COMBINATORIAL LANDSCAPES*

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Abstract. Fitness landscapes have proven to be a valuable concept in evolutionary biology, combinatorial optimization, and the physics of disordered systems. A fitness landscape is a mapping from a configuration space into the real numbers. The configuration space is equipped with some notion of adjacency, nearness, distance or accessibility. Landscape theory has emerged as an attempt to devise suitable mathematical structures for describing the "static" properties of landscapes as well as their influence on the dynamics of adaptation. In this review we focus on the connections of landscape theory with algebraic combinatorics and random graph theory, where exact results are available.

Key words. fitness landscape, genotype phenotype map, random graphs, correlation functions, neutrality, coherent algebras, sequential dynamical systems, combinatorial optimization

AMS subject classifications. 05C90, 15-02

1. Introduction.

The concept of a *fitness landscape* originated in the 1930s in theoretical biology [210, 211]. A fitness landscape is a kind of "potential function" underlying the dynamics of evolutionary optimization. Implicit in this notion is both a *fitness function* f that assigns a fitness value to every possible genotype (or organism), and the arrangement of the set of genotypes in some kind of abstract space that provides some notion of accessibility or reachability.

Models of disordered systems, in particular spin glasses, naturally lead to the notion of landscapes [16, 123]: Each spin configuration is assigned an energy by virtue of the Hamiltonian that specifies the model; the dynamic properties invoke a collection of transitions between configurations. In complete analogy, the folding of biopolymers, including proteins [27, 38, 138] and nucleic acids [53, 51] is determined by energy landscapes.

In combinatorial optimization the fitness function is usually referred to as the *cost function*, and a *move-set* allows to inter-convert the elements of the *search space* [64]. The application of evolutionary models to combinatorial optimization problems has lead to the design of so-called *evolutionary algorithms* such as Genetic Algorithms, Evolutionary Strategies, and Genetic Programming [146, 110, 86, 99, 55].

Conceptually, there is a close connection with the *potential energy surfaces* (PES) of theoretical chemistry [124, 79]: As a consequence of the validity of the Born-Oppenheimer approximation, the PES provides the potential energy $U(\vec{R})$ of a molecule with n atoms as a function of its nuclear geometry $\vec{R} \in \mathbb{R}^{3n}$. Electoral Landscapes are used to explain party platform behavior in spatial voting models [108, 170]. Not surprisingly, fitness landscapes have emerged as one of the unifying themes in the literature on complex systems [142, 99, 61, 30].

In formal terms, a landscape consists of three ingredients

1. A set X of configurations,

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2. a notion $\mathcal{X}$ of neighborhood, nearness, distance, or accessibility on X, and
3. a fitness function $f : X \to \mathbb{R}$.

The set X together with the "structure" $\mathcal{X}$ forms the configuration space. The definition of $\mathcal{X}$ is purposefully left vague at this point and will made precise below.

Example: The Traveling Salesman Problem (TSP). The TSP is probably the most frequently studied combinatorial optimization problem. Hundreds of publications and books have been devoted to this problem and a large variety of solution techniques have been proposed [112]. The TSP is deceptively easy to state: *A Salesman wants to visit n distinct cities and then return home. The goal is to minimize the overall traveling distance while visiting each city not more than once.* The problem is well known to belong to the class of NP-hard problems [64, 6].

The TSPs apparent simplicity on the one hand and the difficulty of finding optimal solutions on the other hand has established it as a test bed for new heuristics and exact algorithms. However, the TSP is not only of theoretical value; there exist many industrial applications to the TSP and its variants.

For the purpose of this contribution we are interested in the properties of the landscape of the TSP rather than in algorithms for "solving" it. A very pragmatic reason for this is that one may hope that problems with similar landscapes will lend themselves to similar solutions.

The ingredients are simple enough: The configurations are the $n!$ permutations of the n cities. A tour is permutation $\pi = (\pi(1), \ldots, \pi(n))$ that lists the cities in the order in which they are visited. Given the travel cost C_{kl} from city l to city k we can write down the cost function in the form

$$f(\pi) = \sum_{i=1}^{n-1} C_{\pi(i+1),\pi(i)} + C_{\pi(1),\pi(n)} \,, \tag{1.1}$$

where the last term corresponds to returning home.

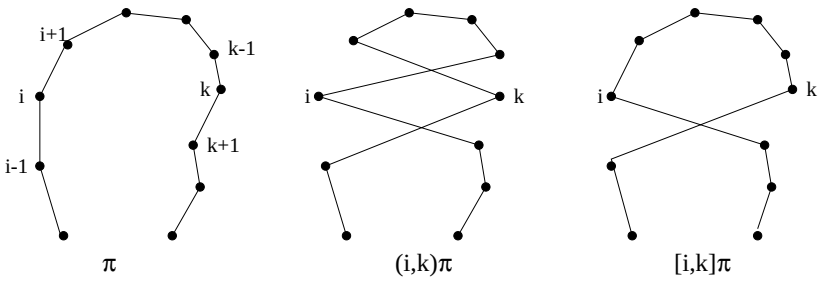


FIG. 1.1. *Transposition $(i,k)\pi$ (middle) and reversal $[i,k]\pi$ (right) of the TSP tour π (left).*

But what is the "structure $\mathcal{X}$" on the set of configurations? Many heuristic algorithms for the TSP work by gradually modifying a tour. Two operators are particularly common: the transposition of cities and the reversal of parts of the tour, Fig. 1.1.

