Complex Adaptations and the

Structure of Recombination Spaces

Günter P. Wagner[a,*] and Peter F. Stadler[b,c]

[a]Dept. of Ecology and Evolutionary Biology, Center for Computational Ecology,
Yale University, New Haven, CT 06520, USA

[b]Institut für Theoretische Chemie — Theoretische Biochemie
Universität Wien, A-1090 Vienna, Austria

[c]Santa Fe Institute, Santa Fe NM 87501, USA

*Mailing Address:
Günter P. Wagner
Dept. of Ecology and Evolutionary Biology, Center for Computational Ecology,
Yale University, New Haven, CT 06520, USA
E-Mail: `gpwag@peaplant.biology.yale.edu`

Abstract

According to the Darwinian theory of evolution, adaptation results from spontaneously generated genetic variation and natural selection. Mathematical models of this process can be seen as describing a dynamics on an algebraic structure which in turn is defined by the processes which generate genetic variation (mutation and/or recombination). The theory of complex adaptive system has shown that the properties of the algebraic structure induced by mutation and recombination is more important for understanding the dynamics than the differential equations themselves. This has motivated new directions in the mathematical analysis of evolutionary models in which the algebraic properties induced by mutation and recombination are at the center of interest. In this paper we summarize some new results on the algebraic properties of recombination spaces. It is shown that the algebraic structure induced by recombination can be represented by a map from the pairs of types to the power set of the types. This construct is called P-structure. Utilizing this approach deep commonalties between the recombination spaces defined by string recombination models and the corresponding point mutation spaces can be shown. Each fitness landscape which is elementary for point mutation is also elementary for string recombination. This is an unexpected result because of the fundamentally different nature of mutation and recombination processes.

1. Introduction

Evolutionary change is caused by the spontaneously generated genetic variation and its subsequent fixation by drift and/or selection. Consequently, the main focus of evolutionary theory has been to understand the genetic structure and dynamics of populations. This objective of neo-Darwinian theory influenced the mathematical face of evolutionary theory. It mainly consists of mathematical statistics, necessary to understand the genetic structure of populations and the stochastic forces acting on it, and dynamical systems theory, which is used to model natural selection. In recent years, however, algebraic methods and approaches have gained increasing prominence in evolutionary theory. This development has been stimulated to some extend by the application of evolutionary models to design so-called evolutionary algorithms, for instance the Genetic Algorithms, Evolution Strategies, and Genetic Programming, as well as the theory of complex adaptive systems. In addition the availability of large amounts of sequence data for phylogenetic analysis generated a demand for a deeper understanding of combinatorial optimization problems. In both cases mathematical problems arose that are beyond the reach of traditional evolutionary models. Here we will deal with developments motivated by the analysis of complex adaptations and genetic algorithms.

Given the bi-phasic nature of the evolution process, in which the genetic variation is generated independently from the natural selection acting in it, the generic structure of an evolutionary model can be written as

$$x' = S\left(\{x, w\}\right) + T\left(\{x, t\}\right) \tag{1}$$

where x describes the frequency distribution over types (genotypes, gametes, etc.) and $S\left(\{x, w\}\right)$ is a term describing the selection forces acting on x. The parameters w are also called fitness function, since it is a mapping from the set of types into the real numbers. The second term $T\left(\{x, t\}\right)$ describes the transmission processes, by determining the probability which transforms one type into another by mutation and/or recombination [1] Hence, evolution models can be seen as dynamical systems which live on an algebraic structure determined by the genetic processes like mutation and recombination.

If one considers just a limited number of types (or some highly symmetrical cases) the behavior of the system can be understood by the selection forces plus perturbations caused by the transmission processes (see [8] for a review of mutation-selection theory). The dynamical systems approach, however, turned out to be less informative if applied to systems containing a large number of types and/or highly irregular fitness functions. These situations occur for instance in the application of mutation/recombination selection algorithms and if one wants to understand the evolution of complex adaptations. In these situations, the algebraic structure on which the dynamical system is realized is more important to understand the behavior of the system than the dynamical equations themselves. The reason is that the global behavior of a genetic algorithm, for instance, is mostly determined by the accessibility of better types by mutation and recombination from the already realized types. Accessibility of a type is largely determined by the mutation/recombination steps necessary to reach the type and whether the intermediary types are selectively advantageous or not. Metaphorically, the dynamics of a mutation-selection process can be seen as a walk on a landscape, where uphill moves are preferred. The ability to evolve certain types of organisms is influenced by the topological features of the fitness landscape. This realization led to what is now called "landscape theory".

The idea of landscape models has several roots. In evolutionary theory it can be traced back to Wright's ideas about adaptive landscapes, (see [48, pp. 304-317], and became important in theories of molecular evolution and the origin of life [15, 14, 20, 22, 35, 38, 47, 50, 49]. and in evolutionary computer science [36]. Similar developments exist in physics, where free energy landscapes are considered, and in search theory [53]. The main challenge to landscape theory is to determine which features of the fitness landscape determine the evolvability of the systems on the landscape.

A landscape results from the combination of three elements. A set of types V, which in genetics can be genotypes or gametes, a set of operators which act on the types to create other types, and a fitness function f. Operators induce a topological structure $\mathcal{X}$ on V; we call $(V, \mathcal{X})$ the configuration space. A fitness function imposed on a configuration space is then a landscape in which terms like peak, valley, etc. are defined. A simple example of a configuration space is the set of strings of characters, like A, G, C and T, and point mutations. In this case, the configuration space can be represented as a graph, where all the types that can be converted into each other by replacing one character by another are connected by an edge. The resulting graph is known as Hamming graph, sequence space, or point mutation space. The ease with which the point mutation space is constructed comes from the fact that the mutation operator has only one argument and the resulting topology can be represented as a simple graph.

In biology and genetic algorithm theory, the landscape concept can only be useful if it can accommodate the action of recombination. There are two chief difficulties in achieving this. One is that recombination is an operator with two arguments, and the other is that the probability of a particular recombination event depends on the frequency of matings between the two types. The latter in turn depends on the frequency of types in the population and the structure or the configuration space is thus population dependent. In this contribution we deal only with the first problem by assuming that all types are equally frequent.

The most immediate consequence of the fact that recombination acts on two arguments is that the recombination induced configuration space can not be represented as a simple graph on the set of types. These leaves two alternatives:

- One can either change the nature of the vertex set and have pairs of types as vertices. Then one obtains again a (di-)graph, since each elementary recombination event creates up to two strings. This approach was pioneered by Culberson [11] and Jones [36]. It creates two new difficulties, however:
  (1) recombination spaces with pairs of strings as vertices are difficult to compare with the corresponding mutation spaces which have single strings as vertices.
  (2) The pairs of strings representing the vertices in this construction have no reality in the structure of the population, in particular if mating is not strictly monogamous.
- The alternative is to make the edges more complex and used a hypergraph representation. In [23] it was shown that recombination spaces can be represented as hypergraphs, where the hyperedges represent the set of all recombinants that can come from the recombination of two types. With this construction is was easy to show that string recombination spaces and point mutations spaces are homomorphic.

