings in GAs. For this purpose, we employ a theory originally developed by Eigen and his colleagues [2, 3]. They proposed a system of ordinary differential equations (ODEs) which describe the rate of population changes of self-replicative macromolecules, such as RNA or DNA, for the investigation of the origin and evolution of life. Each equation contains a term which keeps the total population size constant. In the analysis of their ODEs, they conceived a notion of “quasi-species” which is defined as a distribution of species dominated by one or several sequences. As a result, Eigen's theory is sometimes called the quasi-species theory.

In population genetics, Eigen's theory corresponds to a multilocus model of asexually reproducing haploid organisms. Higgs pointed out the relationship between Eigen's theory and haploid models, and derived the stationary distributions of populations in some fitness landscapes [4]. Wiehe, Baake, and Schuster investigated two (coupled and decoupled) versions of selection-mutation equations for diploid organisms [5]. They obtained these equations by modifying the ODEs of Eigen. In their study they also gave the equations for haploid organisms. We employ the coupled version of their haploid equations to describe the time dependence of allele frequencies.

In section 2, the system of ODEs is presented for the time-dependent description of the allele frequencies in GAs. An explicit form of a selection-mutation matrix which appears in the system is given, and a procedure for solving the equations is presented. We show that eigenvectors of the mutation matrix are Walsh monomials. In section 3, we give several formulae for small mutation rates obtained using two approximations: the neglect of back mutations and perturbation theory. We apply them to three examples of fitness landscapes. Comparisons between Eigen's theory and GA experiments by numerical calculations are presented in section 4. Finally in section 5, we present a discussion of the results.

2. Selection-mutation model

In this section, we present a system of ODEs for simulating time-dependent behavior of GAs. We also describe a method to solve this system. If the fitness value of each allele is a function of Hamming distance from the fittest allele, we can derive a simplified form of ODEs (Hamming class formalism).

2.1 Equations of evolution

We consider an infinitely large population reproducing with selection and mutation, but neglect crossover. We adopt a single-locus multiple-allele model; that is, binary strings of length l are treated as one gene having $n = 2^l$ alleles. Let $x_i(t)$ be the relative frequency of the i th allele B_i at generation t , which satisfies the normalization condition

$$\sum_{i=0}^{n-1} x_i(t) = 1. \quad (2.1)$$

The selection procedure is the proportional selection used in the "simple genetic algorithm" by Goldberg [6]. We start with a system of ODEs for describing evolutionary behavior of GAs,

$$\frac{dx_i(t)}{dt} = \frac{\sum_{j=0}^{n-1} A_{ij}x_j(t)}{f(t)} - x_i(t) \quad (i = 0, \dots, n-1), \quad (2.2)$$

$$\bar{f}(t) = \sum_{i=0}^{n-1} f_i x_i(t), \quad (2.3)$$

where f_i is the fitness of the i th allele and $\bar{f}(t)$ stands for the average fitness of a population at generation t . Here, A_{ij} is an element of selection-mutation matrix A which represents the combined effect of selection and mutation. The matrix A can be decomposed into two parts, matrices F and M , which represent the effects of selection and mutation, respectively. The selection matrix F is a diagonal matrix whose i th diagonal element is f_i . We assume that all fitness values are positive and are not time dependent. The selection-mutation matrix A is given by

$$A_{ij} = (MF)_{ij} = M_{ij}f_j. \quad (2.4)$$

Here, M is the mutation matrix whose element M_{ij} stands for the probability of mutation from allele B_j to allele B_i per generation and satisfies the condition $\sum_i M_{ij} = 1$. We assume that strings are reproduced with mutation rate p per bit per generation. Then the mutation matrix M is described as

$$M_{ij} = (1 - p)^{l-d(i,j)} p^{d(i,j)}, \quad (2.5)$$

where $d(i, j)$ denotes the Hamming distance between alleles B_i and B_j .

By rescaling the time axis

$$\tau = \int_0^t \frac{1}{\bar{f}(t')} dt',$$

the system of ODEs in equation (2.2) can be transformed to Eigen's evolution equation [5],

$$\frac{dx_i(\tau)}{d\tau} = \sum_{j=0}^{n-1} A_{ij}x_j(\tau) - x_i(\tau)\bar{f}(\tau), \quad (i = 0, \dots, n-1). \quad (2.6)$$

Since the right-hand side of equation (2.6) contains the second order term in x , this equation is nonlinear. However, it is shown by Thompson and McBride [8] and independently by Jones, Enns, and Rangnekar [9] that a transformation

$$x_i(\tau) = y_i(\tau) \exp \left(- \int^\tau \bar{f}(t') dt' \right) \quad (2.7)$$

takes the nonlinear equation into the linear equation

$$\frac{dy_i(\tau)}{d\tau} = \sum_{j=0}^{n-1} A_{ij}y_j(\tau). \quad (2.8)$$

We can easily solve this system by calculating the spectrum of A . However, it should be noted that the solution of the transformed system does not satisfy the normalization condition, equation (2.1). But the solution of the original system can be obtained by a transformation [9]

$$x_i(\tau) = y_i(\tau) / \sum_{j=0}^{n-1} y_j(\tau). \quad (2.9)$$

If mutation is absent; that is, $p = 0$, equation (2.2) becomes

$$\frac{dx_i(t)}{dt} = \frac{f_i x_i}{f} - x_i, \quad (2.10)$$

and the solution is given by

$$x_i(\tau) = a_i \exp(f_i \tau) / \sum_{j=0}^{n-1} a_j \exp(f_j \tau), \quad (2.11)$$

where constants a_j are determined by the initial distribution of alleles in the population. If only one allele has the maximum fitness value, the stationary solution at $t \rightarrow \infty$ is given by

$$x_i = \begin{cases} 1 & i = 0 \\ 0 & \text{otherwise,} \end{cases} \quad (2.12)$$

where $i = 0$ denotes the allele of the highest fitness.

In the case of no selection ($f_0 = \dots = f_{n-1} = 1$), the system is solely determined by mutation,

$$\frac{dy_i(\tau)}{d\tau} = \sum_{j=0}^{n-1} M_{ij} y_j. \quad (2.13)$$

Since all elements M_{ij} do not depend on time, we can get the solution by calculating eigenvalues and the corresponding eigenvectors of M . Rumschitzki developed a method to calculate eigenvalues and eigenvectors of matrices appearing in Eigen's systems [10]. By using the procedure of Rumschitzki described in Appendix A, we can obtain the eigenvalues of M ,

$$(1 - 2p)^k \quad \text{with multiplicity} \quad \binom{l}{k}, \quad (k = 0, \dots, l). \quad (2.14)$$

It is also shown in Appendix A that the eigenvectors of M are the Walsh monomials, which have been widely used in the GA literature (e.g., [11]).

