Perturbation Theory and the Renormalization Group in Genetic Dynamics

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Abstract. Although much progress has been made in recent years in the theory of GAs and GP, there is still a conspicuous lack of tools with which to derive systematic, approximate solutions to their dynamics. In this article we propose and study perturbation theory as a potential tool to fill this gap. We concentrate mainly on selection-mutation systems, showing different implementations of the perturbative framework, developing, for example, perturbative expansions for the eigenvalues and eigenvectors of the transition matrix. The main focus however, is on diagrammatic methods, taken from physics, where we show how approximations can be built up using a pictorial representation generated by a simple set of rules, and how the renormalization group can be used to systematically improve the perturbation theory.

1 Introduction

Although much progress has been made in recent years in furthering our theoretical understanding of Genetic Algorithms (GAs) and Genetic Programming (GP) using coarse-grained formulations (see, for instance, [1–5]), most of this progress has been either at the formal level, for instance in the derivation of exact Schema Theorems, or at the qualitative level where, for example, a deeper understanding of the role of recombination has been gained. Such coarse-grained formulations have also led to a unified theoretical framework for both GAs and GP. However, there remains a conspicuous absence of tools by which the dynamics of evolutionary algorithms (EAs) may be systematically approximated.

The Statistical Mechanics approach [6] offers one possibility but, as emphasised in [7] - *"...it is not a mechanical, procedural method. Some insight about what is important and what is inessential is required"*. Instead of passing directly to a "macroscopic" view, as is done in the statistical mechanics approach, one may wonder if any progress can be made at a more microscopic level? Common wisdom is almost uniformly pessimistic as to whether microscopic formulations can offer a way forward. In this paper we try to argue that perhaps the situation

is not as bleak as it first seems, proposing perturbative methods in their various guises as a potential way forward. Of course, perturbation theory appears ubiquitously throughout the physical sciences, as well as in pure and applied mathematics and engineering.

In biology it has been used, for instance, by Eigen and collaborators [8] to analyse the quasi-species model. It has frequently been utilised at a formal level (see, for example [9]) to determine the stability or convergence properties of fixed points of the dynamics. More recently [10], it was used to consider the evolution of the cumulants of a mutation-selection system. The analysis there however, was restricted to a single elementary landscape. As far as we are aware, perturbative techniques have not been considered in the context of Evolutionary Computation (EC). Furthermore, they have not been considered in conjunction with the renormalization group in either biology or EC.

In this paper, as perturbative methods can be implemented in a myriad of different ways, we will give only a simple introduction to a few aspects of the general methodology. Sticking mainly to mutation-selection systems, we briefly discuss the perturbative construction of the eigenvalues and eigenvectors of the transition matrix. However, we concentrate most of our attention on generating perturbative expansions diagrammatically. This has the advantage of being transparent and intuitive, as it concentrates on constructing the different routes by which a given physical process may be realized. Although we use a one-bit system to make a concrete illustration we also consider multi-locus systems on a range of fitness landscapes in order to show that the methodology is not restricted purely to the standard "toy" models. Note that, in standard fashion, we will consider the population dynamics in the infinite population limit. However, as our main interest is in the transition matrix that determines the Markov chain that describes the dynamics, the results herein can be straightforwardly taken over to the finite population model, where a sampling of the multinomial distribution based on this transition matrix is carried out (see [11] Chapters 5 and 6 for a nice introduction to this).

2 An Introduction to Genetic Dynamics

We begin with the fundamental equations that describe the dynamics of a large class of EAs. We consider the three basic genetic operators - mutation, $\mathcal{M}$, selection, $\mathcal{F}$, and recombination, $\mathcal{R}$ - and, without loss of generality, will consider them acting in the causal order $\mathcal{MRF}$ on a population vector $\mathbf{P}(t)$, whose covariant components, $P_I(t)$, represent the probability to find an object - string, tree etc. - I at time t. For fixed length strings of length N and alleles of cardinality n, $I = i_1 \dots i_N$ is a multi-index with $i_1 \dots i_N \in [0, n-1]$. $\mathcal{M}$ and $\mathcal{F}$ in their turn are naturally represented as matrices, ${M_I}^J$ and ${F_I}^J$, with the latter generally being a diagonal matrix with elements proportional to ${\delta_I}^J$, where ${\delta_I}^J = 1$ for $I = J$ and 0 otherwise. In the case of proportional selection for instance, ${F_I}^J = (f_I/\bar{f}(t)){\delta_I}^J$, where f_I is the fitness of string I and $\bar{f}(t)$ the average population fitness. ${M_I}^J$ is the probability that string J mutates to string I, the

matrix elements being given by $p^{d_{IJ}}(1-p)^{N-d_{IJ}}$, with d_{IJ} being the Hamming distance between strings I and J and p the mutation probability.

Mathematically, as matrices, M and F are linear machines[4] which take as input (co-/contra)-variant vectors (row/column vectors in the case of matrix algebra) and give as output (contra-/co)-variant vectors. The intuitive interpretation is that each element of these matrices acts on a component of $\mathbf{P}$ as input to give another, possibly the same, component, as output. Recombination, on the other hand, naturally takes as input a pair of strings and gives as output a string[5]. Mathematically, it is therefore represented naturally as a mixed tensor, ${R_I}^{JK}$, with two contra- and one co-variant indices, which is a linear machine that takes as input two co-variant (row) vectors and gives as output a single contra-variant (column) vector. The dynamics can then be written in the covariant form (covariant here meaning that it is written such that its transformation properties under a coordinate transformation are manifest and follow from the simple linear rule of equation (3) below)

$$P_I(t+1) = \sum_{JK} {H_I}^{JK} P_J(t) P_K(t) \tag{1}$$

where ${H_I}^{JK} = \sum_{LMN} {M_I}^L {R_L}^{MN} {F_M}^J {F_N}^K$.

The reader may wonder: Why this particular interpretation of the mathematical nature of the dynamics? The answer is that using tensors is the most natural way to represent the geometrical properties of the fundamental objects in a theory under coordinate transformations. The next question is: why are the coordinate transformation properties of interest? The answer is that the dynamics can be greatly simplified when written in the most appropriate coordinate system providing greater insight and facilitating quantitative analysis. Additionally, writing equations in covariant form ensures that any statement valid in one coordinate system will be valid in any. A coordinate transformation is understood here as a linear map between bases and is explicitly realized by a matrix Λ. One may then enquire as to what is the most appropriate basis [13]? For instance, for binary strings the standard basis in the configuration space is the *δ-basis*, B_δ. The *δ-basis* is the set of 2^N characteristic functions defined on the hypercube, C_N, embedded in $\mathbb{R}^N$ - N-dimensional Euclidean space - one function for each of the 2^N vertices of C_N. Each characteristic functions is "delta-like", having non-zero values only at the corresponding vertex of the cube. For example, the basis function at the origin is $\bar{x}_1\bar{x}_2\ldots\bar{x}_N$ and so

$$B_\delta = \{\bar{x}_1\bar{x}_2\ldots\bar{x}_N,\, \bar{x}_1\bar{x}_2\ldots x_N,\, \ldots,\, x_1x_2\ldots x_N\}\,. \tag{2}$$

If we restrict all the basis functions to the vertices of C_N, each x_i, $1 \le i \le N$, takes the values 0 and 1 and $\bar{x}_i \equiv e - x_i$, where e takes the value 1 at each

[4] We will here use the language of tensor analysis. Readers unfamiliar with this may consult an introductory text such as [12].

[5] Although the output is really a pair of strings, determination of the first child completely fixes the second.

corner of the unit cube. Arranging the basis elements in columns to form the vector $\mathbf{x}_\delta = (\bar{x}_1 \dots \bar{x}_1, \dots, x_1 \dots x_N)^T$, one implements a transformation to a new basis $\mathbf{x}_{\delta'}$ via $\mathbf{x}_{\delta'} = \Lambda \mathbf{x}_\delta$. A tensor $T_{I_1 \dots I_r}{}^{J_1 \dots J_s}$ transforms under a basis transformation between δ and δ' as

$$T_{I'_1 \dots I'_r}{}^{J'_1 \dots J'_s} = \sum_{\substack{I_1 \dots I_r \\ J_1 \dots J_s}} \Lambda_{I'_1}{}^{I_1} \dots \Lambda_{I'_r}{}^{I_r} T_{I_1 \dots I_r}{}^{J_1 \dots J_s} (\Lambda^{-1})_{J_1}{}^{J'_1} \dots (\Lambda^{-1})_{J_s}{}^{J'_s} \tag{3}$$

Further insight into the dynamics can be obtained by explicitly subtracting out the linear "cloning" term from the recombination operator to obtain

$$P_I(t+1) = \sum_J M_I{}^J \left((1-p_c) P'_J + p_c \sum_{KLm} \frac{1}{2} \big(p(m) + p(\bar{m}) \big) \lambda_J{}^{KL}(m) P'_K P'_L \right) \tag{4}$$

where $P'_I(t) = \sum_J F_I{}^J P_J(t)$ is the probability to select string I, p_c is the probability that recombination takes place and $p(m)$ is the probability to implement the recombination mask m, $\bar{m}$ denoting the conjugate mask. Finally, $\lambda_I{}^{JK}(m)$ is an interaction term between strings I, J and K and represents the conditional probability that, given the selection of parent strings J and K, a child string of type I is produced when recombination is implemented using a mask m. It takes values 0 and 1. Equation (4) has a straightforward intuitive interpretation. The first term in brackets represents the probability that a string is "cloned", while the second term represents the probability that a string is created via recombination. An analogous functional form also holds for the case of GP [2, 14].