We prefer the second approach, i.e., leaving each type as a vertex and increase the complexity of the edges. Hypergraphs are still not completely satisfactory, however, since they do not indicate which pair of types produces which set of recombinants, i.e., which hyperedge arises from which mating. This led to the invention of P-structures [57], which are a mappings of pairs of types to the hyperedges of the hypergraph (see section 3). With P-structures it is now possible to apply Fourier decomposition theory to recombination landscapes, an approach that proved useful in the case of mutation-based landscapes.

2. Landscapes on Graphs

2.1. Fourier Series on Graphs

Landscapes on finite undirected graphs are discussed in detail in ref. [54]. A finite graph $\Gamma = (V, E)$ is faithfully described by its *adjacency matrix* $\mathbf{A}$ with entries $\mathbf{A}_{xy} \stackrel{\text{def}}{=} 1$ if $\{x, y\}$ is an edge of Γ and $\mathbf{A}_{xy} \stackrel{\text{def}}{=} 0$ otherwise. We shall write $N \stackrel{\text{def}}{=} |V|$ for the total number of configurations. The number of neighbors of a vertex $x \in V$ is called the *degree* of x; by $\mathbf{D}$ we denote the diagonal matrix of the vertex degrees. It turns out that the *graph Laplacian* $-\Delta \stackrel{\text{def}}{=} \mathbf{D} - \mathbf{A}$ provides a more convenient description of Γ. This matrix is related to the more familiar differential operator Δ in continuous spaces, see [3, 28, 44, 51]. The graph Laplacian $-\Delta$ is non-negative definite, and the smallest eigenvalue $\lambda_0 = 0$ has multiplicity 1 if and only if Γ is a connected graph. A graph is *regular* if all vertices have the same vertex degree, i.e., $\mathbf{D} = D\mathbf{I}$, where $\mathbf{I}$ is the identity matrix and D is the common degree of all vertices. Our prime interest here is sequence spaces which are regular of degree $D = (\alpha - 1)n$, where n is the sequence length and α is the number of different letters in the alphabet. Throughout this section we shall assume that Γ is regular and connected.

Let $f : V \to \mathbb{R}$ be a *fitness function.* A series expansion $f(x) = \sum_{i=1}^{N} a_i \varphi_i(x)$, where the φ_i form a complete and orthonormal system of eigenfunctions of the graph Laplacian $-\Delta$, is termed a *Fourier series* expansion of f on Γ. Note that we write $\varphi_i(x)$ to mean the x-component of the vector φ_i throughout this paper. A landscape is called *elementary* if it is of the form $f(x) = c + \varphi(x)$, where c is an arbitrary constant and φ is an eigenvector of the graph-Laplacian belonging to an eigenvalue $\lambda > 0$, see [29, 54]. Elementary landscapes form an important class because the landscape of the most intensively studied combinatorial optimization problems, such as the travelling salesman problem [40], the graph bipartitioning problem, or the graph coloring problem, are of this type when the configuration space (graph) Γ is chosen in a natural way [29].

For boolean hypercubes defined on the alphabet $\{+1, -1\}$, a Fourier basis can easily be determined explicitly. The *p-spin function* or *Walsh function*

$$\varepsilon_I(x) \stackrel{\text{def}}{=} \prod_{j\in I} x_j \qquad \text{with} \quad I \subseteq \{1, \ldots, n\} \quad \text{and} \quad p = |I| \tag{2}$$

is an eigenvector of $-\Delta$ belonging to the eigenvalue $\lambda_p = 2p$, see e.g., [59]. We remark that Derrida's p-spin Hamiltonians [13, 12], which are important models in spin glass physics, are superpositions of these basis functions containing only contributions with a single interaction order $p > 0$. This is to say that the p-spin Hamiltonians are eigenfunctions of the Laplacian of the Boolean hypercube.

A *schema* is a hyperplane in sequence space. It is defined by the set H of "fixed" bits and their values h_i, $i \in H$. In symbols: $\mathcal{H} = \{x \in V | \forall i \in H : x_i = h_i\}$. Schemata and Walsh functions have been used extensively in the analysis of GA behavior, see e.g. [25, 26, 27, 41, 46]. In order to connect to this line of work we repeat here the explicit expressions for the average fitness of schema $\mathcal{H}$ and for the variance on $\mathcal{H}$ in our notation:

$$f(\mathcal{H}) = \sum_{I\subseteq H} a_I \varepsilon(h) \qquad \text{var}(\mathcal{H}) = \sum_{I\subseteq H} \left\{ \sum_{K\not\subseteq H} a_K a_{K\triangle I} \right\} \varepsilon_I(h)\,, \tag{3}$$

where $I\triangle J$ denotes the symmetric difference of the sets I and J. Note that these quantites are superpositions of Walsh functions with index set $I \subseteq H$ evaluated at the fixed bits of the schema. It is interesting that $f(\mathcal{H})$ depends only on Fourier coefficients a_I with $I \in H$, while $\text{var}(\mathcal{H})$ depends only on coefficients with $I \not\subseteq H$. A generalization of Walsh functions to non-binary strings in discussed in [18].

2.2. Correlation Functions

If a simple algebraic description of a landscape is not available we need a condensed description of its salient features. This is because the extremely large number of configurations, for instance $N = 4^n$ for RNA sequences or $N = n!$ for n-city travelling salesman problems, renders a complete "listing" infeasible. Correlation measures relating the values of nearby configurations with each other seem to be a natural approach.

Defining mean and variance[1] of a landscape f by

$$\overline{f} \stackrel{\text{def}}{=} \frac{1}{N}\sum_{x\in V} f(x) \qquad \text{and} \qquad \sigma_f^2 \stackrel{\text{def}}{=} \frac{1}{N}\sum_{x\in V}\left(f(x)-\overline{f}\right)^2 = \overline{f^2}-\overline{f}^2 \tag{4}$$

we note that $\sigma_f^2 = 0$ if and only if f is constant, i.e., for *flat* landscapes. Two types of *correlation functions* have been investigated. Eigen and co-workers [14] introduced

$$\rho(d) \stackrel{\text{def}}{=} \frac{\langle f(x)f(y)\rangle_{d_H(x,y)=d} - \overline{f}^2}{\sigma_f^2}\,, \tag{5}$$

where the notation $\langle\,.\,\rangle_{d(x,y)=d}$ indicates the mean value is calculated from all pairs of sequences x, y with Hamming distance [30] $d_H(x,y) = d$. An alternative approach has been explored by Weinberger [58]. A simple random walk $\{x_0, x_1, \ldots\}$ on the vertex set of Γ generates a "time series" $\{f(x_0), f(x_1), \ldots\}$ with the autocorrelation function

$$r(s) \stackrel{\text{def}}{=} \frac{\langle f(x_t)f(x_{t+s})\rangle_{x_0,t} - \langle f(x_t)\rangle_{x_0,t}\,\langle f(x_{t+s})\rangle_{x_0,t}}{\sqrt{\left(\langle f(x_t)^2\rangle_{x_0,t} - \langle f(x_t)\rangle_{x_0,t}^2\right)\,\left(\langle f(x_{t+s})^2\rangle_{x_0,t} - \langle f(x_{t+s})\rangle_{x_0,t}^2\right)}} \tag{6}$$