In the model including selection and mutation, it seems very difficult to obtain the explicit expression for the spectrum of the selection-mutation matrix A . Here, we describe some results concerning the properties of the eigenvalues of A . In Appendix B, we show that all eigenvalues of A are real if all fitness values are positive. It is also verified that the largest eigenvalue is nondegenerate and positive.

2.2 Hamming class formalism

In GA applications, we frequently encounter a case where fitness values of alleles depend only on their Hamming distances from an optimum allele. In such a case the system of evolution equations can be reduced to a considerably smaller size. We treat alleles having the same Hamming distance i from the optimum allele as one group and call them Γ_i ($i = 0, \dots, l$). It may

be reasonable to assume that, when the solution approaches a stationary distribution, alleles within the same Hamming class distribute uniformly. Then the evolution equations are reduced to

$$\frac{dz_i(t)}{dt} = \frac{\sum_{j=0}^l A_{ij}^H z_j(t)}{\bar{f}(t)} - z_i(t), \quad (i = 0, \dots, l), \quad (2.15)$$

where z_i denotes the relative frequency of Γ_i . The selection-mutation matrix in the Hamming class formalism is given by

$$A_{ij}^H = M_{ij}^H f_j^H, \quad (2.16)$$

where f_j^H stands for the fitness value of allele(s) within Γ_j . An element of M^H representing the collective effect of mutations from Γ_j to Γ_i is

$$M_{ij}^H = \sum_{k=\text{kmin}}^{\text{kmax}} \binom{j}{k} \binom{l-j}{i-k} (1-p)^{l-i-j+2k} p^{i+j-2k}, \quad (2.17)$$

where $\text{kmin} = \max(0, i+j-l)$, and $\text{kmax} = \min(i, j)$ [5]. The mutation matrix M^H is no longer symmetric, but still satisfies the condition $\sum_i M_{ij}^H = 1$.

3. Approximation for weak mutation

In this section, we present theoretical results applicable to systems evolving with small p . First, we develop approximation methods for calculating a stationary distribution of alleles by neglecting terms corresponding to “back mutations” in equation (2.2). Second, we describe the results of the perturbation theory that can express a stationary distribution of alleles in the power series of p . The obtained formulae are applied to three fitness landscape examples.

3.1 Neglect of back mutations

We follow the approach of Higgs who applied the quasi-species theory to population genetics [4]. His theory of a haploid organism reproducing asexually is a powerful tool for analyzing the behavior of GAs. We assume a fitness landscape depending only on Hamming distances from an optimum allele and apply the Hamming class formalism. If the mutation rate p is small and the length l of strings is sufficiently large, we may neglect back mutations, which are mutations from Γ_j to Γ_i with $i < j$. This approximation is valid only for small j . In the case of large j , the frequency z_j may be negligibly small in the total system and we can also ignore back mutations. With this approximation, the mutation matrix M^H is approximately given by retaining the term of the lowest power in p , $k = \text{kmax} = \min(i, j) = j$, in the summation of equation (2.17),

$$M_{ij}^H = \binom{l-j}{i-j} (1-p)^{l-i+j} p^{i-j}, \quad (0 \leq j \leq i \leq l), \quad (3.1)$$

and otherwise M_{ij}^H is zero. Here we used the fact that matrix elements corresponding to back mutations ($i < j$)

$$M_{ij}^H = \binom{j}{i} (1-p)^{l+i-j} p^{j-i}$$

are smaller than the elements given by equation (3.1) for large l and small j . Then the equations in the Hamming class formalism take the simple form

$$\frac{dz_i(t)}{dt} = \sum_{j=0}^i \binom{l-j}{i-j} (1-p)^{l-i+j} p^{i-j} f_j^H z_j(t) / \bar{f}(t) - z_i(t). \quad (3.2)$$

We introduce a variable $U = lp$ which may be more appropriate than p for describing the effect of weak mutation. The new value U stands for the mutation rate per string per generation. Since we assumed large l and small p , the mutation matrix approximately takes the form of a Poisson distribution

$$M_{ij}^H = \frac{U^{i-j}}{(i-j)!} \exp(-U), \quad (i \geq j). \quad (3.3)$$

At equilibrium, in which $dz_i/dt = 0$, we have these relations among allele frequencies:

$$z_i = \sum_{j=0}^i \binom{l-j}{i-j} (1-p)^{l-i+j} p^{i-j} f_j^H z_j / \sum_{j=0}^l f_j^H z_j \quad (3.4)$$

$$\simeq \sum_{j=0}^i \frac{U^{i-j}}{(i-j)!} \exp(-U) f_j^H z_j / \bar{f}. \quad (3.5)$$

By setting $i = 0$ in equation (3.5), we have a very interesting relation

$$\bar{f} = f_0^H \exp(-U) = f_0^H \exp(-lp). \quad (3.6)$$

This result for the mean fitness was already noted by Kimura and Maruyama [12] in their analysis of the mutational load $(f_0^H - \bar{f})/\bar{f}$. The important point is that the above relation is quite general, imposing no restriction on the form of fitness landscape.

Now we consider two special examples of fitness landscapes. One is the multiplicative landscape defined by

$$f_i^H = (1-r)^i \quad (0 < r < 1). \quad (3.7)$$

If we take the limit $l \rightarrow \infty$, we can obtain the stationary distribution for this landscape by using equation (3.5)

$$z_i = \frac{(U/r)^i}{i!} \exp\left(-\frac{U}{r}\right), \quad (3.8)$$

which was given by Haigh [13]. On the other hand, Higgs gave an approximate solution for finite string length l by using equation (3.4) [4]

$$\bar{f} = (1 - p)^l, \quad (3.9)$$

$$z_i = \binom{l}{i} (1 - p/r)^{l-i} (p/r)^i, \quad (3.10)$$

where the following identity was used

$$\binom{l-j}{i-j} \binom{l}{j} = \binom{l}{i} \binom{i}{j}.$$

It can be noted that the stationary distribution of alleles becomes a binomial distribution determined by only one parameter p/r . This result also suggests that each bit behaves independently of other bits in the multiplicative landscape.