Despite the covariance of (1), the facility of its analysis and its physical interpretation are basis-dependent. The dynamics is governed by the mutation matrix $M_I{}^J$, the tensor $\lambda_I{}^{JK}(m)$, the mask probability distribution $p(m)$ and the fitness values f_I, hidden inside P'_I or $F_I{}^J$. In this sense the EA is a "black box" whose output depends on a large set of parameters. It therefore behoves us to look for symmetries and regularities that may be exploited in order to effect a coarse graining which makes manifest the effective degrees of freedom of the dynamics in terms of which the dynamics looks simplest. However, this in its turn depends on choosing an appropriate coordinate system wherein a particular regularity is more clearly seen. For instance, in a selection dominated regime, the string basis is the most appropriate one, as the selection matrix F is diagonal in this basis, i.e. the strings themselves are the appropriate effective degrees of freedom. However, when mutation is the dominant operator, a basis transformation to the Walsh basis, $\hat{\mathbf{x}}$, using the transformation matrix

$$\Lambda^w \equiv 2^{-N/2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^{\otimes N} \tag{5}$$

is useful, where $\otimes N$ is the Nth tensor power of the matrix. The power of the Walsh transform is that it diagonalizes the mutation matrix M so that its matrix elements are $(1-2p)^{|I|} \delta_I{}^J$, $|I|$ being the order of the Walsh mode I. Similarly,

when recombination is the dominant operator a basis transformation to the Building Block or monomial basis [13, 15], $\mathbf{x}_{BB}$, is appropriate using

$$\Lambda^{BB} \equiv \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}^{\otimes N} \tag{6}$$

The advantage of this transformation is that the tensor ${\lambda_I}^{JK}$ becomes skew-diagonal on the indices J and K for any string I [13, 15], thus showing that recombination builds strings by explicitly combining the Building Blocks of that string.

3 Exact Solutions of the Dynamics

As the key element of a perturbative approach is the development of a power series expansion around a known exact limit, it is important to have a good understanding of the different limits in which an exact solution for the dynamics may be found. There are no known exact solutions of equation (4) in the presence of all three genetic operators.[6] However, solutions in the absence of one or more of the operators may be found[7].

3.1 Explicit Solutions

Selection Only In the case of selection only the evolution equations (4) are uncoupled and essentially linear in the variables $P_I(t)$, the apparent non-linearity in $\bar{f}(t)$ having as its origin nothing more than the normalisation of the probabilities, $\sum_I P_I(t) = 1$. Passing to unnormalised variables $x_I(t)$, defined via

$$P_I(t) = \frac{x_I(t)}{\sum_I x_I(t)} \tag{7}$$

leads to an explicit solution

$$P_I(t) = \frac{f_I^t P_I(0)}{\sum_I f_I^t P_I(0)} \tag{8}$$

In general, an exponential number of fitness values must be specified. However, in many cases the map will be many-to-one and the phenotypic dynamics may simplify accordingly. The fixed point of (8) is $P_I^* = \lim_{t\to\infty} P_I(t) \to 1 \iff f_I > f_J \ \ \forall \ \ J \ \ \text{such that} \ \ P_J(0) \neq 0$. Note that this fixed point depends on the initial conditions and hence is not universal. In the case where all strings are represented however, the fixed point is the global maximum of the fitness landscape in the case where this maximum is unique.

[6] Note however, that exact solutions may be found [16] for the case of modified recombination operators, such as genepool recombination, and certain specific fitness landscapes, such as functions of unitation.

[7] A more leisurely derivation of many of the results in this section can be found in [11].

Mutation Only In the case of mutation only, the equations (4) remain linear, but are coupled in the string basis. Passing to the Walsh basis using the basis transformation (5) one finds the solution

$$\hat{P}_I(t) = (1-2p)^{|I|t}\hat{P}_I(0) \tag{9}$$

each eigenvalue denoted by $|I|$ being associated with ${}^{N}C_{|I|}$ degenerate eigenvectors. Thus, just as the exact solution for selection only is diagonal in the string basis the exact solution for mutation only is diagonal in the Walsh basis. The fixed point of the dynamics is given by $\lim_{t\to\infty}\hat{P}_I(t) = 2^{-N/2}{\delta_I}^0$ and corresponds to the centre of the simplex, i.e. equal proportions of every genotype. The bigger is $|I|$, the faster the decay of the associated transient to the fixed point.

Recombination Only Finally, in the case of recombination only, although an exact solution is not known for discrete time and arbitrary crossover, a solution is known in the continuous time limit for one-point crossover [3]. The solution is

$$P_I(t) = \sum_{n=0}^{N-1} \mathrm{e}^{\frac{-np_c}{N-1}}(1-\mathrm{e}^{\frac{-p_c}{N-1}})^{N-n}\mathcal{P}(n+1) \tag{10}$$

where $\mathcal{P}(n+1) = \sum_i \Pi_{n_i=1}^{N-n} P_{n_i}(0)$. Each $P_{n_i}(0)$ is the initial probability for the Building Block n_i which crossover could combine to give genotype I. The product is over the different numbers, n_i, of Building Blocks and the sum is over the different possible permutations for a given number. For example, for $N=3$, for $I=111$ $\mathcal{P}(1) = P_{1**}(0)P_{*1*}(0)P_{**1}(0)$, $\mathcal{P}(2) = P_{11*}(0)P_{**1}(0) + P_{1**}(0)P_{*11}(0)$ (two permutations) and $\mathcal{P}(3) = P_{111}(0)$.

3.2 Formal Solutions

Above we considered explicit exact solutions. One can also get useful information by considering formal, or implicit, exact solutions. An example of this is the case of mutation and selection where the problem is linear and so the trick of passing to unnormalised variables, $x_I(t)$, remains valid. In this setting the equation $x_I(t+1) = \sum_K {W_I}^K x_K(t)$, where the matrix W has elements ${W_I}^K = \sum_J {M_I}^J f_J {\delta_J}^K$, can be simply iterated to obtain the formal solution

$$P_I(t) = \frac{\sum_J (W^t)_I{}^J P_J(0)}{\sum_{IJ}(W^t)_I{}^J P_J(0)} \tag{11}$$

The solution is formal in that (W^t) is the t-th power of an exponentially large matrix. If W can be diagonalized via a similarity transformation, which we assume, then we may interpret this as a basis transformation $\tilde{\mathbf{x}} = \tilde{\Lambda}\mathbf{x}_\delta$, where the $\tilde{\mathbf{x}}$ are the normalised eigenvectors of W. Under this transformation $P_I(t) \to$

$\tilde{P}_I(t) = \sum_J \tilde{\Lambda}_I{}^J P_J(t)$ and $W \to \tilde{W}$, where $\tilde{W}$ is diagonal with elements $\lambda_I \delta_I{}^J$ and λ_I is the eigenvalue corresponding to eigenvector I. One thus finds

$$\tilde{P}_I(t) = \frac{\lambda_I^t \tilde{P}_I(0)}{\sum_I \lambda_I^t \tilde{P}_I(0)} \tag{12}$$

The general solution in the original string basis can be found by inverting the basis transformation using $\tilde{\Lambda}$ to find

$$P_I(t) = \frac{\sum_{JK} \tilde{\Lambda}_I{}^J \lambda_J^t (\tilde{\Lambda}^{-1})_J{}^K P_K(0)}{\sum_{IK} \lambda_I^t (\tilde{\Lambda}^{-1})_I{}^K P_K(0)} \tag{13}$$

Note the functional form as a sum of exponentials, where, as W has only positive entries, at least the biggest eigenvalue is positive. For example, for one-bit

$$P_0(t) = N\left(A_{00}\lambda_0^t + A_{01}\lambda_1^t\right) \tag{14}$$

where $A_{00} = (\tilde{\Lambda}_0{}^0(\tilde{\Lambda}^{-1})_0{}^0 P_0(0) + \tilde{\Lambda}_0{}^0(\tilde{\Lambda}^{-1})_0{}^1 P_1(0))$ and $A_{01} = (\tilde{\Lambda}_0{}^1(\tilde{\Lambda}^{-1})_1{}^0 P_0(0) + \tilde{\Lambda}_0{}^1(\tilde{\Lambda}^{-1})_1{}^1 P_1(0))$ are the amplitudes of the different exponents and where $N = \sum_{IK} \lambda_I^t (\tilde{\Lambda}^{-1})_I{}^K P_K(0)$ is a normalisation constant. The asymptotic behaviour is dominated by the largest eigenvalue, $\lambda_{\max}$, associated with a corresponding eigenvector $\tilde{x}_{\max}$. The corresponding component of $\mathbf{P}$ in this basis is $\tilde{P}^*_{\max}$. In terms of the original string basis the fixed point is $P^*_I = \tilde{\Lambda}_I{}^{\max}$, independent of the initial population.