The notation $\langle\,.\,\rangle_{x_0,t}$ emphasizes that the expectation is taken over all "times" t and all initial conditions x_0. We will refer to $r(s)$ as the *"random walk" correlation*

[1] There is nothing "statistical" about $\overline{f}$ or σ_f^2. Both quantities are functionals of f. They should not be mistaken for the averages over different instances that are commonly used in a statistical mechanics type analysis of what one might call statistical models of landscapes (random fields) [43].

function of the landscape f on Γ. A simple random walk [52] on a graph Γ has transition matrix $\mathbf{T} \stackrel{\text{def}}{=} \mathbf{A}\mathbf{D}^{-1}$. It can be shown [54] that

$$r(s) = \frac{1}{\sigma_f^2}\left[\frac{1}{N}\langle f, \mathbf{T}^s f\rangle - \overline{f}^2\right] \tag{7}$$

for a regular graph Γ. The two correlation measures $r(s)$ and $\rho(d)$ are closely related to each other, since $r(s) = \sum_{d=0}^{d_{\max}} \phi_{sd}\rho(d)$, where $d_{\max}$ is diameter of the graph Γ and ϕ_{sd} is the probability that a simple random walks of s steps ends in distance d from its starting point [58]. In particular, the nearest neighbor correlation satisfies $\varrho = r(1) = \rho(1)$.

It has been shown [54] that there is an intimate relationship between the Fourier expansion of a landscape and the form of its correlation functions $\rho(d)$ and $r(s)$. For sequence spaces[2] (Hamming graphs) one has

Proposition 1. [54] Let f be a non-flat landscape on the sequence space (Hamming graph) $\mathcal{Q}_\alpha^n$. Then the following statements are equivalent:

(i) f is elementary with $\lambda = p\alpha$.

(ii) The "random walk" correlation function is exponential,

$$r(s) = \varrho^s = (1-\lambda/D)^s = \left(1 - \frac{\alpha}{\alpha-1}\frac{p}{n}\right)^s . \tag{8}$$

(iii) The "direct" correlation function is a Krawtchouk polynomial,

$$\rho(d) = \omega_p^{n,\alpha}(d) \stackrel{\text{def}}{=} \frac{1}{\binom{n}{p}(\alpha-1)^p}\sum_{j=0}^{p}(-1)^j(\alpha-1)^{p-j}\binom{d}{j}\binom{n-d}{p-j} . \tag{9}$$

Since any landscape on Γ is necessarily a superposition of elementary landscapes, their correlation functions are superpositions as well. Let $f = \sum_j a_j\varphi_j$ be a Fourier expansion of f, and denote by λ_p the distinct eigenvalues of $-\Delta$. Furthermore, let I_p be the set of all indices k for which $\Delta\varphi_k + \lambda_p\varphi_k = 0$. The value $p = 0$

[2] Analogous results hold for all distance regular graphs.

corresponds to the flat component of the landscape. Defining the *amplitude* of the p-ary interactions as

$$B_p \overset{\text{def}}{=\!=} \frac{\sum_{k\in I_p} |a_k|^2}{\sum_{k\neq 0} |a_k|^2} . \tag{10}$$

we have $B_p \geq 0$ and $\sum_p B_p = 1$. As a by-product of the proof of Proposition 1 it can be shown [54] that the Fourier expansion of f translates directly into an expansion of the correlation functions:

Proposition 2. $r(s) = \sum_{p\neq 0} B_p(1-\lambda_p/D)^s$ and $\rho(d) = \sum_{p\neq 0} B_p\omega_p^{n,\alpha}(d)$.

Given a landscape, the crucial information about its correlation structure is therefore contained in the amplitudes B_p which describe the relative importance of the different elementary components and the eigenvalues λ_p which describe the ruggedness of the individual components.

2.3. Ruggedness

The eigenstructure of the graph Laplacian offers a promising formalism for relating the correlation structure of a landscape to the geometry of its local optima. In fact, the geometric structure of an elementary landscape is closely related to the eigenvalue of the graph Laplacian to which f belongs.

- The solutions of the *Laplace equation* $\Delta f = 0$ form the *harmonic functions* on Γ. It is well known that there are no non-trivial harmonic functions on finite connected graphs; see, e.g., [4, 51]. The harmonic functions are therefore the flat landscapes.
- Define the sets $V_+ = \{x \in V | f(x) \geq 0\}$ and $V_- = \{x \in V | f(x) \leq 0\}$ of all vertices on which f is non-negative or non-positive, respectively, and denote the corresponding induced subgraphs by Γ_+ and Γ_-. The connected components of Γ_+ and Γ_- are called the *nodal domains* of f. The second smallest eigenvalue λ_1 of the graph Laplacian $-\Delta$, which is positive for all connected graphs, is called the *algebraic connectivity* of Γ. A theorem by Fiedler [16, 17], see also

[7, Thm.2.5.7], states that both Γ_+ and Γ_- are connected in this case, i.e., there are exactly two nodal domains. Following a suggestion by Kauffman [37] we term this type of landscape *Fujijama" landscapes* because they consist of a single "mountain" Γ_+. For Hamming graphs a much stronger result holds: Fujijama landscapes have no non-global minima or maxima [53].

- The geometry of the nodal domains of a landscape f is of course a very important characteristic of the landscape. Courant's *nodal domain* theorem[3], which has been proved recently for graphs [10], states that, if all eigenvalues of $-\Delta$ are labeled in ascending order, $0 = \lambda_0 \leq \lambda_1 \leq \ldots \leq \lambda_{N-1}$, then the number of nodal domains of an eigenfunction f belonging to λ_k is at most $k+1$.
- Grover [29] observed that the local optima have a characteristic distribution on elementary landscapes: Let $z_{\min}$ and $z_{\max}$ be a local minimum and a local maximum, respectively. Then $f(z_{\min}) \leq \bar{f} \leq f(z_{\max})$. In other words, all local maxima are in Γ_+ and all local minima are in Γ_- if f is an eigenvector of $-\Delta$.
- A heuristic argument [56] suggests that there should be approximately one local optimum of a landscape in a ball with a radius determined by the *correlation length*
$$\ell \stackrel{\text{def}}{=\!=} \sum_{s=0}^{\infty} r(s)\,. \tag{11}$$
Numerical computations [21, 39, 55, 56] show that this estimate is remarkably accurate for elementary landscapes fulfilling a certain maximum entropy condition.