Another example of landscape is the single-peaked landscape defined by

$$f_i^H = \begin{cases} 1 & (i = 0) \\ 1 - r & (\text{otherwise}). \end{cases} \quad (3.11)$$

Only one allele has a high fitness, and all other alleles have a lower fitness ($0 < r < 1$). This landscape has been studied intensively by Eigen and other researchers because of the interesting behavior observed in the solution [3, 5]. An approximate solution for this landscape was also given by Higgs [4]

$$\begin{aligned} z_0 &= 1 - lp/r, \\ z_i &= (lp/r)^i (1 - lp/r) \quad (i \geq 1), \end{aligned} \quad (3.12)$$

where $lp \ll 1$ and $r \ll 1$ are assumed.

3.2 Application of the perturbation theory

To obtain the stationary distribution of alleles, we have to carry out the diagonalization of matrix A in equation (2.8). However, in the case of weak mutation, we have an approximation method to calculate the relative frequencies of alleles by using the perturbation theory [14]. This method has wide applicability and does not assume a special form of fitness landscapes.

The selection-mutation matrix A is divided into two parts, $A^{(0)}$ and Φ . The unperturbed part $A^{(0)}$ is a diagonal matrix whose i th diagonal element is $\lambda_i \equiv A_{ii}^{(0)} = A_{ii}$. We assume that the remaining part $\Phi = \{\phi_{ij}\} = A - A^{(0)}$ is small enough, so we treat it as a perturbation on $A^{(0)}$. Note that $\phi_{ij} = A_{ij}$ for $i \neq j$ and $\phi_{ii} = 0$. We also assume that λ_0 , the maximum eigenvalue of $A^{(0)}$, is not degenerate. This means the uniqueness of an optimum allele. The procedure giving an approximate stationary distribution of alleles is described in Appendix C. We show here the results of the second-order perturbation

approximation. The approximate solution for equation (2.8) at $t \rightarrow \infty$ is given as the power series expansion in ϕ

$$y_0 = 1, \quad (3.13)$$

$$y_i \simeq \frac{\phi_{i0}}{\lambda_0 - \lambda_i} + \sum_j' \frac{\phi_{ij}\phi_{j0}}{(\lambda_0 - \lambda_i)(\lambda_0 - \lambda_j)}, \quad (i \geq 1), \quad (3.14)$$

where the prime on \sum_j' denotes the omission of the term $j = 0$.

By substituting the expressions for $\lambda_i = A_{ii}$ and $\phi_{ij} = A_{ij}$ from equations (2.4) and (2.5) into equation (3.14), we can obtain the approximate solution for y_i . We will calculate y_i to second order in p . When the allele i is a member of Hamming class k , we can write the first term in equation (3.14) as

$$\frac{\phi_{i0}}{\lambda_0 - \lambda_i} = \frac{f_0}{f_0 - f_i} p^k (1 - p)^{-k} \simeq \frac{f_0}{f_0 - f_i} (p + p^2)^k, \quad (i \in \Gamma_k). \quad (3.15)$$

This term represents the one-step mutation process from the optimum allele to a mutant allele with k point mutations. Since this calculation is restricted to second order in p , only y_i with $i \in \{\Gamma_1, \Gamma_2\}$ have nonzero terms in equation (3.15). The second term in equation (3.14) contains the quantities $\phi_{ij}\phi_{j0}$ in the summation. This term represents the process of two-step mutation $0 \rightarrow j \rightarrow i$. For ϕ_{ij} , it should be noted that $\phi_{ii} = 0$ and that $\phi_{ij} = o(p^2)$ or higher order in p when both i and j are members of the same Hamming class. Within the approximation to second order in p , the only remaining terms in the summation in equation (3.14) are those of $j \in \Gamma_1$ and $i \in \Gamma_2$. Furthermore, if we fix the subscript i , corresponding to an allele with two point mutations, only two terms within the summation of j remain in the calculation. Each term corresponds to an allele having one point mutation at either of the two point mutations in the allele i .

The results for y_i are summarized as follows:

$$\begin{aligned} y_i &\simeq \frac{f_0}{f_0 - f_i} (p + p^2) = F_i p + F_i p^2, & (i \in \Gamma_1) \\ y_i &\simeq \frac{f_0}{f_0 - f_i} \left(1 + \sum_j'' \frac{f_j}{f_0 - f_j} \right) p^2 = F_i (1 + G) p^2, & (i \in \Gamma_2), \end{aligned} \quad (3.16)$$

where we have used the abbreviations

$$F_i = \frac{f_0}{f_0 - f_i}, \quad G = \sum_j'' \frac{f_j}{f_0 - f_j}.$$

Here \sum_j'' stands for the summation of the above mentioned two terms in Γ_1 . By using the approximation for small p , $1/(1+ap+bp^2) \simeq 1-ap-bp^2+a^2p^2$, we obtain

$$x_0 = \frac{y_0}{\sum_i y_i} \simeq 1 - F^{(1)} p + \{F^{(1)}\}^2 p^2 - F^{(1)} p^2 - F^{(2)} (1 + G) p^2, \quad (3.17)$$

where

$$F^{(1)} = \sum_{j \in \Gamma_1} F_j, \quad F^{(2)} = \sum_{j \in \Gamma_2} F_j.$$

We also obtain the relations

$$\begin{aligned} x_i &\simeq F_i p + F_i(1 - F^{(1)})p^2, & (i \in \Gamma_1), \\ x_i &\simeq F_i(1 + G)p^2, & (i \in \Gamma_2). \end{aligned} \quad (3.18)$$

3.3 Perturbation expansion in Hamming class formalism

When we apply the perturbation theory to GAs in the Hamming class formalism, we derive

$$\begin{aligned} z_0 &= 1 - g_1 lp + g_1^2 l^2 p^2 - g_1 lp^2 - g_2 \left(h_1 + \frac{1}{2} \right) l(l-1)p^2, \\ z_1 &= g_1 lp - g_1^2 l^2 p^2 + g_1 lp^2, \\ z_2 &= g_2 \left(h_1 + \frac{1}{2} \right) l(l-1)p^2, \end{aligned} \quad (3.19)$$

where

$$g_1 = \frac{f_0^H}{f_0^H - f_1^H}, \quad g_2 = \frac{f_0^H}{f_0^H - f_2^H}, \quad h_1 = \frac{f_1^H}{f_0^H - f_1^H}.$$

In this section we present the formulae obtained by the perturbation theory for the following three examples of fitness landscapes.