4 Perturbation Theory

Perturbation theory is an ubiquitous tool in the physical sciences. However, in all its guises its conceptual basis is the same - finding approximate solutions as power series expansions with respect to a "small" parameter, ϵ, around a known solution. Conceptually, the methodology is simple. In the context at hand one writes P_I (or the unnormalised variable x_I) as a power series in ϵ

$$P_I(t) = \sum_{n=0}^{\infty} \epsilon^n P_I^{(n)}(t) \tag{15}$$

where the expansion coefficients $P_I^{(n)}$ are to be determined. One assumes that the operator $H_I{}^{JK}$ can be written in the form $H_I{}^{JK} = D_I{}^{JK} + \epsilon O_I{}^{JK}$, where $O_I{}^{JK}$ is the perturbation operator and the solution of $P_I(t+1) = \sum_{JK} D_I{}^{JK} P_J(t) P_K(t)$ is known. One subsequently substitutes the ansatz (15) into equation (1) and matches powers of ϵ^n from both sides of the equation. For instance, to $O(1)$ and $O(\epsilon)$ one finds

$$P_I^{(0)}(t+1) = \sum_{JK} D_I{}^{JK} P_J^{(0)}(t) P_K^{(0)}(t) \tag{16}$$

$$P_I^{(1)}(t+1) = \sum_{JK} \Big(D_I{}^{JK} P_J^{(1)}(t) P_K^{(0)}(t) + D_I{}^{JK} P_J^{(1)}(t) P_K^{(0)}(t) \; + O_I{}^{JK} P_J^{(0)}(t) P_K^{(0)}(t) \Big) \tag{17}$$

The solution of (16) is assumed known. Once $P_I^{(0)}$ has been determined then equation (17) is a linear inhomogeneous difference equation for $P_I^{(1)}$ where the inhomogeneity is a known function of $P_I^{(0)}$. This equation can be solved using as initial condition $P_I^{(1)}(0) = 0$.[8] The solution to $O(\epsilon)$ is thus $P_I(t) = P_I^{(0)}(t) + \epsilon P_I^{(1)}(t) + O(\epsilon^2)$. The formal expansion parameter ϵ can now be put to one.[9]

5 Perturbation theory for Mutation-Selection Systems

To illustrate the general methodology we restrict attention to the case of mutation and selection. This problem is, in principle, straightforward, requiring only the eigenvalues and eigenvectors of the matrix MF. However, computationally this is extremely difficult for large matrices.

First, we transform to the unnormalised variables defined in (7), $x_I(t)$, remembering that we can consider them in either the string or the Walsh basis. The equation to be solved is

$$x_I(t+1) = \sum_{JK} M_I{}^J F_J{}^K x_K(t) \tag{18}$$

where, without change of notation, we now take F to have elements $F_I{}^J = f_I \delta_I{}^J$, the scalar $\bar{f}(t)$ having been removed by the change to unnormalised variables. The idea now is to solve this approximately by some perturbative expansion around some known exact limit. From section 3, two natural limits are the limits $M_I{}^J \to \delta_I{}^J$ and $F_I{}^J \to \delta_I{}^J$, associated with zero mutation and zero selection gradient respectively. In this case one writes

$$M_I{}^J = (\delta_I{}^J + \epsilon dM_I{}^J) \tag{19}$$

$$F_I{}^J = (\delta_I{}^J + \epsilon dF_I{}^J) \tag{20}$$

where dM and dF are the perturbation operators and contain the deviations of M and F from the unit matrix. Thus, in the case of selection we are using dF to measure deviations from a constant fitness value, which we take to be one. For example, for one bit, in the string basis the deviations are given by

$$dM = \begin{pmatrix} -p & p \\ p & -p \end{pmatrix} \qquad \text{and} \qquad dF = \begin{pmatrix} f_0 & 0 \\ 0 & f_1 \end{pmatrix} \tag{21}$$

with f_0 and f_1 measuring deviations from flat fitness, while in the Walsh basis

$$\widehat{dM} = \begin{pmatrix} 0 & 0 \\ 0 & -2p \end{pmatrix} \qquad \text{and} \qquad \widehat{dF} = \frac{1}{2}\begin{pmatrix} (f_0+f_1) & (f_0-f_1) \\ (f_0-f_1) & (f_0+f_1) \end{pmatrix} \tag{22}$$

[8] We can naturally set $P_I^{(n)}(0) = 0 \;\forall\; n \neq 0$. This is intuitive, in that ϵ gauges the effect of the perturbation which perturbs the initial population *after* $t = 0$.

[9] ϵ is only taken to be small in a formal sense here in order to generate systematic power series expansions. Physically, the relevant small parameter for mutation-selection systems is the mutation rate, or the deviation from a flat fitness landscape, and it is these parameters that will govern the accuracy of the approximation.

Alternatively, given that (18) is exactly solvable when $W = MF$ is any diagonal matrix, we could divide W into a diagonal part, D, and an off-diagonal part, O, and write $W = D + \epsilon O$.

5.1 Perturbative construction of Eigenvalues and Eigenvectors

There are several alternatives for constructing a perturbation theory depending on what quantities one wishes to construct. In EC the string proportions, $P_I(t)$, are of direct interest. Hence, it is natural to implement a formalism that focuses directly on them. However, there is another implementation that focuses more on the perturbative construction of the eigenvalues and eigenvectors of W.

We assume, as in section 3.2, that W can be diagonalized via a basis transformation $W \to \tilde{W} = \tilde{\Lambda} W \tilde{\Lambda}^{-1}$. In distinction to section 3.2 though, where it was assumed that $\tilde{\Lambda}$ could be determined exactly, we will here construct the transformation perturbatively. As the eigenfunctions of the unperturbed problem form a complete set of basis functions - string or Walsh basis functions - one may consider the basis transformation $\tilde{\mathbf{x}} = \tilde{\Lambda}\mathbf{x}$ as an expansion of the exact eigenfunctions of W in terms of the unperturbed ones (i.e. of M or F alone), where $\mathbf{x}$ will refer to the unperturbed eigenfunctions. One now seeks perturbative solutions by writing power series expansions for the eigenvalues, λ_i and the expansion coefficients, $\tilde{\Lambda}_i{}^j$

$$\lambda_i = \sum_{n=0}^{\infty} \epsilon^n \lambda_i^{(n)}; \qquad \tilde{\Lambda}_i{}^i = \sum_{n=0}^{\infty} \epsilon^n \tilde{\Lambda}_i{}^{i(n)}; \qquad \tilde{\Lambda}_i{}^j = \sum_{n=1}^{\infty} \epsilon^n \tilde{\Lambda}_i{}^{j(n)} \tag{23}$$

where we are using lower case letters i and j to index the eigenvectors and eigenvalues. Note that the expansion of the non-diagonal elements of $\tilde{\Lambda}$ starts at $O(\epsilon)$, in distinction to the diagonal ones. This recognises the fact that only the presence of the perturbation can induce such non-diagonal terms. In the basis where $\tilde{W}$ is diagonal, an eigenvector $\tilde{\mathbf{x}}^i$ with components $\tilde{x}^i_I$ is a solution of

$$\sum_J \tilde{W}_I{}^J \tilde{x}^i_J = \lambda_i \tilde{x}^i_I \tag{24}$$

Substituting the ansatz (23) into (24), matching coefficients of ϵ^n and using the fact that the unperturbed eigenfunctions are orthogonal, i.e. $\sum_J x_i^J x^j{}_J = 0$ for $i \neq j$, one finds to $O(\epsilon)$

$$\lambda_i = \lambda_i^{(0)} + \epsilon \sum_{JK} x_i^J O_J{}^K x^i_K \tag{25}$$