The correlation length ℓ defined in equ.(11) is also closely related to the spectrum: we have
$$\ell = \sum_{p\neq 0} B_p \sum_{s=0}^{\infty} (1-\lambda_p/D)^s = D \sum_{p\neq 0} B_p \lambda_p^{-1}\,, \tag{12}$$
i.e., the correlation length of a landscape is determined by the harmonic mean of the eigenvalues of the Laplacian λ_p of the configuration space weighted by the amplitudes B_p of the landscape. For an elementary landscape we have in particular $\ell = D/\lambda_p$. In addition, there is ample evidence that the correlation length ℓ of a landscape is closely related to the performance of optimization heuristics, see e.g., [42, 19, 20, 50].

[3] The original version of this theorem holds for Riemannian manifolds, see [9].

3. P-Structures and Hypergraphs

3.1. Weighted and Unweighted P-Structures

Search processes using mutations, i.e., rules to modify individual configurations, impose a graph structure on V by assigning edges between configurations that are accessible from each other by a single "move". The search in genetic algorithms works quite differently: two configurations from a population are chosen and a so-called crossover (or recombination) operator creates "offsprings" from the two "parents". In this section we introduce a discrete mathematical structure which allows for a discussion of recombination-like search by methods from algebraic graph theory.

Definition. Let V be a finite set with power set $\mathcal{P}(V)$. A *P-structure*[4] is a pair $(V, \mathcal{R})$ where $\mathcal{R} : V \times V \to \mathcal{P}(V)$. We say that the P-structure is *symmetric* if $\mathcal{R}(x, y) = \mathcal{R}(y, x)$ for all $x, y \in V$.

The *support* pf the P-structure $(V, \mathcal{R})$ is the (pseudo)digraph supp$\mathcal{R}$ with vertex set V and edge set $E_{\mathcal{R}} \stackrel{\text{def}}{=} \big\{(x, y) \in V \times V \,\big|\, \mathcal{R}(x, y) \neq \emptyset \big\}$. Note that supp$\mathcal{R}$ has a loop at vertex x whenever $\mathcal{R}(x, x) \neq \emptyset$. We set $M \stackrel{\text{def}}{=} |E_{\mathcal{R}}|$. In the case of symmetric P-structures then we can regard supp$\mathcal{R}$ as an undirected pseudograph (possible with loops). Throughout this paper we shall assume $\mathcal{R}(x, y) \neq \emptyset$ for all $x, y \in V$, i.e., supp$\mathcal{R}$ will always be the complete di-graph with loops and thus $M = N^2$.

A *hypergraph* [2] consists of a vertex set V and a collection $\mathcal{E}$ of (not necessarily) distinct subsets of V which are called (hyper)edges. The hypergraph imag$\mathcal{R}$ with vertex set V and (hyper)edge multiset $\mathcal{E} \stackrel{\text{def}}{=} \{\mathcal{R}(x, y) \in \mathcal{P}(V) \,|\, \mathcal{R}(x, y) \neq \emptyset$ and $x, y \in V\}$ is the called the *image* of $(V, \mathcal{R})$. This construction has been

[4]The term "P-structure" has been chosen because its image set is the **p**ower set of V.

used in [23] in order to represent the structure of recombination on a finite set of genotypes. The hypergraph imag$\mathcal{R}$ has in general multiple edges. In particular, if $\mathcal{R}$ is symmetric, any set $\mathcal{R}(x,y)$ appears at least twice if $x \neq y$.

The *(unweighted) incidence matrix* $\mathbf{H}$, which is defined component-wise by

$$\mathbf{H}_{x,(y,z)} \stackrel{\text{def}}{=} \begin{cases} 1 & \text{if } x \in \mathcal{R}(y,z) \\ 0 & \text{otherwise}, \end{cases} \tag{13}$$

uniquely determines the P-structure $(V,\mathcal{R})$. It seems natural to generalize equ.(13) by introducing arbitrary positive weights $\mathbf{H}_{x,(y,z)}$ whenever $x \in \mathcal{R}(y,z)$. This is necessary to reflect the fact that certains types in $\mathcal{R}(y,z)$ are produced more frequently than others. In this case we shall call $\mathbf{H}$ the incidence matrix of a *weighted* P-structure and set

$$\eta(y,z) \stackrel{\text{def}}{=} \sum_{x\in V} \mathbf{H}_{x,(y,z)} \,. \tag{14}$$

For an unweighted P-structure we have $\eta(y,z) = |\mathcal{R}(y,z)|$, which is the degree of the hyperedge $\mathcal{R}(y,z)$ in imag$\mathcal{R}$.

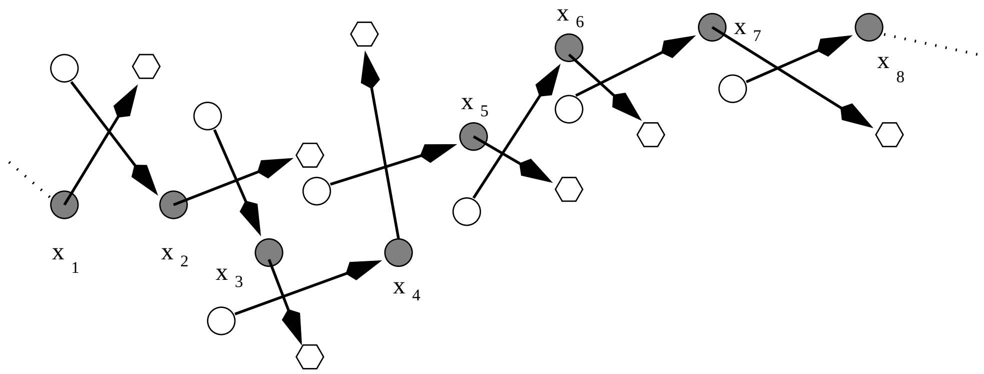

Figure 1: Random Walk on V induced by the mapping $\mathcal{R}$.

From the incidence matrix $\mathbf{H}$ we define the *transition matrix* of a (weighted or unweighted) P-structure by

$$S_{xy} \stackrel{\text{def}}{=} \frac{1}{V} \sum_{z\in V} \mathbf{H}_{x,(y,z)} \eta(y,z)^{-1} \,. \tag{15}$$

It describes how the map $\mathcal{R}$ can be used to generate a random walk on V: Starting with an arbitrary pair of parents, $\mathcal{R}$ produces a set of offsprings (possibly with different weights). From those we choose one (with a probability proportional to its weight) and mate it with a random element of V. The procedure is repeated. The offsprings selected at each step form a walk $\{x_0, x_1, \ldots\}$ on V, see figure 1. Obviously, $\mathbf{S}$ is the transition matrix of the corresponding Markov process. In [57] we argue that $\mathbf{S}$ (with a different normalization) can be interpreted as a generalization of the adjacency matrix of a graph.