1. Additive landscape: $f_i^H = l - i$.
2. Multiplicative landscape: $f_i^H = (1 - r)^i$.
3. Single-peaked landscape: $f_0^H = 1$, $f_i^H = 1 - r \quad (i \geq 1)$.

The additive landscape defined here is essentially the same as that used in the “counting ones” problem. Though this landscape includes an allele of zero fitness value, it is straightforward to extend the results of Appendix B to this case.

The stationary distributions for these landscapes can easily be obtained. For the additive landscape we get

$$\begin{aligned} z_0 &= 1 - lU + \frac{1}{4}(2l + 5)(l-1)U^2, \\ z_1 &= lU - (l^2 - 1)U^2, \quad z_2 = \frac{1}{4}(2l - 1)(l-1)U^2, \end{aligned} \quad (3.20)$$

where $U = lp$.

For the multiplicative landscape we obtain

$$\begin{aligned} z_0 &= 1 - lu + \frac{1}{2}(l - 2r + 1)lu^2, \\ z_1 &= lu + (r - l)lu^2, \quad z_2 = \frac{1}{2}l(l-1)u^2, \end{aligned} \quad (3.21)$$

where we define $u = p/r$. For large l we get

$$z_0 = 1 - lu + l^2 u^2 / 2, \quad z_1 = lu - l^2 u^2, \quad z_2 = l^2 u^2 / 2.$$

For the single-peaked landscape we obtain

$$\begin{aligned} z_0 &= 1 - lu + \frac{1}{2}(rl - 3r + 2)lu^2, \\ z_1 &= lu + (r - l)lu^2, \quad z_2 = \frac{2 - r}{2}l(l - 1)u^2, \end{aligned} \quad (3.22)$$

where $u = p/r$. For large $l \gg 1$ but small $r \ll 1$

$$z_0 = 1 - lu, \quad z_1 = lu - l^2 u^2, \quad z_2 = l^2 u^2.$$

4. Numerical calculations

Here we compare the theoretical results derived in the previous sections with GA calculations. The GAs on the additive, multiplicative, and single-peaked fitness landscapes were used as examples. Figure 1 demonstrates the time dependence of the relative frequencies in three fitness landscapes with string length $l = 3$. A population size of $N = 1024$ and mutation rate $p = 0.1$ were used in the GAs. All calculations started at generation $t = 0$ with the uniform initial distribution $x_i(0) = 1/2^l$. It can be seen that Eigen's model performs very close to GA calculations in all cases.

Figure 2 shows the results of the theoretical prediction and actual GA calculations with string length $l = 8$ on the three landscapes. The theoretical calculations were performed using ODEs in the Hamming class formalism equation (2.15). We used a population size $N = 4096$ and mutation rate $p = 0.01$. Though there are noticeable discrepancies between theoretical and GA calculations in the transient regions, both calculations agree very well in the stationary regions.

Figure 3 shows the theoretical results for the mutation rate dependence of the stationary distributions of Hamming classes with $l = 8$ in the three landscapes. The calculations were performed in the Hamming class formalism. There is a close resemblance between the distributions in the additive and multiplicative landscapes, but that in the single-peaked landscape is quite different from the others. As the mutation rate p increases in the additive and multiplicative landscapes, the frequency of the fittest class Γ_0 decreases very rapidly, and alternatively Γ_1 appears as the main component. With the further increase of p , Γ_2 becomes dominant instead of Γ_1 , and in this way the next Hamming class occupies the main part in the population one after another. The distribution in the single-peaked landscape exhibits striking contrast to other landscapes. We observe a phase-transition-like behavior around $p = 0.04$. Below this critical p , the distribution behaves in the same manner as those of other landscapes, but it changes drastically above this point, where all alleles are distributed uniformly in the population. This critical $p = p_c$ is called the *error threshold*. For more detailed discussions, see [5, 7, 15].

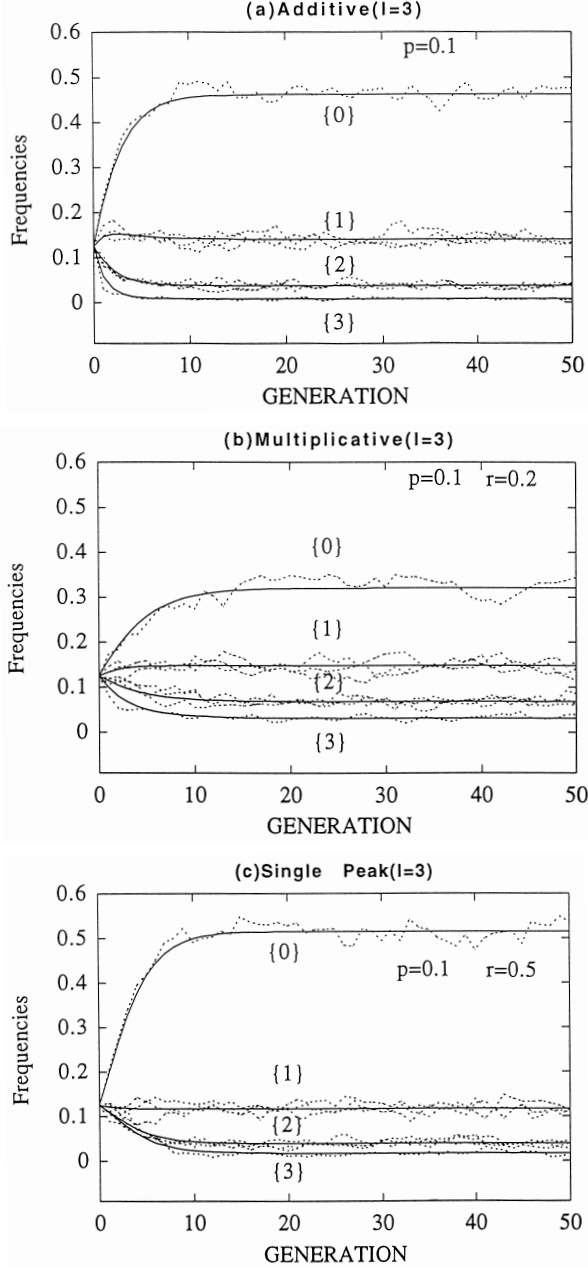


Figure 1: Evolution of population distributions in GAs on three fitness landscapes; (a) additive, (b) multiplicative, and (c) single-peaked. Solid lines are the results of Eigen's evolution model and dotted lines show GA calculations. The symbol $\{i\}$ stands for the strings in the Hamming class i . For example, $\{0\} = \{000\}$, $\{1\} = \{001, 010, 100\}$ and so on.