where O is the perturbation operator. To be more concrete, consider the example of one-bit with perturbation operator $O_I{}^J = dF_I{}^J$. In this case it is appropriate to work in the Walsh basis using equation (22). In this basis, as $\hat{M}$ is diagonal, the unperturbed eigenvalues, $\lambda_+ = 1$ and $\lambda_- = (1-2p)$, can be read off directly from it. The corresponding eigenvectors are $x_+ = (1\ 0)^T$ and $x_- = (0\ 1)^T$. The $O(\epsilon)$ contribution to λ_+, $\lambda_+^{(1)}$, is

$$\lambda_+^{(1)} = \frac{1}{2}(1\ 0) \begin{pmatrix} (f_0+f_1) & (f_0-f_1) \\ (1-2p)(f_0+f_1) & (1-2p)(f_0-f_1) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{(f_0+f_1)}{2} \tag{26}$$

where, once again, f_0 and f_1 refer to deviations from flat fitness. The analogous expression for λ_- is found by substituting (1 0) for (0 1) in (26) to find $\lambda_-^{(1)} = (1-2p)(f_0+f_1)/2$. Thus, to $O(\epsilon)$ the two eigenvalues are

$$\lambda_+ = \left(1 + \frac{\epsilon(f_0+f_1)}{2}\right) \tag{27}$$

$$\lambda_- = (1-2p)\left(1 + \frac{\epsilon(f_0+f_1)}{2}\right) \tag{28}$$

In order to construct a solution of the form (13), as well as the eigenvalues we also need the basis transformation matrix $\tilde{\Lambda}$ that relates the exact basis to the string or Walsh basis. The columns of the transformation matrix are, in fact, just the eigenvectors of W. Hence, a perturbative calculation of the eigenvectors is equivalent to an expansion of the elements of $\tilde{\Lambda}$. For our example one-bit case, as we are working in the Walsh basis, it is the eigenvectors of $\hat{W}$. Explicitly, for the coefficients of the transformation between unperturbed and perturbed eigenstates, to $O(\epsilon)$ one finds $\tilde{\Lambda}_i{}^{i(1)} = 0$ and for $j \neq i$

$$\tilde{\Lambda}_i{}^{j(1)} = \frac{\sum_{IJ} x_i^I O_I{}^J x_J^j}{(\lambda_i^{(0)} - \lambda_j^{(0)})} \tag{29}$$

For one bit, for the case $\hat{O}_I{}^J = \widehat{dF}_I{}^J$

$$\tilde{\Lambda}_+^{-(1)} = \frac{1}{4p}(1\ 0)\begin{pmatrix} (f_0+f_1) & (f_0-f_1) \\ (1-2p)(f_0+f_1) & (1-2p)(f_0-f_1) \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{(f_0-f_1)}{4p} \tag{30}$$

With the expansion coefficients in hand the exact eigenvectors $\tilde{\mathbf{x}}$ may be calculated, which are then used to compute the basis transformation matrix $\tilde{\Lambda}$. As seen in section 3.2 it is in fact this matrix which provides important information, such as the fixed points of the dynamics, the eigenvalues merely governing the approach to the fixed point.

5.2 Diagrammatic Perturbative Construction of P_I

Although conceptually straightforward and well known, the above methodology for calculating eigenvalues and eigenvectors is complicated to implement beyond leading order, especially in terms of calculating the expansions of the eigenvectors, and these are essential if one wishes to construct expressions for the $P_I(t)$ and, in particular, if the asymptotic behaviour in the vicinity of any fixed point is required. Additionally, when there are several eigenvectors that correspond to the same eigenvalue, orthogonal combinations of the associated eigenvectors must be found. We thus consider now how to calculate the $x_I(t)$ directly. Initially, we will consider a general fitness landscape and arbitrary string length and population, as a great deal of useful information can be gleaned from the general case without having to specialise to a particular problem.

We will illustrate the methodology in the context of an expansion around the no selection limit (the corresponding expansion around zero mutation is very similar). In this case it is appropriate to first do a coordinate transformation to the Walsh basis. In the Walsh basis, the solution of the unperturbed (i.e. no selection and no crossover) system is

$$\hat{x}_I(t) = (1-2p)^{|I|t}\hat{x}_I(0) \tag{31}$$

One can interpret (31) and, in particular, a factor $(1-2p)^{|I|(t-t')}$ as describing the propagation in time, between t' and t, of an elementary "excitation" of type I[10] which can be represented diagrammatically as a straight line, as shown in Figure 1(a). As $(1-2p) < 1$ the excitation decays exponentially, the rate of decay depending on the order of the Walsh coefficient. The only excitation that does not decay is the zeroth order one which corresponds to the uniform population limit in the string basis. The presence of the perturbation, in this case selection, can be interpreted as an interaction between the excitation and some external operator and can be represented diagrammatically by a wavy line as shown in Figure 1(b). These diagrams are a simple, intuitive mnemonic for the algebraic

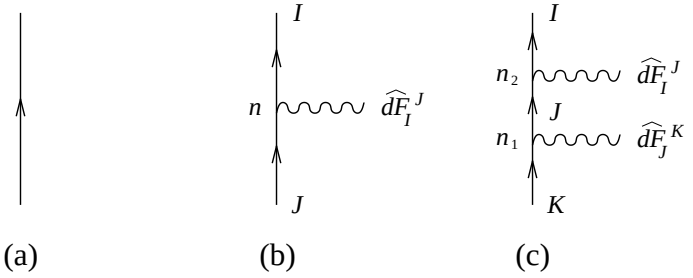

Figure 1. Diagrammatic representation of the $O(1)$, $O(\epsilon)$ and $O(\epsilon^2)$ perturbative terms [(a), (b) and (c) respectively.]

expression

$$\hat{x}_I(t) = (1-2p)^{|I|t}\hat{x}_I(0) + \epsilon \sum_J \sum_{n=0}^{t-1} (1-2p)^{|I|(t-n)} \widehat{dF}_I{}^J (1-2p)^{|J|n} \hat{x}_J(0), \tag{32}$$

The two terms represent the different physical processes that can contribute to $O(\epsilon)$ to the appearance of a Walsh mode I at time t. The first term, corresponding to Figure1(a), represents the process where the mode I was present at $t = 0$ and propagates forward to t. The second term, corresponding to Figure 1(b) however, represents the probability that it is produced by first starting with a mode J at $t = 0$, which then propagates to time $t = n$. At $t = n$ it interacts

[10] In the Walsh basis this excitation is analogous to a normal mode, while in the string basis these elementary excitations are obviously the strings themselves.

with the Walsh-transformed perturbation selection operator, $\widehat{dF}_I{}^J$ to produce the mode I, which then propagates from $t = n$ to t. $\sum_J$ represents the fact that one must consider all possible initial starting states as potential contributions, while $\sum_{n=0}^{t-1}$ represents the possibility that the interaction may take place at any one of the t time steps of the evolution.

One may sum the second term (32) to find

$$\hat{x}_I(t) = (1-2p)^{|I|t}\hat{x}_I(0)+\epsilon(1-2p)^{|I|t}\sum_J \frac{\left(1-(1-2p)^{(|J|-|I|)t}\right)}{1-(1-2p)^{(|J|-|I|)}}\widehat{dF}_I{}^J\hat{x}_J(0) \quad (33)$$

There are three distinct cases to take into account: $|I| < |J|$, $|I| > |J|$ and $|I| = |J|$. In the first case the contribution from the corresponding interactions only modifies the amplitude of the zeroth-order transient behaviour, associated with $(1-2p)^{|I|t}$, from 1 to $1+\sum_{|J|>|I|}\widehat{dF}_I{}^J\hat{x}_J(0)/(1-(1-2p)^{(|J|-|I|)})$, where the sum is over those Walsh modes for which $|J| > |I|$. When $|I| > |J|$ the contribution from the interaction dominates, leading to a decay for $\hat{x}_I(t)$ of the form $(1-2p)^{|J|t}$, which is slower than $(1-2p)^{|I|t}$. Finally, in the limit $|J| \to |I|$ there is an apparent singularity in the dynamical factor. However, $\lim_{|J|\to|I|}(1-(1-2p)^{(|J|-|I|)t})/(1-(1-2p)^{(|J|-|I|)}) = t$. This term is the analog of a secular term as found in perturbative solutions of ordinary differential equations [17]. At first glance it invalidates perturbation theory, as it leads to a linearly growing perturbation in time. However, as this term is suppressed by the exponential decay, $(1-2p)^{|I|t}$, it does not affect the value found for the fixed point except, at first glance, for the zeroth mode. That this is not a problem can be seen by returning to the normalised variables P_I via equation (7). First we pass to the normalised Walsh variables, $\hat{P}_I$, which are related to the $\hat{x}_I$ via

$$\hat{P}_I(t) = \frac{1}{2^{\frac{N}{2}}}\frac{\hat{x}_I(t)}{\hat{x}_0(t)} \quad (34)$$

with $\hat{P}_0(t) = 1/2^{N/2}$ just the Walsh transformed constraint $\sum_I P_I(t) = 1$. Substituting (33) into (34) and expanding the denominator in ϵ one finds to $O(\epsilon)$

$$\begin{aligned}\hat{P}_I(t) = (1-2p)^{|I|t}\hat{P}_I(0) + \epsilon(1-2p)^{|I|t}\sum_J \frac{\left(1-(1-2p)^{(|J|-|I|)t}\right)}{1-(1-2p)^{(|J|-|I|)}}\widehat{dF}_I{}^J\hat{P}_J(0) \\ - \epsilon(1-2p)^{|I|t}2^{\frac{N}{2}}\hat{P}_I(0)\sum_J \frac{\left(1-(1-2p)^{|J|t}\right)}{1-(1-2p)^{|J|}}\widehat{dF}_0{}^J\hat{P}_J(0) \quad (35)\end{aligned}$$