3.2. Symmetries of P-Structures

Let us now turn to the symmetries of P-structures. An *automorphism* of a (weighted or unweighted) P-structure $(V,\mathcal{R})$ is a mapping $\psi : V \to V$ with the property

$$\mathbf{H}_{\psi(x),(\psi(y),\psi(z))} = \mathbf{H}_{x,(y,z)} \qquad \text{for all} \quad x,y,z \in V\,. \tag{16}$$

The set of all automorphisms of a P-structure forms of course a group (under composition) which we shall denote by $\mathbf{Aut}[V,\mathcal{R}]$. Any automorphism of a P-structure is a graph automorphism of $\mathrm{supp}\mathcal{R}$ and $\mathrm{bbg}\mathcal{R}$ as well as a hypergraph automorphism of $\mathrm{imag}\mathcal{R}$. Therefore $\mathbf{S}$ is also invariant under P-structure automorphisms [57]. This observation will be of particular importance for our discussion.

A permutation group is said to act *transitively* of a set V if for any two elements $x,y \in V$ there is a group element $\psi \in \mathbf{Aut}[V,\mathcal{R}]$ such that $y=\psi(x)$. A permutation group on V is *generously transitive* [6, 24] if for any two elements $x,y\in V$ there is a group element ψ such that $\psi(x)=y$ and $\psi(y)=x$. We say that $(V,\mathcal{R})$ is *vertex transitive* (*generously transitive*) if $\mathbf{Aut}[V,\mathcal{R}]$ acts (generously) transitively on V. This is analogous to the corresponding definition for graphs.

Consider now the *orbits* of $\mathbf{Aut}(V,\mathcal{R})$ on the set $V\times V$ of vertex pairs, that is, the sets of the form

$$\mathcal{X} = \left\{ (x,y) \middle|\, \exists\psi \in \mathbf{Aut}[V,\mathcal{R}] : \quad x=\psi(x_0),\, y=\psi(y_0) \right\} \tag{17}$$

that are generated by applying all P-structure automorphism to a pair (x_0, y_0) of reference vertices. To each orbit $\mathcal{X}$ we can associate a characteristic matrix $\mathbf{X}$, with entries $\mathbf{X}_{xy} = 1$ if $(x, y) \in \mathcal{X}$ and $\mathbf{X}_{xy} = 0$ otherwise. These matrices are by construction invariant under all P-structure automorphisms and they form a basis of a matrix algebra $\mathcal{A}[V, \mathcal{R}]$ which is coherent in the sense of Higman [31, 32, 33], see e.g., [6, chap.2] for detailed discussion. We note that $\mathbf{I}, \mathbf{J}, \mathbf{S} \in \mathcal{A}[V, \mathcal{R}]$.

If the group $\mathbf{Aut}[V, \mathcal{R}]$ is generously transitive then $\mathcal{A}[V, \mathcal{R}]$ is a commutative algebra consisting of symmetric matrices. It is the so-called Bose-Mesner algebra [5] of a (symmetric) association scheme, see [6, 24] for details. For our purposes only the following proposition, which is a trivial rewriting of well known properties of symmetric association schemes, will be of importance.

Proposition 3. Suppose the P-structure $(V, \mathcal{R})$ is generously transitive. Then there is a common basis $\{\varphi_k\}$, $1 \leq k \leq N$, of eigenvectors for all matrices $\mathbf{Y} \in \mathcal{A}[V, \mathcal{R}]$. We shall call $\{\varphi_k\}$ a *Fourier basis* of the (generously transitive) P-structure.

3.3. The Backbone Graph of a P-Structure

The set of pairs (x, y), $x \neq y$, with $\mathcal{R}(x, y) = \{x, y\}$ plays a special role in a P-structure. Such a pair can be interpreted as an analogue of a fixed point (under repeated application of $\mathcal{R}$) which implies an intuitive notion of "closeness". The set of all such edges introduces a digraph on V which we call the *backbone graph* bbg$\mathcal{R}$ of $(V, \mathcal{R})$. P-structures do not necessarily have non-trivial backbone graphs: if imag$\mathcal{R}$ does not contain (hyper)edges of degree 2 then bbg$\mathcal{R}$ is the "discrete" graph that does not contain any edges. However, if bbg$\mathcal{R}$ is a connected graph then it defines **a** natural metric on V. We shall see in the next section that the backbone graph of certain string recombination P-structures are exactly the Hamming graphs. The adjacency matrix of the backbone graph bbg$\mathcal{R}$, $\mathbf{G}$, is of course also contained in the algebra $\mathcal{A}[V, \mathcal{R}]$.

Definition. Suppose bbg$\mathcal{R}$ is a connected graph and let $d : V \times V \to \mathbb{R}$ be the associated metric distance on V. We say that the P-structure is distance transitive with respect to its backbone (*b.d.transitive*) if for any two pairs (x, y) and (u, v) with $d(x, y) = d(u, v)$ there is an automorphism $\psi \in \mathbf{Aut}[V, \mathcal{R}]$ such that $x = \psi(u)$ and $y = \psi(v)$. Connectedness of bbg$\mathcal{R}$ is a crucial condition in the above definition; it cannot be relaxed.

Theorem 1. [57] If $(V, \mathcal{R})$ is a b.d.transitive P-structure then its Bose-Mesner algebra $\mathcal{A}[V, \mathcal{R}]$ coincides with the adjacency algebra of the backbone graph bbg$\mathcal{R}$, i.e., $\mathcal{A}[V, \mathcal{R}]$ is generated by $\mathbf{G}$.

The algebraic properties of a b.d.transitive P-structure are therefore determined already by its backbone graph, or more precisely by the adjacency algebra of bbg$\mathcal{R}$. The adjacency algebra of graphs is discussed in some detail in [3]. The backbone graph of a b.d.transitive P-structure is of course always distance transitive. We shall see in the next sections that some important recombination P-structures are b.d.transitive.

4. String Recombination Structures

4.1. Crossover Operators and Recombination Structures

Gitchoff and Wagner [23] used the following axioms to describe the action of a recombination in terms of what we call here P-structures.

Definition. A P-structure $(V,\mathcal{R})$ is a *recombination structure* if for all $x,y,z\in V$ holds:

(i) $\mathcal{R}(x,x)=\{x\}$.

(ii) $\mathcal{R}(x,y)=\mathcal{R}(y,x)$.