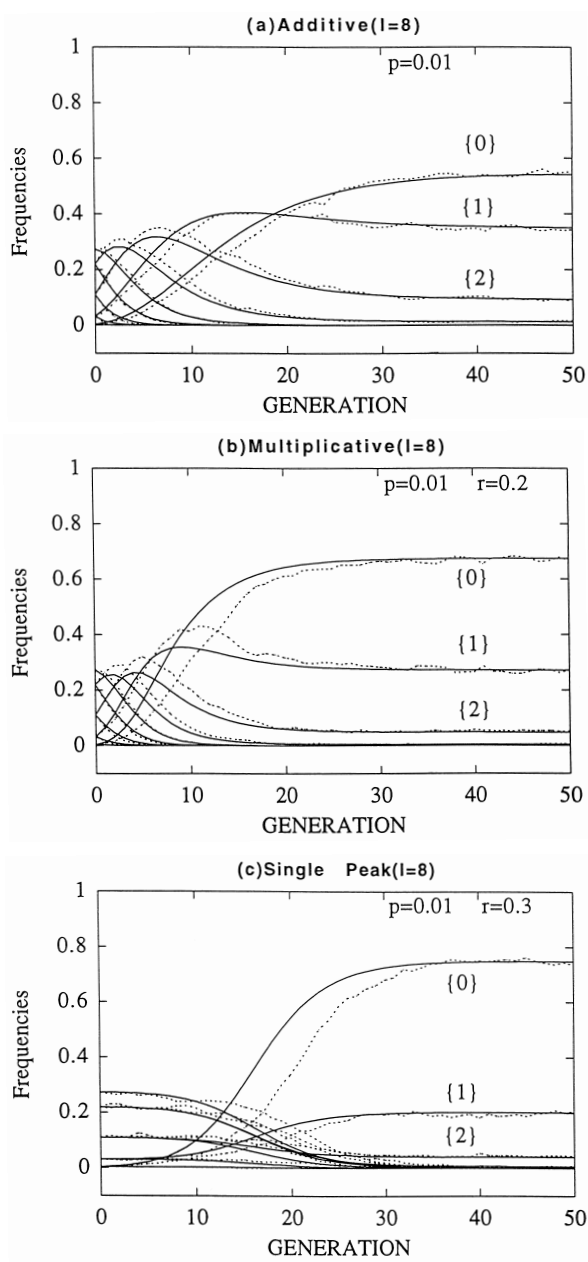


Figure 2: Evolution of population distributions as in Figure 1.

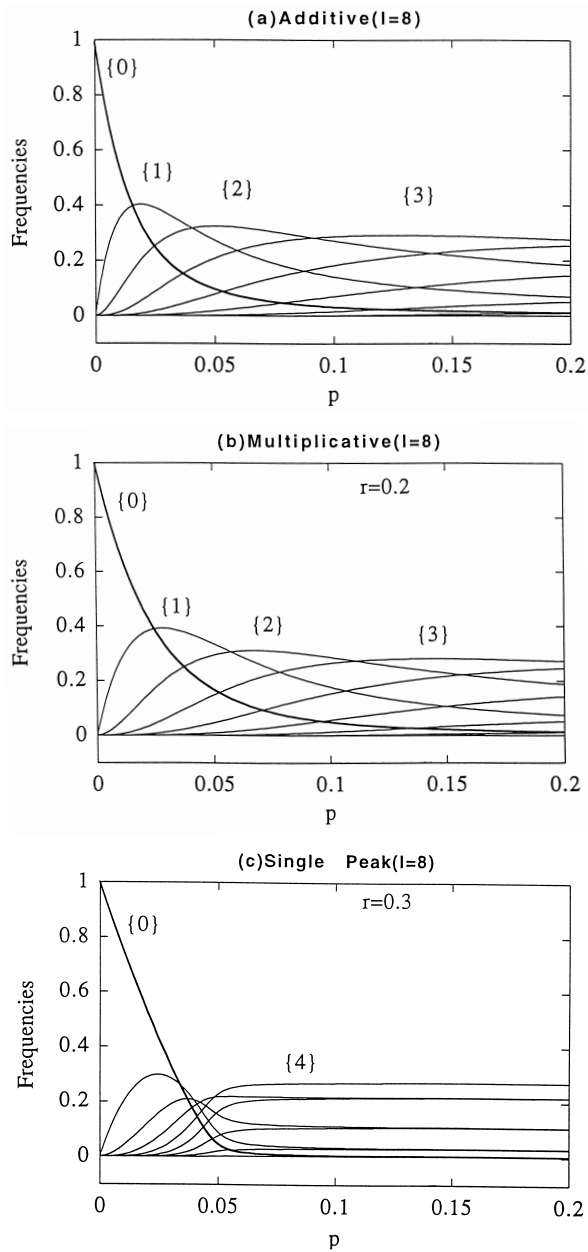


Figure 3: Mutation rate dependence of the stationary distributions of Hamming classes in three landscapes.

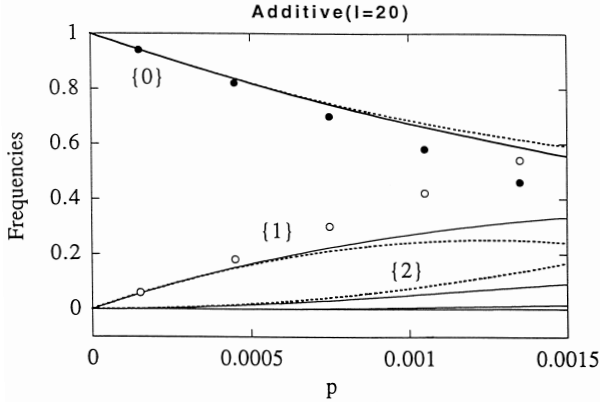


Figure 4: Perturbation approximation in the additive landscape. Solid lines for the exact calculation, dotted lines for the second-order perturbation, and symbols \bullet and \circ for the first-order perturbation.

In Figure 4, a comparison of the perturbation approximation with the exact solution is presented for the stationary distribution of the additive landscape with string length $l = 20$. It should be noted that the stationary distribution of this landscape has a particular l dependence. As we have already derived in equations (3.20) through (3.22), the relative frequency z_0 is approximately given by $1 - l^2 p + o(p^2)$ in the additive landscape and by $1 - lp/r + o(p^2)$ in other landscapes. The additive landscape has an l^2 dependence in the first order of p while other landscapes have an l dependence. Therefore this fact suggests that we should choose smaller p for the additive landscape than values used for other landscapes.