Taking the limit $t \to \infty$ one finds the fixed point for $|I| \neq 0$

$$\hat{P}_I^* = \frac{\epsilon}{2^{\frac{N}{2}}}\frac{\widehat{dF}_I{}^0}{((1-2p)^{-|I|}-1)} \quad (36)$$

Thus, we see that the fixed point associated with the centre of the simplex is modified by selection and is independent of the initial conditions. This is intuitive

given that the non-zero modes are associated with exponentially decaying excitations. We also see that the biggest contribution to the asymptotic behaviour will come from the most important Walsh components of the fitness landscape. For instance, for a unitation type landscape only the $O(1)$ Walsh coefficients of the landscape are non-zero and hence $\hat{P}^*_I = 0$ for $|I| \neq 1$.

To $O(\epsilon^2)$ the corresponding diagram is Figure 1(c) and represents the production of a Walsh mode I by starting with a Walsh mode K which propagates to $t = n_1$, interacts with the perturbation selection operator $\widehat{dF}_J{}^K$ to produce a Walsh mode J, which in its turn propagates from $t = n_1$ to $t = n_2$. This Walsh mode then interacts with the perturbation selection operator $\widehat{dF}_I{}^J$ at $t = n_2$ to produce a Walsh mode I, which finally propagates from $t = n_2$ to t. The corresponding algebraic expression for this second order process is

$$\epsilon^2 \sum_{JK} \sum_{n_2=1}^{t-1} \sum_{n_1=0}^{n_2-1} (1-2p)^{|I|(t-n_2)} \widehat{dF}_I{}^J (1-2p)^{|J|(n_2-n_1)} \widehat{dF}_J{}^K (1-2p)^{|K|n_1} \hat{x}_K(0) \quad (37)$$

Once again, one must sum over different possible initial and intermediate states, J and K, and sum over the different possibilities for the times at which the excitations interact with the selection operator. Note that causally the second interaction with the selection operator must come *after* the first one, hence the sum over n_2 begins at $t = 1$ not $t = 0$. Evaluating (37) and adding to (32) one obtains to second order

$$\begin{aligned} \hat{x}_I(t) = (1-2p)^{|I|t} \hat{x}_I(0) + \epsilon (1-2p)^{|I|t} \sum_J \frac{\left(1-(1-2p)^{(|J|-|I|)t}\right)}{1-(1-2p)^{(|J|-|I|)}} \widehat{dF}_I{}^J \hat{x}_J(0) \\ + \epsilon^2 (1-2p)^{|I|t} \sum_{JK} \left(\frac{(1-2p)^{(|J|-|I|)}\left(1-(1-2p)^{(|J|-|I|)(t-1)}\right)}{\left(1-(1-2p)^{(|K|-|J|)}\right)\left(1-(1-2p)^{(|J|-|I|)}\right)} \right. \\ \left. - \frac{(1-2p)^{(|K|-|I|)}\left(1-(1-2p)^{(|K|-|I|)(t-1)}\right)}{\left(1-(1-2p)^{(|K|-|J|)}\right)\left(1-(1-2p)^{(|K|-|I|)}\right)} \right) \widehat{dF}_I{}^J \widehat{dF}_J{}^K \hat{x}_K(0) \end{aligned} \quad (38)$$

As at $O(\epsilon)$, one must take care over the limits $|I| = |J|$, $|J| = |K|$, $|I| = |K|$ or $|I| = |J = |K|$. Note that this expression is valid for an arbitrary fitness landscape as long as the selection pressure is weak. To get back to the probabilities $P_I(t)$ from the $\hat{x}_I(t)$ is straightforward. One first passes to the variables $\hat{P}_I(t)$ using equation (34). One is then faced with a choice - to expand the denominator, $\hat{x}_0$, as a power series in ϵ into the numerator, or to evaluate it numerically without this last expansion. Schematically, it is the difference between writing at $O(\epsilon)$: $\hat{P}_I = (1/2^{N/2})(\hat{x}_I/\hat{x}_0) = (a_I + \epsilon b_I)(a_0 + \epsilon b_0)^{-1}$, where both numerator and denominator are now evaluated numerically for a given landscape, or writing $(a_0 + \epsilon b_0)^{-1} \approx (a_0 - \epsilon b_0)$ and *then* evaluating the expression numerically. The true spirit of perturbation theory is to do the latter and we shall follow that procedure here. However, under certain circumstances it is possible to envision the former. Finally, one passes to the $P_I(t)$ using the inverse Walsh transform from (5).

This diagrammatic formulation gives a powerful pictorial representation of the underlying problem, wherein the different diagrams represent the different ways in which a process may occur - for instance, production of a particular string. The problem then may be turned around to be associated with the specification of the *rules*[11] by which the diagrams that represent the different possibilities may be constructed. In fact, one may take these rules as being a definition of the theory, as their particular form depends on the theory in question, e.g. selection only, selection and mutation etc.. In the case at hand, for mutation and selection with an expansion around the zero selection limit, the rules for constructing a solution to a given perturbative order are:

1. Draw all possible topologically distinct diagrams contributing to the process under study to the desired perturbative order
2. To each internal line attach a propagator $(1-2p)^{|I|(t-t')}$
3. At each interaction vertex insert a factor $\epsilon \widehat{dF}_I^{\ J}$
4. Sum over all internal times associated with the interaction vertices
5. Sum over intermediate states on internal lines

These rules are also valid when expanding around the zero mutation limit if the propagator is replaced by $f_I^{(t-t')}$ and the vertex factor by $\epsilon \widehat{dM}_I^{\ J}$. Note that in calculating $x_I(t)$ we summed over all possible initial states as we were interested ultimately in $P_I(t)$ not in the conditional probability $P(I,t|J,t')$. One may, of course, always revert to the algebraic formulation if there is any doubt or ambiguity over constructing the diagrams and their associated algebraic expressions.

In order to give a feeling for the capabilities of the method we present some results for the case of $N = 7$ and with various fitness landscapes. We use a mutation probability $p = 0.1$ which, it is worth noting given that we are formally in the "high" mutation perturbation limit, is not much different from typically used rates. The three fitness landscapes we consider are representative of different classes of landscape - consisting of the Eigen model ("needle-in-a-haystack"), counting ones (unitation models) and a model where fitnesses are assigned to strings randomly (akin to a Kauffman NK-model with $N = K$). Specifically: for the Eigen landscape $f_{1111111} = 1.5$ and $f_I = 1.0$ for $I \neq 1111111$; for counting ones $f_I = 1 + (0.5/7)\sum_i 1_i$; and finally for the random landscape $f_I \in [1, 1+R]$, where R is a random number chosen with uniform probability from the interval $[0, 0.5]$. In all three cases the parameters have been chosen so that the maximum deviation from fitness value 1 is 0.5, corresponding to a 50% difference in fitness between the fittest string and the least fit string, i.e. a 50% "planarity deviation", i.e. the deviation from the no-selection limit. As ϵ is set to one this is a good test of the approximations as the corresponding perturbation is not then particularly "small". In all cases a random initial population was chosen.

In Figures 2-4 we compare the perturbative approximations of $\bar{f}(t)$ to $O(\epsilon)$ and $O(\epsilon^2)$ with the exact solution, obtained by explicitly integrating equation

[11] In physics, in quantum field theory, these rules are known as Feynman rules.

(18). Notice that the $O(\epsilon^2)$ approximation gives uniformly better results (by a factor of between 2 for the Eigen model and 10 for counting ones) in the asymptotic regime but not necessarily for the transients. This is due to the presence of secular terms, which are also responsible for artefacts like the peak in the second order curve in Figure 4.