(iii) $\{x,y\}\subseteq\mathcal{R}(x,y)$.

(iv) For all $z\in\mathcal{R}(x,y)$ holds $|\mathcal{R}(x,z)|\le|\mathcal{R}(x,y)|$.

The effect of a crossover operator χ is to separate two subsets of string positions. By abuse of notation we shall write χ for the set of string positions that are exchanged among the two parent-strings; $\bar\chi$ is the complement of χ in $\{1,\dots,n\}$. Hence there is a one-to-one correspondence between the set of crossover operators acting on strings of length n and the partitions of $\{1,\dots,n\}$ into two non-empty subsets. In addition it will sometimes be convenient to consider the identity operator ι with $\iota(y,z)=\{y,z\}$ as crossover operator. We have therefore $\chi(y,z)=\{x,\bar x\}$ with

$$x_k=\begin{cases} y_k & \text{if} \quad k\in\chi\\ z_k & \text{if} \quad k\in\bar\chi\end{cases}\qquad \bar x_k=\begin{cases} y_k & \text{if} \quad k\in\bar\chi\\ z_k & \text{if} \quad k\in\chi\end{cases}\tag{18}$$

We follow here the spirit of [36] when we regard a crossover operator as producing pairs of sequences rather than a single sequence from a pair of “ancestors”. For each crossover operator we define the weighted incidence matrix

$$\mathbf{H}^{\chi}_{x,(y,z)}=\begin{cases} 2 & \text{if} \quad x=y=z\\ 1 & \text{if} \quad x\in\chi(y,z) \qquad \text{and } y\neq z\\ 0 & \qquad\text{otherwise}\end{cases}\tag{19}$$

Now consider a family $\mathcal{F}$ of crossover operators acting on strings of length n. The family $\mathcal{F}$ gives rise to a (weighted) P-structure with

$$\begin{aligned} \mathcal{R}(y,z) &= \big\{ x \in V \big| \exists \chi \in \mathcal{F} : x \in \chi(y,z) \big\} \\ \mathbf{H}_{x,(y,z)} &= \sum_{\chi \in \mathcal{F}} \pi(\chi) \mathbf{H}^{\chi}_{x,(y,z)} \end{aligned} \tag{20}$$

The weights $\pi(\chi)$ of the individual crossover operators within the family $\mathcal{F}$ can be assigned arbitrarily, and may thus reflect the genetic map distance of the polymorphic loci. In combinatorial optimization the uniform distribution $\pi(\chi) = 1/|\mathcal{F}|$ is commonly used.

In [57] we have investigated the unweighted version of this P-structure in some detail. The arguments used there extend without difficulties to the weighted P-structures defined in equ.(19) and (20). The unweighted version assumes that all possible recombination products occur with equal probability. This assumption is not necessarily satisfied in a GA simulation. For instance, if 1-point crossover is simulated by chosing a recombination point from a uniform distribution, then the frequency distribution of the recombinants depends on the position of the non-conserved letters in the strings. The weighted P-structure in equ.(20) is designed to produce the correct frequencies.

Lemma 1. [57] Let $\mathcal{F}$ be a family of crossover operators. Then the associated P-structure is a recombination structure if and only if $\iota \in \mathcal{F}$.

The fact that $\iota \in \mathcal{F}$ is required can be regarded as a mere technicality implied by property (iii). We conclude hence that the Gitchoff-Wagner definition of a recombination structure indeed captures the most salient features of crossover.

The first three of the following four examples are discussed in more detail in [23], where it is also shown that they fulfil the axioms of a recombination structure.

$\mathcal{R}_1$ *One-Point Crossover* is defined by the collection of all crossover operators $\times_k$ for which $\times_k = \{1, \ldots, k\}$ with $1 \le k \le n$. Note that $\times_n = \iota$ is the identity.

$\mathcal{R}_2$ *Two-Point Crossover* consists of all compositions $\times_k \circ \times_l$, $1 \le k, l \le n$. $\mathcal{R}_2$ hence contains the "pure" 2-point crossover operations as well as all 1-point operators and the identity.

$\mathcal{R}_\Omega$ *Uniform Crossover* allows for all possible recombinations to take place.

$\mathcal{R}_\diamondsuit$ *Single-Position-Exchange* is closely related to mutation. Here we have $\chi = \{k\}$ plus the identity.

Definition. A string recombination structure is *separable* if for any two positions k, l there is a crossover operator $\chi \in F(\mathcal{R})$ such that either $\diamondsuit_k$ or $\diamondsuit_l$ is contained in the product representation of χ, but not both. In other words, there is a crossover operator that separates the sequence positions k and l.

The four string recombination P-structures $\mathcal{R}_\Omega$, $\mathcal{R}_1$, $\mathcal{R}_2$, and $\mathcal{R}_d iamondsuit$ are separable. An example of a recombination P-structure that is not separable is a subset F' of 1-point X-over operators that allow for crossover only at certain "crossover spots" but not at all sequence positions. As a consequence certain adjacent positions can never be separated by recombination. Pure 2-point recombination is also non-separable: positions 1 and n of the string are always transmitted together.

4.2. Symmetries of String Recombination Structures

String recombination P-structures have considerable symmetry. The following two results forms the basis for most of our analysis:

Theorem 2. [57] The automorphism group $\mathbf{Aut}(\mathcal{Q}_\alpha^n, \mathcal{R})$ of a string recombination structure is generously transitive.

Corollary. The matrix $\mathbf{S}$ is symmetric for all string recombination P-structures.

Theorem 3. [57] The backbone graph of a string recombination P-structure $(\mathcal{Q}_\alpha^n, \mathcal{R})$ is the Hamming graph $\mathcal{Q}_\alpha^n$ if and only if it is separable.

If a separable recombination P-structure is b.d.transitive then its Fourier basis coincides with the Fourier basis of corresponding point-mutation space (Hamming space) and we can immediately compare mutation with recombination. In particular, if $(\mathcal{Q}_2^n, \mathcal{R})$ is b.d.transitive then the p-spin (Walsh) functions form a Fourier basis and the eigenvalues of $\mathbf{S}$ depend only p.

Let us now consider the special case of binary strings, and suppose that the string recombination P-structure $(\mathcal{Q}_2^n, \mathcal{R})$ is separable. We have seen in the previous section that in this case the adjacency matrix of the Boolean hypercube $\mathbf{A}$ is contained in the Bose-Mesner algebra $\mathcal{A}[\mathcal{Q}_2^n, \mathcal{R}]$, and hence a Fourier basis for this algebra consists of eigenvectors of $\mathbf{A}$. We have even more information on the eigenvectors: If φ is a Fourier basis function, then it must be a superposition of p-spin functions with a common value of p. In ref. [57] we conjecture that the p-spin (Walsh) functions themselves form a Fourier basis on any string recombination structure on $\mathcal{Q}_2^n$. While we still have no complete proof, this conjecture is stronly supported by theorem 5 in the following section.