Figure 5 shows a comparison among the exact solution, an approximation based on the neglect of back mutations, and the second-order perturbation theory for the stationary distribution of the multiplicative landscape with $l = 20$. When z_0 decreases to 0.7 with increasing p , the results of the second-order perturbation begin to deviate rapidly from the exact solution as in Figure 4. On the other hand, the approximation obtained by neglecting back mutations gives a surprisingly good agreement with the exact solution. This fact may suggest that there is a deeper relationship between this approximation and the exact solution.

In Figure 6, a comparison of two approximations with the exact solution is presented for the single-peaked landscape with $l = 20$. While the exact solution and the perturbation calculations are virtually identical for z_0 , the second-order perturbation calculation deviates remarkably from the exact one for z_2 in large p . Though the agreement is not complete, the approximation neglecting back mutations also reproduces the exact solution.

Figure 7 shows the results of three calculations of the average fitness in the multiplicative landscape with $l = 20$. The solid line shows the exact solution, the dotted line represents the approximation (3.6) $\bar{f} = \exp(-lp)$,

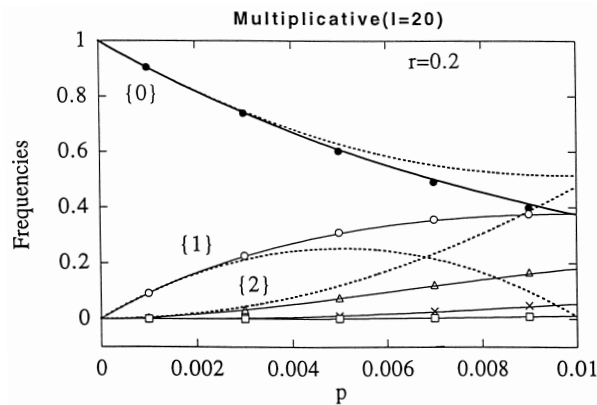


Figure 5: Comparison of approximations with the exact solution in the multiplicative landscape. Solid lines for the exact calculation; dotted lines for the second-order perturbation; and symbols •, ○, and □ for the approximation by neglecting back mutations.

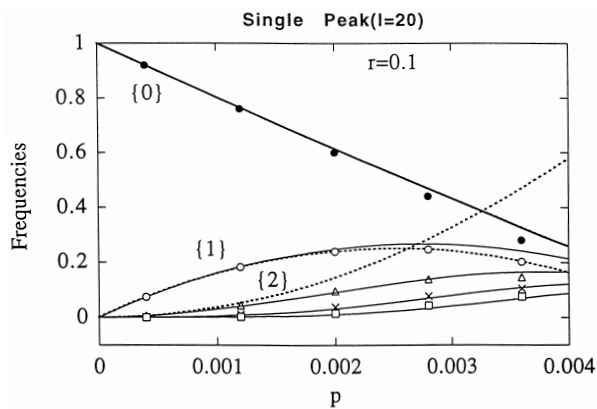


Figure 6: Comparison of two approximations with the exact solution in the single-peaked landscape as in Figure 5.

and the symbol ○ shows another approximation (3.9) $\bar{f} = (1 - p)^l$. The two approximations are virtually identical, and agree very well with the exact average fitness.

5. Discussion

In this paper the use of Eigen's theory for understanding the behavior of allele frequencies in GAs has been studied. The system of ODEs with the selection-mutation matrix A excellently reproduced the GA experiments of a large population size. It can be seen from equations (2.2) and (2.4) that

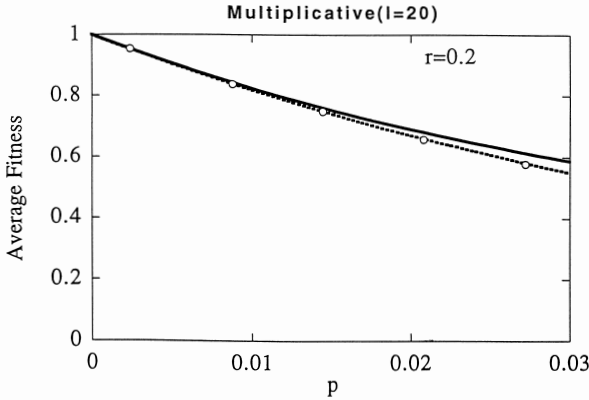


Figure 7: Comparison of two approximations with the exact solution for the average fitness in the multiplicative landscape.

the allele frequencies are determined by the combined effect of selection and mutation. Therefore it is essential to obtain the spectrum of the matrix A for predicting GA behavior. In particular, the stationary distribution of alleles is completely determined by the eigenvector corresponding to the maximum eigenvalue of this matrix. Therefore it will become a powerful tool if an analytic procedure can be found to calculate the eigenvectors and eigenvalues of A in its general form. It seems, however, very difficult to derive explicit expressions for them. Rumschitzki tried to derive a full solution for matrix A [10]. He calculated the eigenvalues of A in the single-peaked landscape with $l = 2$ using the REDUCE system. The obtained solution has a very complicated form and, therefore, he concluded that it may not be possible to solve the general case exactly. Thus the spectrum of the matrix A can usually only be obtained by numerical methods.

The GA model of this paper, based on Eigen's theory, is a deterministic one which assumes an infinitely large population and neglects the effect of genetic drift caused by random sampling. Since all practical GAs use small populations, it is inevitable to extend the present theory to the stochastic one. The relation between the deterministic and stochastic theories in GAs has been discussed in [16] and references therein. The stochastic approach based on Eigen's model has been attempted by Nowak and Schuster [15]. They obtained an expression for the population size dependence of the error threshold in the single-peaked landscape. However, their theory is still not satisfactory enough to be used in GAs.

There are two instructive examples thoroughly investigated in population genetics. Both examples use a two-allele model of one-bit strings denoted by alleles a and a' with finite population size N . One is a system without selection and mutation, the other is a system including mutation. Kimura's diffusion model [17] makes it possible to calculate the probability density

$\phi(x, t)$ of the relative frequency x at generation t of allele a . The probability density function $\phi(x, t)$ is obtained by solving a Fokker–Planck equation with the initial condition $\phi(x, 0) = \delta(x - x_0)$, where δ is the Dirac delta function.