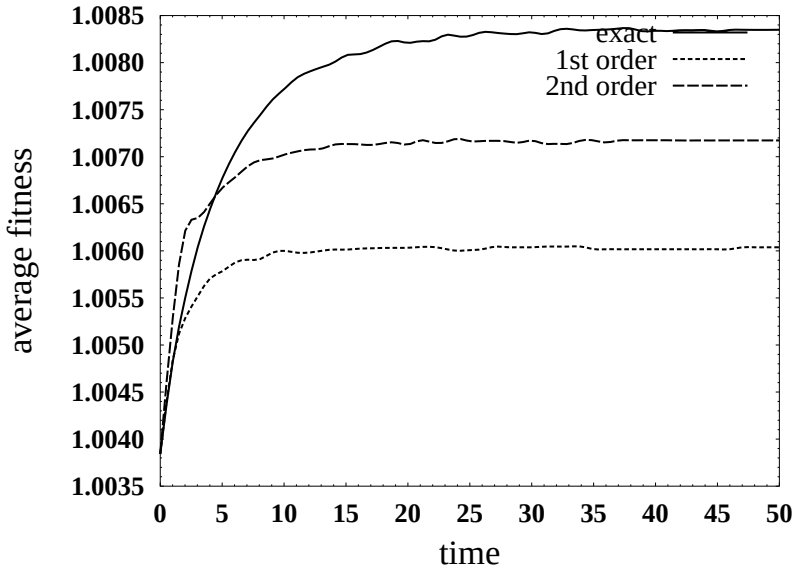

Figure 2. Average fitness for 7-bit Eigen model with 50% deviation from flat fitness limit

Note that even at $O(\epsilon)$ the results are asymptotically very accurate with deviations from the exact answer being less than about 0.1%. The population fitness in this sense is quite robust in terms of approximations.

A more sensitive object is the proportion of optimal strings in the population as a function of time. In Figures 5-7 we see graphs of precisely this quantity. For the Eigen model the optimal sequence is the "master sequence", i.e. the needle - chosen to be 1111111 - while for the counting ones landscape it is the string 1111111. For the random landscape the optimal sequence was found by examining all 128 strings. Note that asymptotically the quality of the approximation is quite sensitive to the landscape considered. At $O(\epsilon)$ the error for the Eigen model is about 28% whereas it is only about 2% for the counting ones landscape. The $O(\epsilon^2)$ results are better than the $O(\epsilon)$ results, as one might expect, except in the case of the counting ones landscape which is both interesting, somewhat counterintuitive and worthy of further investigation. We also repeated the experiments for $N = 3$ with very similar results, the approximation being generally somewhat worse for this shorter string length. This is to be expected as for

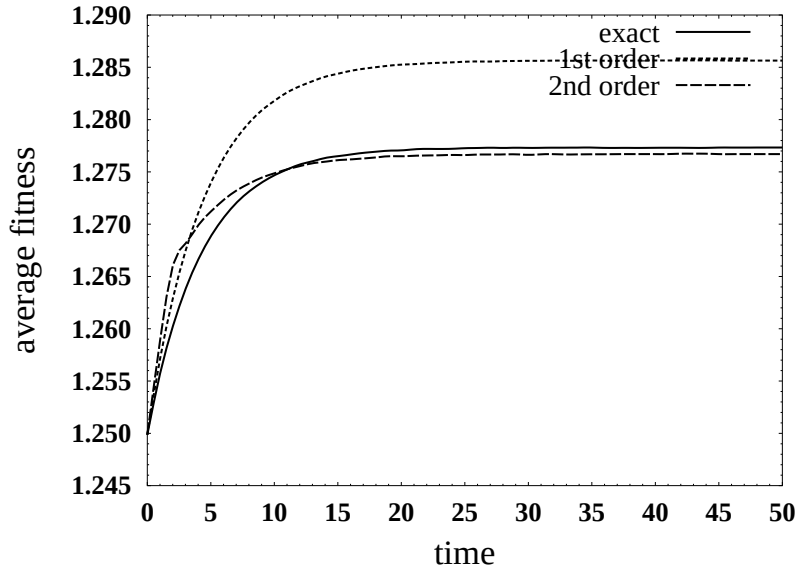

Figure 3. Average fitness for 7-bit counting ones model with 50% deviation from flat fitness limit

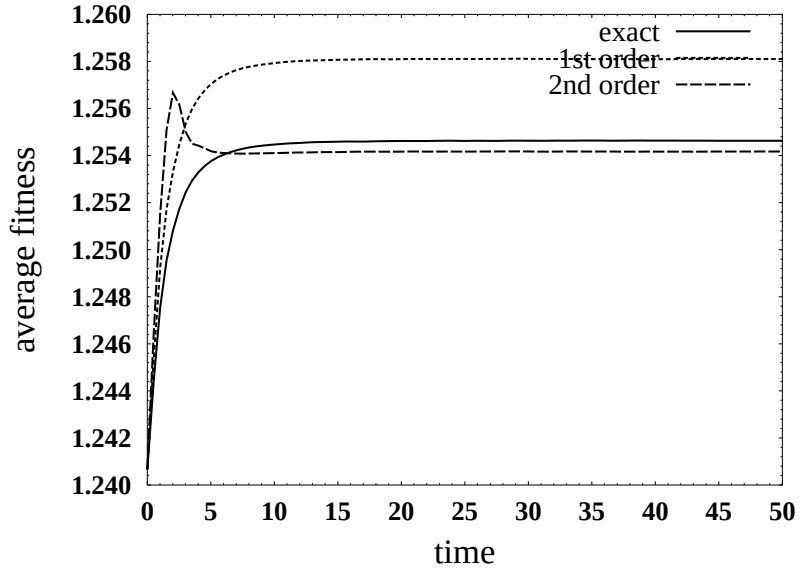

Figure 4. Average fitness for 7-bit random landscape model with 50% deviation from flat fitness limit

shorter strings the neglect of mutation events where a higher proportion of bits change is less valid.

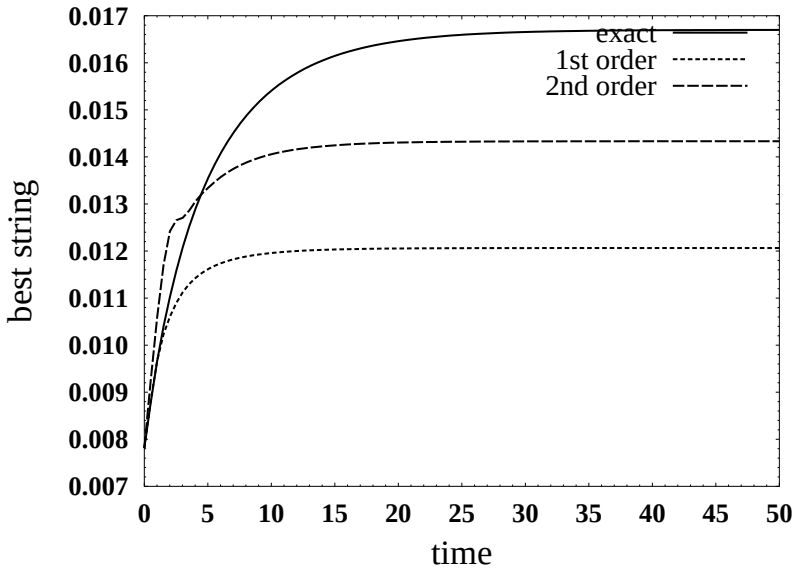

Figure 5. Proportion of optimal strings for 7-bit Eigen model with 50% deviation from flat fitness limit

6 Perturbation theory for Mutation-Selection Systems - A Simple Example

This section gives a fairly complete analysis of the case of one bit. Naturally, this is meant only to illustrate the general techniques and the relationship between the different methodologies in a transparent context. In this case a state is represented by the two-component vector $\begin{pmatrix} x_1(t+1) \\ x_0(t+1) \end{pmatrix}$ and $F = \begin{pmatrix} f_0 & 0 \\ 0 & f_1 \end{pmatrix}$