Theorem 4. [57] The recombination P-structures $(\mathcal{Q}_2^n, \mathcal{R}_\diamond)$ and $(\mathcal{Q}_2^n, \mathcal{R}_\Omega)$ are distance transitive with respect to their backbone graphs.

Corollary. The matrix elements $\mathbf{S}_{xy}$ of the recombination P-structures $(\mathcal{Q}_2^n, \mathcal{R}_\diamond)$ and $(\mathcal{Q}_2^n, \mathcal{R}_\Omega)$ depend only on the Hamming distance $d_H(x, y)$.

This result justifies to some extent Culberson's approach to used the Hamming distance as the canonical distance in the context of recombination operators [11]. The results of Manderick and co-workers [42] and Jones' "fitness distance correlation" [36] are also based on correlation lengths with respect to Hamming distance.

4.3. Correlation in String Recombination Landscapes

A random walk with transition matrix $\mathbf{S}$ was used in [34] in order to generate the "times-series" for a numerical correlation analysis of Nk landscapes under recombination. The samples of fitness values $\{f(x_0), f(x_1), \ldots\}$ collected along such a walk forms a "time-series" that generalizes Weinberger's [58] procedure for mutation spaces. The autocorrelation function of this time series is defined as in equ.(6).

A generalized Laplace operator on V can be associated with any symmetric non-negative matrix $N \times N$ matrix $\mathbf{C}$ by defining

$$-\Delta_{\mathbf{C}} f(x) \stackrel{\text{def}}{=} \sum_{y\in V} \mathbf{C}_{xy} \Big[f(x) - f(y) \Big] . \tag{21}$$

The operator $-\Delta_{\mathbf{C}}$ has therefore the off-diagonal entries $-\mathbf{C}_{xy}$, while the diagonal is determined by $(-\Delta_{\mathbf{C}})_{xx} = \sum_{y\neq x} \mathbf{C}_{xy}$. Laplacians are special cases of Schrödinger operators, see e.g. [10].

Since the search by P-structures is associated with $\mathbf{S}$ we suggest to characterize the ruggedness of a landscape f on a string recombination structure in terms of the spectrum of the Laplacian

$$-\Delta_{\mathbf{S}} = \mathbf{I} - \mathbf{S}\,. \tag{22}$$

This has to be compared with the mutation Laplacian $-\Delta_{\text{mut}} = \mathbf{I} - (1/D)\mathbf{A}$, which is associated with the adjacency matrix $\mathbf{A}$ of the mutational space. Even more conveniently, we may directly compare the spectra of the transition matrices $\mathbf{S}$ and $(1/D)\mathbf{A}$ whose eigenvalues are the nearest neighbor correlations $r(1)$ of the corresponding random walk "time" series.

The ruggedness of a landscape can be quantified by its location in the spectrum of the Laplacian associated with the search strategy. For instance, landscapes on the boolean hypercube become more rugged as the interaction order p increases. Conversely, we propose to measure the suitability of a particular search procedure by comparing the values of B_k and λ_k that are obtained for the same fitness function f with *different* Laplacians. The absolute location of λ_k in the Laplacian spectrum depends to a certain extent on the normalization of the Laplacian — for instance, there is a factor of 2 between the usual definition of the graph Laplacian and the definition of the Laplacian on hypergraphs, see [45]. The crucial information is thus contained in the relative location. Using the correlation function $r(s)$ or the correlation lenght ℓ directly suffers from a similar problem: The diagonal entries in the transition matrix that is used to define $r(s)$ are to a certain extent arbitrary; again, the ordering of the corresponding eigenvalues is not affected by this ambiguity.

Definition. A landscape $f : V \to \mathbb{R}$ is *elementary for $\mathcal{F}$-recombination* if there is a constant $\bar{f}$ such that $f - \bar{f}$ is an eigenfunction of $\mathbf{S}$.

Again, elementary landscapes are characterized by exponential autocorrelation functions along the walk defined by $\mathbf{S}$. This follows immediately from the discussion in [54]: we find

$$r(s) = \frac{1}{\sigma_f^2}\left[\frac{1}{|V|}\langle f, \mathbf{S}^s f\rangle - \overline{f}^2\right] \tag{23}$$

in complete analogy with the mutation case equ.(7). It will be useful to have an explicit representation of $\mathbf{S}$ in terms of the individual contributions of the crossover operators in $\mathcal{F}$. Assuming that $\pi(\chi)$ is normalized to 1 we find that $\eta(y,z) = 2\sum_{\chi\in\mathcal{F}}\pi(\chi) = 2$ for all $y, z \in V$. Thus

$$\mathbf{S}^{\chi}_{xy} = \frac{1}{2}\sum_{z\in V}\mathbf{H}^{\chi}_{x,(y,z)} \qquad \text{and} \qquad \mathbf{S} = \sum_{\chi\in\mathcal{F}}\pi(\chi)\mathbf{S}^{\chi}\,. \tag{24}$$

The central result of our work is the following theorem, the proof of which will be presented elsewhere:

Theorem 5. The p-spin or Walsh function ε_I is an eigenfunction of $\mathbf{S}^{\chi}$ with eigenvalue

$$\lambda_I^{\chi} = \begin{cases} 1 & \text{if} \quad I = \emptyset \\ 1/2 & \text{if} \quad I \subseteq \chi \text{ or } I \subseteq \bar{\chi} \\ 0 & \qquad\text{otherwise} \end{cases} \tag{25}$$

Corollary 1. Let ε_I be a $|I|$-spin function and let $\mathcal{S}$ be the transition matrix of the weighted string recombination structure associated with an arbitrary family