When there is no selection and mutation, only genetic drift is present. The function ϕ satisfies the Fokker–Planck equation,

$$\frac{\partial \phi}{\partial t} = \frac{1}{2N} \frac{\partial^2}{\partial x^2} \{x(1-x)\phi\}.$$

The solution of this equation has an interesting property. As the number of generations increases, ϕ is approximately given by

$$\phi(x, t) \sim 6x_0(1-x_0) \exp(-t/N), \quad (0 < x < 1).$$

Thus, when $t \rightarrow \infty$, ϕ approaches 0 in the region of $0 < x < 1$; both boundaries $x = 0$ and $x = 1$ act as absorbing barriers in this case. In this model, the mean value of x is not dependent on t and given by $x = x_0$. The infinite population model also gives the result that $x(t) = x_0$ at all t . This fact tells us that close attention should be paid when the results of an infinite population model are interpreted.

On the contrary, another example produces an optimistic result. When mutation is present in an infinite population system, the differential equation for describing $x(t)$ is $\dot{x} = -px + p(1-x)$, where \dot{x} stands for the time derivative of x . The solution of this equation is given by $x(t) = 1/2 + (x_0 - 1/2) \exp(-2pt)$, and approaches $1/2$ as $t \rightarrow \infty$. On the other hand, the diffusion model predicts the stationary distribution of x as [17]

$$\phi(x) \sim Cx^{2Np-1}(1-x)^{2Np-1} \quad (t \rightarrow \infty),$$

where C stands for the normalization constant. This distribution has a peak at $x = 1/2$ and becomes more and more like $\delta(x - 1/2)$ as N increases. Thus, in this example, the infinite population model is a good approximation to the stochastic approach. In any case, the development of the stochastic theory of Eigen's model may answer the question of what is the relation between finite and infinite population models in GAs.

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Appendix A. Spectrum of the mutation matrix

Let M_l be a mutation matrix for l -bit strings. In this appendix we added the subscript l to distinguish the length of strings. The mutation matrix M_1 plays the role of a building block and is given by

$$M_1 = \begin{pmatrix} s_0^1 & s_1^1 \\ s_0^1 & p \\ s_1^1 & 1-p \end{pmatrix},$$

where s_0^1 and s_1^1 denote one-bit strings 0 and 1, respectively. The eigenvalues of M_1 are 1 and $1 - 2p$, and corresponding eigenvectors can be represented by the Hadamard matrix

$$H_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

where the columns of H_1 give the eigenvectors.

If we have the mutation matrix M_{l-1} for $(l-1)$ -bit strings, we can recursively construct the mutation matrix M_l for l -bit strings. It is convenient to arrange l -bit strings in the order $0s_0, \dots, 0s_{m-1}, 1s_0, \dots, 1s_{m-1}$, where s_0, \dots, s_{m-2} , and s_{m-1} stand for the $m = 2^{l-1}$ $(l-1)$ -bit strings. This ordering is equivalent to that of the binary representation of unsigned integers in the ascending order. In this ordering, the matrix M_l is given by

$$M_l = \begin{pmatrix} (1-p)M_{l-1} & pM_{l-1} \\ pM_{l-1} & (1-p)M_{l-1} \end{pmatrix} = M_1 \otimes M_{l-1},$$

where \otimes stands for the Kronecker product.

Applying this equation repeatedly, we can easily show

$$M_l = \underbrace{M_1 \otimes M_1 \otimes \dots \otimes M_1}_l. \quad (\text{A.1})$$

In the same way, the eigenvalue matrix H_l is also represented by the Kronecker products of H_1

$$H_l = \underbrace{H_1 \otimes H_1 \otimes \dots \otimes H_1}_l, \quad (\text{A.2})$$

where each column vector of the Hadamard matrix H_l gives the eigenvector of M_l . The eigenvalues of M_l are also represented by using two eigenvalues of M_1 , 1 and $1 - 2p$. The terms appearing in the expansion

$$(1 + 1 - 2p)^l = \sum_{k=0}^l \binom{l}{k} (1 - 2p)^k$$

give the eigenvalues,

$$(1 - 2p)^k \text{ with multiplicity } \binom{l}{k}, \quad (k = 0, \dots, l). \quad (\text{A.3})$$

From this expression we can show that the maximum eigenvalue of M_l is 1 with multiplicity one.

The eigenvectors of the mutation matrix given by equation (A.2) can also be represented by the Walsh monomials. Here we may use the fact that one of the representations of the Walsh monomials is given by the Hadamard matrix. Let $s = x_l x_{l-1} \dots x_1$ be an l -bit string with each bit $x_i \in \{0, 1\}$ at position i . In the binary representation, an integer j ($0 \leq j \leq 2^l - 1$) is also

given by $j = j_l j_{l-1} \dots j_1$, where $j_i \in \{0, 1\}$. We define auxiliary variables $y_i \in \{1, -1\}$ by

$$x_i = \frac{1}{2}(1 - y_i), \quad (i = 1, \dots, l).$$

By using these definitions, we can calculate the $n = 2^l$ Walsh monomials

$$\psi_j(S_k) = \prod_{i=1}^l y_i^{j_i}, \quad (k = 0, \dots, n-1), \quad (\text{A.4})$$

where $S_k = y_l y_{l-1} \dots y_1$ stands for the k th auxiliary string. The ordering of the auxiliary strings S is the same as that of the corresponding l -bit strings s , which has been defined above. The j th eigenvector of the mutation matrix M_l is

$$\mathbf{v}_j = (\psi_j(S_0), \psi_j(S_1), \dots, \psi_j(S_{n-1}))^t, \quad (j = 0, \dots, n-1), \quad (\text{A.5})$$

where t denotes transpose. The eigenvector corresponding to the maximum eigenvalue 1 is given by $\mathbf{v}_0 = (1, 1, \dots, 1)^t$.

Appendix B. Spectrum of the selection-mutation matrix

In this appendix we show that the eigenvalues of the selection-mutation matrix $A = MF$ are all real and the maximum eigenvalue is nondegenerate and positive. We assume that fitness values f_i are all positive. Since elements of the matrix A are given by $A_{ij} = M_{ij} f_j$, they are all positive when $p \neq 0, 1$. The Perron–Frobenius theorem states that a matrix whose elements are all positive has a real and positive eigenvalue whose magnitude is greater than the magnitudes of other eigenvalues. It has also been shown that this eigenvalue is nondegenerate, and that one can choose all elements of the corresponding eigenvector to be nonnegative.