6.1 The Exact Solution

The exact solution is determined by calculating the eigenvalues and eigenvectors of $W = MF$. The eigenvalues are the solutions of the 2^N-dimensional characteristic equation, which in this case is quadratic with solutions

$$\lambda_{\pm} = \frac{1}{2}\left[(1-p)(f_1+f_0) \pm \beta_0\right], \tag{39}$$

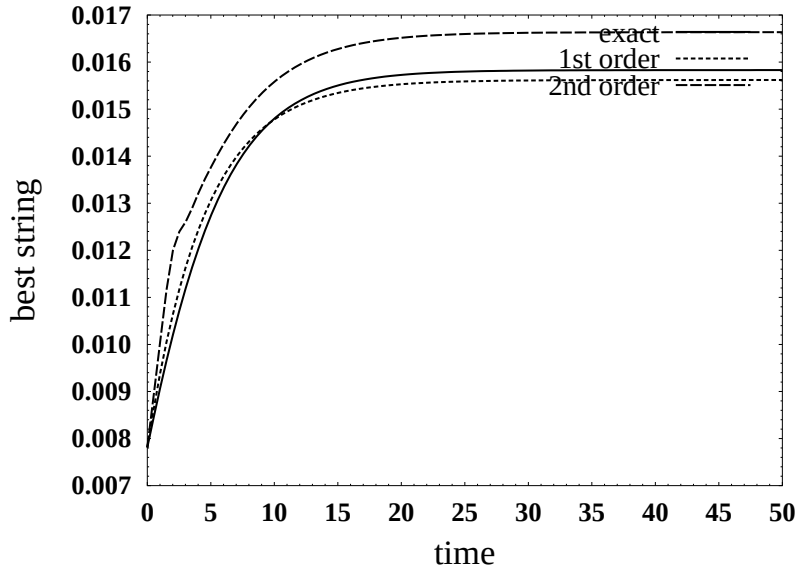

Figure 6. Proportion of optimal strings for 7-bit counting ones model with 50% deviation from flat fitness limit

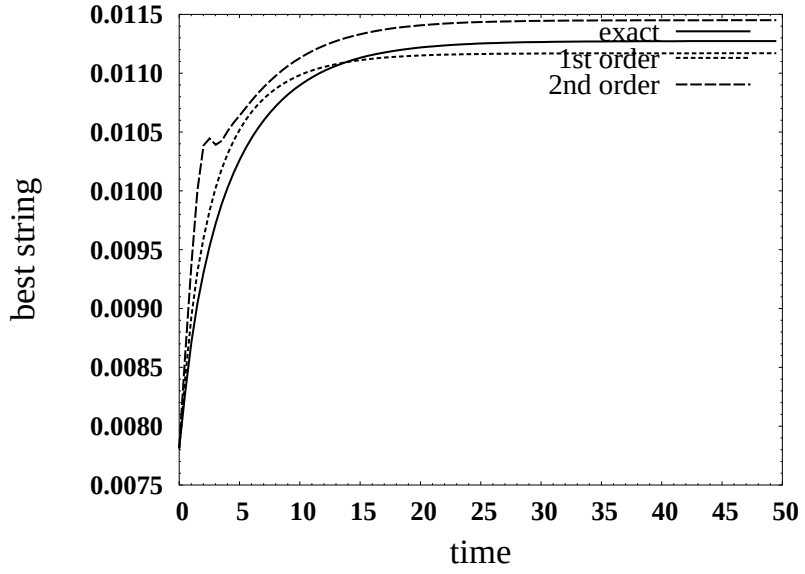

Figure 7. Proportion of optimal strings for 7-bit random landscape model with 50% deviation from flat fitness limit

where $\beta_0 = [(1-p)^2(f_1+f_0)^2 - 4(1-2p)f_1f_0]^{1/2}$. The corresponding eigenvectors are

$$\lambda_+ \to \begin{pmatrix} \alpha \\ b\alpha \end{pmatrix}, \qquad \lambda_- \to \begin{pmatrix} \beta \\ a\beta \end{pmatrix}, \tag{40}$$

where $a = \dfrac{-(1-p)f_1 + \lambda_-}{pf_0}$ and $b = \dfrac{-(1-p)f_1 + \lambda_+}{pf_0}$ and the normalisation factors are $\alpha = (1+b^2)^{-1/2}$ and $\beta = (1+a^2)^{-1/2}$. The transformation that diagonalizes W is implemented using the similarity-transformation matrix

$$\tilde{\Lambda} = \frac{1}{\alpha\beta(b-a)} \begin{pmatrix} -\alpha & b\alpha \\ \beta & -a\beta \end{pmatrix}, \tag{41}$$

which relates the eigenvector basis, $\tilde{x}_I$ and the string basis x_I via $\tilde{x}_I = \tilde{\Lambda}_I{}^J x_J$. The solution in the eigenvector basis is $\tilde{x}_I(t) = \lambda_I^t \tilde{x}_I(0)$ which, changing basis back to the string basis, gives the solution

$$x_I(t) = A_{I-}\lambda_-^t + A_{I+}\lambda_+^t \tag{42}$$

which is of the general form posited in equation (14). Explicitly, the four amplitudes, A_{ij}, $i = 0, 1$ and $j = \pm$, are

$$A_{1-} = \left(\frac{(\lambda_- - (1-p)f_0)x_1(0) + pf_0x_0(0)}{\lambda_- - \lambda_+} \right) \tag{43}$$

$$A_{1+} = \left(\frac{(-\lambda_+ + (1-p)f_0)x_1(0) - pf_0x_0(0)}{\lambda_- - \lambda_+} \right) \tag{44}$$

$$A_{0-} = \left(\frac{(\lambda_- - (1-p)f_1)x_0(0) + pf_1x_1(0)}{\lambda_- - \lambda_+} \right) \tag{45}$$

$$A_{0+} = \left(\frac{(-\lambda_+ + (1-p)f_1)x_0(0) - pf_1x_1(0)}{\lambda_- - \lambda_+} \right) \tag{46}$$

If we consider weak selection, i.e. $f_I \to (1+\epsilon f_I)$, or weak mutation, i.e. $M_I{}^J \to \delta_I{}^J + \epsilon d M_I{}^J$, then the eigenvalues (42) can be perturbatively expanded in ϵ. To $O(\epsilon)$ for weak mutation

$$\lambda_- = f_0(1-p) \qquad \lambda_+ = f_1(1-p) \tag{47}$$

While for weak selection, with $f_I \to 1 + f_I$,

$$\lambda_- = (1-2p)\left(1 + \frac{(f_0+f_1)}{2}\right) \quad \lambda_+ = \left(1 + \frac{(f_0+f_1)}{2}\right) \tag{48}$$

where we have put $\epsilon = 1$. The corresponding amplitudes for the case of weak selection can be found by expanding (43-46) to this order.

6.2 Diagrammatic Perturbation Theory

In this case one evaluates explicitly equations (33) or (38), corresponding to the diagrams in Figure 1, depending on the order of perturbation theory required.

To $O(\epsilon)$ the solutions for the case of weak selection are

$$\hat{x}_0(t) = \left(1 + \epsilon \widehat{dF}_0{}^0 t\right) \hat{x}_0(0) + \epsilon \left(\frac{1-(1-2p)^t}{2p}\right) \widehat{dF}_0{}^1 \hat{x}_1(0) \tag{49}$$

$$\hat{x}_1(t) = (1-2p)^t \left(1 + \epsilon \widehat{dF}_1{}^1 t\right) \hat{x}_1(0) + \epsilon \left(\frac{1-(1-2p)^t}{2p}\right) (1-2p) \widehat{dF}_1{}^0 \hat{x}_0(0) \tag{50}$$

which agree with the expressions derived from the exact solution *after* expanding in powers of ϵ *both* the amplitudes (43-46) and the factors λ^t, where the eigenvalues are given by (39), when expanded to $O(\epsilon)$. Notice the secular term linear in t. Schematically, this arises from expanding $\lambda^t = (a+\epsilon b+\epsilon^2 c+...)^t \approx a^t(1+\epsilon(b/a)t)$ to $O(\epsilon)$. Passing to the variables $\hat{P}_I(t)$, one finds $\hat{P}_0(t) = 1/2^{1/2}$ and

$$\hat{P}_1(t) = \frac{(1-2p)^t}{2^{\frac{1}{2}}} \left(\hat{P}_1(0) + \epsilon \widehat{dF}_1{}^1 \left(\frac{1-(1-2p)^{-t}}{1-(1-2p)^{-1}}\right) - \epsilon \widehat{dF}_1{}^0 \hat{P}_1^2(0) \left(\frac{1-(1-2p)^t}{1-(1-2p)}\right)\right) \tag{51}$$

Thus, we see that the secular terms cancel out of the $\hat{P}_I$ and hence out of the probabilities P_I. This however, is a property only of the one-bit case. For $N > 1$, generically they will remain. Although they do not destroy the validity of the perturbation expansion entirely, due to the presence of exponential suppression factors $(1-2p)^{|I|t}$, they do remain somewhat problematic, as we know that the exact functional form is a sum of pure exponentials. A polynomial times an exponential does not fit this pattern. This can be further understood by considering the contributions from $O(\epsilon^2)$.

$$\begin{aligned}\hat{x}_0(t) = 1^t \Bigg[& \Bigg(1 + \epsilon t \widehat{dF}_0{}^0 + \frac{\epsilon^2}{2} \widehat{dF}_0{}^0 \widehat{dF}_0{}^0 t(t-1) \\ & + \epsilon^2 \widehat{dF}_0{}^1 \widehat{dF}_0{}^1 \frac{(1-2p)}{2p}(t-1)\Bigg) \hat{x}_0(0) \\ & + \left(\frac{\epsilon}{2p} \widehat{dF}_0{}^1 + \frac{\epsilon^2}{2p} \widehat{dF}_0{}^0 \widehat{dF}_0{}^1 (t-1)\right) \hat{x}_1(0)\Bigg] \\ + (1-2p)^t \Bigg[& \left(-\frac{\epsilon}{2p} \widehat{dF}_0{}^1 - \frac{\epsilon^2}{2p} \widehat{dF}_0{}^1 \widehat{dF}_1{}^1 (t-1)\right) \hat{x}_1(0) \\ & + \epsilon^2 \widehat{dF}_0{}^1 \widehat{dF}_0{}^1 \frac{(1-2p)}{4p^2} \hat{x}_0(0)\Bigg]\end{aligned} \tag{52}$$

which agree with the expressions derived from the exact solution when expanded to $O(\epsilon^2)$.