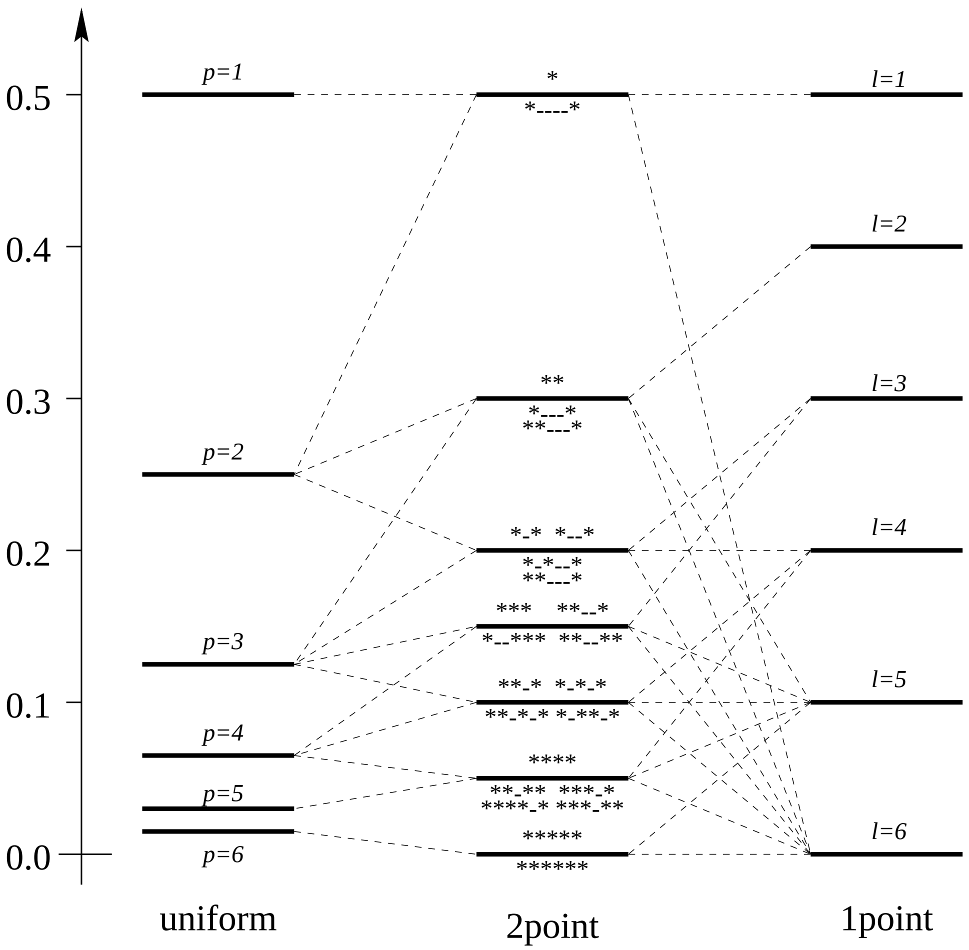

Figure 2: Spectrum λ_I for uniform, 1-point, and 2-point crossover. In both the 1-point and the 2-point crossover family we have omitted the identity ι, hence the smallest eigenvalue is 0.
Note that 2-point crossover yield large eigenvalues for interaction patterns that have small l and p, or small p with the interacting positions located at both ends of the string. These cannot be separared by 2-point crossovers. Including 1-point crossovers into the family will lead to a further splitting of spectrum (along the lines connecting 2-point and 1-point correlation levels). Small values of $\ell(I)$ will lead to increased values of λ_I.

$\mathcal{F}$ of crossover operators. Then ε_I, $I \neq \emptyset$, is an eigenvector of $\mathbf{S}$ with eigenvalues $\lambda_\emptyset^\mathcal{F} = 1$ and

$$\lambda_I^\mathcal{F} = \frac{1}{2|\mathcal{F}|} \left| \left\{ \chi \in \mathcal{F} \,\middle|\, I \subseteq \chi \text{ or } I \subseteq \bar{\chi} \right\} \right| \qquad \text{if } I \neq \emptyset\,. \tag{26}$$

Proof. Follows immediately from the linear decomposition of $\mathbf{S}$ and theorem 1. ∎

Corollary 2. For the family of 1-point cross-over operators we obtain $\lambda_{\emptyset}^{[1]} = 1$ and

$$\lambda_I^{[1]} = \frac{1}{2}\frac{n-\ell(I)}{n-1} \quad \text{if } I \neq \emptyset \tag{27}$$

The eigenfunctions are characterized by the pattern of spin-interactions along the sequence, that is, by the index set I. The *length* of an interaction pattern is $\ell(I) \stackrel{\text{def}}{=} \max I - \min I + 1$. For instance, if $I = \{k, k+1, k+4\}$ for some k, then $\varepsilon_I(x) = x_k x_{k+1} x_{k+4}$ has interaction length $\ell(I) = 5$ and interaction order $p = 3$. We shall write `[**--*]` for this type of eigenfunctions, see Figure 2.

Corollary 3. For the family of uniform cross-over operators we obtain

$$\lambda_I^{[\infty]} = 2^{-|I|}\,. \tag{28}$$

The same result is true for uniform crossover in the unweighted case [57].

It is not easy to find general expressions for more complicated families of crossover operators. In figure 2 we show the spectrum for 2-point crossover (without identity and 1-point crossover) for $n = 6$ as an example. We have, however:

Corollary 4. Let $\mathcal{F}$ be an arbitrary family of crossover operators. Then $\lambda_I^{\mathcal{F}} \geq 0$. If $\mathcal{F}$ contains the identity ι then $\lambda_I^{\mathcal{F}} > 0$ for all I. This is not true for mutation: $\lambda_I^{\text{mut}} = 1 - 2p/n$ becomes negative for $p > n/2$.

5. Discussion

In this paper we have discussed how algebraic methods can be used to analyze complex problems in evolutionary theory and evolutionary computation. The basic notion for the present approach is that of a landscape defined over a configuration space. The topological features of the configuration space are determined by the genetic operators which transform types into each other. Since each operator can in principle induce a different topology, the resulting fitness landscape can be different for each operator. This is reflected in the *One Operator-One Landscape* hypothesis by Jones (1995). Taken literally, this thesis could imply that recombination acts on a completely different landscape than mutation. The consequence could be that mutation and recombination are pursuing different optimization paths, which would be deleterious if both are acting together, as is the case in most higher organisms.

While the *One Operator-One Landscape* hypothesis is still strictly true, the algebraic approach to landscape analysis reveals deep commonalities between string recombination and point mutation landscapes. For instance, already the hypergraph representation of string recombination spaces has revealed that the mutation graph is embedded in the recombination space [23]. Hence, the point mutation space is homomorphic to the string recombination space. In addition, the extension of Fourier decomposition to landscapes on recombination P-structures shows even deeper relationships between mutation and recombination spaces.

As shown in section 4, the algebraic properties of a P-structure are determined by the backbone graph, which in fact is just the mutation space embedded in the recombination hypergraph. As a consequence, exactly those fitness functions which are elementary for mutation spaces are also elementary for string recombination spaces. We also presented analytical results on the spectrum of the P-structure Laplacian, which happen to be identical to the nearest neighbor correlations for a random walk in the recombination space. From these vales a qualitative assessment can be obtained about the relationship between the number and position of interacting sites and the relative evolvability of the systems.

The reason why the results can only be considered qualitative is that the actual transition probabilities depend on the frequency distribution of types in the population. The present formalism is strictly true only if the population is at the very center of the simplex, i.e. if all types are present with the same frequency. Deviations from this state lead to asymmetric transition matrices and many of the symmetries used to derive our results are lost. In principle, however, the approach outlined here can be extended to include population structure in a straight forward manner, even if it means that we may have to use numerical techniques to obtain concrete answers.

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