Furthermore, we can show that the eigenvalues of A are all real. We define a diagonal matrix $F^{1/2}$ such that $F_{jj}^{1/2} = f_j^{1/2}$. The eigenvalue equation which we have to solve is

$$A\mathbf{v}_j = W_j \mathbf{v}_j,$$

where W_j and \mathbf{v}_j are the j th eigenvalue and eigenvector of A , respectively. We rewrite this equation by multiplying the matrix $F^{1/2}$ from the left side:

$$F^{1/2} A \mathbf{v}_j = F^{1/2} M F^{1/2} (F^{1/2} \mathbf{v}_j) = W_j (F^{1/2} \mathbf{v}_j).$$

This is also an eigenvalue equation with the eigenvalue W_j and eigenvector $F^{1/2} \mathbf{v}_j$. Since the matrix $F^{1/2} M F^{1/2}$ is symmetric, we now know that eigenvalues W_j are all real.

Appendix C. Short review of the perturbation theory

We divide the $n \times n$ selection-mutation matrix A into the unperturbed part $A^{(0)}$ and its perturbation Φ , $A = A^{(0)} + \Phi$. The matrix $A^{(0)}$ is a diagonal matrix with $\lambda_i \equiv A_{ii}^{(0)} = A_{ii}$. The perturbation $\Phi = A - A^{(0)}$ has nondiagonal elements $\phi_{ij} = A_{ij}$, and its diagonal elements are $\phi_{ii} = 0$. We already know the eigenvalues and eigenvectors of $A^{(0)}$:

$$A^{(0)}\mathbf{u}_i = \lambda_i\mathbf{u}_i, \quad \mathbf{u}_i = (0, \dots, 0, 1, 0, \dots, 0)^t, \quad (i = 0, \dots, n-1),$$

where the i th element of the eigenvector \mathbf{u}_i is one, and other elements are all zero. It is easy to show that the set of the eigenvectors \mathbf{u}_i is the orthonormal basis, $\mathbf{u}_i^t \cdot \mathbf{u}_j = \delta_{ij}$, for the n -dimensional vector space.

Since our concerns are the maximum eigenvalue of A , denoted by W , and its corresponding eigenvector \mathbf{v} , we derive the perturbation expansions of them. We assume that the maximum eigenvalue of $A^{(0)}$ is λ_0 , and that its eigenvector \mathbf{u}_0 is nondegenerate. It is not necessary to assume the nondegeneracy of other eigenvectors \mathbf{u}_i ($i \geq 1$).

By introducing a parameter δ , we replace Φ by $\Phi\delta$. The parameter δ is set to one when the final results are obtained.

The eigenvalue W , eigenvector \mathbf{v} , and selection-mutation matrix are written

$$\begin{aligned} W &= W^{(0)} + W^{(1)}\delta + W^{(2)}\delta^2 + \dots, \\ \mathbf{v} &= \mathbf{v}^{(0)} + \mathbf{v}^{(1)}\delta + \mathbf{v}^{(2)}\delta^2 + \dots, \\ A &= A^{(0)} + \Phi\delta, \end{aligned} \tag{C.1}$$

and are substituted into the eigenvalue equation

$$A\mathbf{v} = W\mathbf{v}.$$

By comparing the coefficients of equal powers of δ on both sides, we can obtain a set of equations:

$$\begin{aligned} (A^{(0)} - W^{(0)})\mathbf{v}^{(0)} &= 0, \\ (A^{(0)} - W^{(0)})\mathbf{v}^{(1)} &= (W^{(1)} - \Phi)\mathbf{v}^{(0)}, \\ (A^{(0)} - W^{(0)})\mathbf{v}^{(2)} &= (W^{(1)} - \Phi)\mathbf{v}^{(1)} + W^{(2)}\mathbf{v}^{(0)}, \quad \text{etc.} \end{aligned} \tag{C.2}$$

From the first line of equation (C.2) we put

$$\mathbf{v}^{(0)} = \mathbf{u}_0, \quad W^{(0)} = \lambda_0. \tag{C.3}$$

It is to be noted from the left side of the equations in (C.2) that the vectors $\mathbf{v}^{(k)}$ can include an arbitrary multiple of $\mathbf{v}^{(0)}$. We choose the condition for $\mathbf{v}^{(k)}$ such that

$$\mathbf{v}^{(0)t} \cdot \mathbf{v}^{(k)} = 0, \quad k \geq 1. \tag{C.4}$$

The first order term $W^{(1)}$ is given by taking the inner product of \mathbf{u}_0 and the second line of equation (C.2)

$$W^{(1)} = \mathbf{u}_0^t \cdot \Phi \mathbf{u}_0 = \phi_{00} = 0. \tag{C.5}$$

We calculate the first order vector $\mathbf{v}^{(1)}$ by expanding it in terms of the \mathbf{u}_i

$$\mathbf{v}^{(1)} = \sum_{j=0}^{n-1} a_j^{(1)} \mathbf{u}_j.$$

From the condition of equation (C.4), it is shown that $a_0^{(1)} = 0$. We substitute this expansion into the second line of equation (C.2), replace $A^{(0)}\mathbf{u}_j$ by $\lambda_j\mathbf{u}_j$, and multiply \mathbf{u}_i^t from the left to take the inner product. Then we obtain

$$a_i^{(1)} = \frac{\phi_{i0}}{\lambda_0 - \lambda_i}, \quad (i \geq 1). \quad (\text{C.6})$$

The second order term $W^{(2)}$ is

$$W^{(2)} = \mathbf{u}_0^t \cdot \Phi \mathbf{v}^{(1)} = \sum_{j=1}^{n-1} \frac{\phi_{0j}\phi_{j0}}{\lambda_0 - \lambda_j}. \quad (\text{C.7})$$

The second order vector is also given by the expansion in terms of the \mathbf{u}_j

$$\mathbf{v}^{(2)} = \sum_{j=1}^{n-1} a_j^{(2)} \mathbf{u}_j,$$

where $a_0^{(2)} = 0$ from the condition of equation (C.4). Substituting the expansion of $\mathbf{v}^{(2)}$ into the third line of equation (C.2), we obtain

$$a_i^{(2)} = \sum_{j=1}^{n-1} \frac{\phi_{ij}\phi_{j0}}{(\lambda_0 - \lambda_i)(\lambda_0 - \lambda_j)}, \quad (i \geq 1). \quad (\text{C.8})$$

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