Now, from (13), we know on general grounds the functional form of $\hat{x}_I(t)$, i.e. a sum of exponentials with different time independent amplitudes. In (52) there are exponentials, however, the exponents are what one would expect from the mutation only system as the perturbative expansions contain a part whose origin was the expansion of the eigenvalues of the exact expression. The question arises

then - is it possible to restore the general functional form of equation (13)? and thereby improve the approximation, and is it possible to separate out amplitudes from exponents? The answer to both these questions is yes and requires a tool known in physics as the renormalization group.

7 Perturbation Theory and the Renormalization Group

The solution to the two questions just posed begins with the observation that the secular terms invalidate perturbative expressions for $\hat{x}_I(t)$ when, for example, $\epsilon \widehat{dF}_0{}^0 t$ is no longer small. Notice for instance though, the first three coefficients of $\hat{x}_0(0)$ in the amplitude of the exponent of the leading eigenvalue - 1 - are the first three terms in an expansion of $(1 + \epsilon \widehat{dF}_0{}^0)^t$, i.e. an exponential. Notice further that from the exact answer (39) and its expansion to $O(\epsilon)$ for weak selection, as given in (27), that this posited exponential is the same as the perturbative expansion of the exact one. Thus, it would seem that a resummation of the perturbative series in (52) is required. However, given that we only have the first two terms in the equations how can we determine what the series should sum to? and how do we determine what should be summed and what shouldn't? At the heart of the problem is the fact that we are trying to be too greedy with the perturbative approximation. In the regime $\epsilon dFt \ll 1$ there is no problem. However, we wish to investigate the dynamics well away from the initial starting point at $t = 0$. To circumvent this difficulty we will introduce a new initial condition, $\hat{x}_I(\tau)$, at some arbitrary time τ and demand that the parameters $\hat{x}_I(\tau)$ are related to the physical initial conditions $\hat{x}_I(0)$ via

$$\hat{x}_I(0) = \sum_J \hat{Z}_I{}^J(\tau)\hat{x}_J(\tau) \tag{53}$$

and posit a perturbative expansion for the coefficients $Z_I{}^J$

$$\hat{Z}_I{}^J(\tau) = 1 + \sum_{n=1}^{\infty} \epsilon^n \delta_I{}^J a_I \tag{54}$$

The idea now is to "renormalize" (essentially reparameterize) (52) by replacing the $\hat{x}_I(0)$ using (53). It is important to note that the latter is an identity and so we are not changing anything by doing so. However, the coefficients a_I remain to be determined and at our disposal. We use the freedom in their definition to eliminate the secular terms in (52) at the particular time $t = \tau$. We will here carry this out to $O(\epsilon)$, the $O(\epsilon^2)$ and higher calculations being fairly straightforward (though eventually complicated) extensions. To $O(\epsilon)$ one finds

$$a_0 = a_1 = -\epsilon\tau \widehat{dF}_0{}^0 \tag{55}$$

Now, from (53), as $\hat{x}_I(0)$ is independent of τ so must be $\sum_J \hat{Z}_I{}^J(\tau)\hat{x}_J(\tau)$ which therefore must satisfy

$$\sum_J \hat{Z}_I{}^J(\tau+1)\hat{x}_J(\tau+1) = \sum_J \hat{Z}_I{}^J(\tau)\hat{x}_J(\tau) \tag{56}$$

Substituting in $\hat{Z}_I{}^J$ to $O(\epsilon)$ using (55) one finds

$$\hat{x}_I(\tau+1) = (1+\epsilon\widehat{dF}_I{}^I)\hat{x}_I(\tau) \tag{57}$$

which can be iterated to yield

$$\hat{x}_I(\tau) = (1+\epsilon\widehat{dF}_I{}^I)^\tau \hat{x}_I(0) \tag{58}$$

using as initial condition $\hat{x}_I(0)$. Substituting this expression into (52) and using our freedom to choose τ, we set $\tau = t$ to find

$$\hat{x}_0(t) = (1+\epsilon F_0{}^0)^t(\hat{x}_0(0) + \epsilon\frac{\widehat{dF}_0{}^1}{2p}\hat{x}_1(0)) - (1-2p)^t(1+\epsilon F_0{}^0)^t\epsilon\frac{\widehat{dF}_0{}^1}{2p}\hat{x}_1(0) \tag{59}$$

$$\begin{aligned}\hat{x}_1(t) = (1-2p)^t(1+\epsilon F_1{}^1)^t(\hat{x}_1(0) - \epsilon\frac{\widehat{dF}_0{}^1}{2p}\frac{(1-2p)}{2p}\hat{x}_0(0)) \\ +(1+\epsilon F_0{}^0)^t\epsilon\frac{(1-2p)\widehat{dF}_0{}^1}{2p}\hat{x}_0(0)\end{aligned} \tag{60}$$

These expressions are equivalent to the exact solution (42), where the eigenvalues $\lambda_\pm$ and the amplitudes A_{I-} and A_{I+} have been expanded to $O(\epsilon)$. Thus, the renormalization group has resummed the diagrammatic perturbation theory and thereby gives a better approximation than the latter. These statements are true for any N, although we are only illustrating the one-bit problem. In the latter case, when considering the $\hat{P}_I$ or P_I, because to $O(\epsilon)$ the approximate eigenvalues are of the form $\lambda_i^{(0)}(1+\epsilon F_0{}^0)$ for $i = +$ or $-$, and because in the non-renormalization group resummed perturbation theory of section 6.2 the secular terms cancel, the RG and non-RG resummed answers are the same. This is not true beyond lowest order or for $N > 1$.

8 Conclusions

We have introduced and proposed perturbation theory as a candidate tool for analysing the dynamics of EAs. We showed that within the umbrella of perturbative methods there are many different implementations. In the context of mutation-selection EAs we briefly discussed one of the most familiar ones, where the eigenvalues and eigenvectors of the transition matrix are computed perturbatively. This methodology has various drawbacks. In particular, the computation of the perturbed eigenvectors beyond leading order is complicated. Additionally, it lacks intuitive transparency. To ameliorate some of these defects we considered a perturbative calculation of the population variables themselves (really we are computing the transition matrix of the Markov chain $G_I{}^J(t,t')$, which is then used to compute the $P_I(t)$ via $P_I(t) = \sum_J G_I{}^J(t,t')P_J(t')$), using diagrammatic methods familiar from field theory, showing how a pictorial representation of the processes that contribute to the production of a given string could be systematically constructed using a simple set of rules.

As a simple illustration of the results one might expect we showed how the approximate solutions were close to the exact solutions for a variety of landscapes and for strings of length 7, even when the perturbation was quite large, the approximation systematically improving as different orders in ϵ were considered. To make transparent exactly how the methodology works we also considered a simple one-bit example. We showed that a defect of the direct diagrammatic expansion is the existence of "secular" terms and then introduced the renormalization group, which was seen to eliminate these secular terms to give uniform approximations for all t.

We emphasise that this paper is merely an introduction to these techniques and, given the lack of space, a brief one at that. Although we used a toy one bit example to illustrate in as simple a context as possible how the different perturbative implementations work and how they approximate the exact solution, we also showed that using diagrammatic methods one could push on to more realistic problems. How simple it is to implement the renormalization group in that context remains to be seen, as when there exist degenerate unperturbed eigenvectors a non-diagonal matrix renormalization is necessary. As at heart we are calculating the transition matrix for the Markov chain it should be relatively straightforward to include in finite population effects. All in all, we believe there to be a huge space in which further work may be carried out to check to what extent perturbative methods can help narrow the expectation gap between theoreticians and practitioners.

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