An interesting, and rather surprising, observation is that simple heuristic algorithms (such as simulated annealing) work much better with reversals than with transpositions as long as the matrix of travel costs is symmetric $C_{kl} = C_{lk}$. On the other hand, if transpositions are used, it does not matter whether the travel cost matrix is

symmetric $C_{kl} = C_{lk}$. For asymmetric travel cost matrices, however, transpositions work more efficiently [115].

What is it about the landscape that causes such performance differences? We shall encounter a simple answer in terms of so-called amplitude spectra in section 3.3: The correlation of the landscapes is (almost) the same for symmetric and asymmetric C when transpositions are used. The symmetric TSP with reversals has smoother version than with transpositions, while it is the other way around if C is asymmetric.

Landscapes can be studied either from a "static" point of view, focusing on geometric properties such as smoothness, ruggedness, and neutrality, or from a "dynamical" point of view focusing on the features of a dynamical system, for instance an evolving population, that uses the landscape as its substrate. The static point of view will be the main topic of this review as it lends itself readily to a detailed mathematical analysis. Dynamical aspects are much more difficult and mostly tackled by computer simulations.

This contribution is organized as follows: We first identify the structure of configuration spaces either as undirected, unweighted graphs or as reversible Markov chains. This sets the stage for decomposition of landscapes in terms of particular orthonormal bases that take into account the structure of the underlying configuration space. This "spectral" approach concentrates on ruggedness, neutrality and isotropy and is of particular relevance for combinatorial optimization problems and disordered systems. Landscapes arising in biology are based upon an underlying genotype-phenotype map which determines key features of the landscape. We discuss two paradigmatic examples of genotype phenotype maps: RNA secondary structure folding and sequential dynamical systems. The analysis of these examples naturally leads to a random graph theory of neutrality. In section 6 we very briefly review dynamical aspects in landscape theory, in particular simulated annealing and the quasispecies model. We close our discussion with a few remarks on recent trends.

2. Configuration Spaces. There appears to be three distinct approaches to organizing the set of configurations.

1. Sometimes transition probabilities are specified that describe how frequently a system attempts to move from one configuration to another.
2. In computer science one typically specifies a "move set" or "genetic operator" that inter-converts one or more configurations into a new one. Evolutionary biology takes the same point of view, except that the move sets are given by nature rather than being engineered.
3. A rigorous mathematical analysis often starts with specifying a metric or a topology on X. This approach will be discussed in some detail in section 7.1.

We shall see below that move sets and transition probabilities are closely related. Eventually, we obtain an algebraic description of the configuration space in terms of a matrix that may serve as the starting point of *spectral landscape theory*.

2.1. Markov Chains. Regarding X as a set of "states" we may specify transition probabilities $\mathbf{T}_{xy}$ for moving from y to x. The Markov process with transition matrix $\mathbf{T}$ organizes the configuration space. Typically, one requires $\mathbf{T}$ to be ergodic (i.e., every state can be reached from every other state) and reversible, i.e., to satisfy

(E) $\mathbf{T}$ is irreducible, or, equivalently,
there is a unique stationary distribution p on X such that $\mathbf{T}p = p$. Furthermore $p(x) > 0$ for all $x \in X$.

(R) $\mathbf{T}_{xy}p(y) = \mathbf{T}_{yx}p(x)$. This condition is also known as "detailed balance".

In other words, $\mathbf{T}$ is self-adjoined w.r.t. to the scalar product

$$\langle f, g\rangle_p = \sum_x p(x) f(x) g(x)^* \tag{2.1}$$

where $*$ denotes complex conjugation.

A most useful observation is that the matrix $\mathbf{S}$ defined by

$$\mathbf{S}_{xy} = p(x)^{-1/2} \mathbf{T}_{xy} p(y)^{1/2} \tag{2.2}$$

is symmetric and similar to $\mathbf{T}$. Hence given a non-symmetric transition matrix $\mathbf{T}$ and a landscape f we may transform the model to new coordinates with the symmetric operator $\mathbf{S}$ and the transformed landscape

$$f^\sigma(x) = p(x)^{-1/2} f(x) \ . \tag{2.3}$$

This allows for the application of much of the spectral landscape theory in the non-symmetric case as well.

2.2. Move Sets. In its most abstract form a *move set* assigned to a k-tuple $(x_1, \ldots, x_k) \in X^k$ which we refer to as "parents" a list $N(x_1, \ldots, x_k) \subseteq X$ which we call "children". In the following we will restrict our attention to the two most commonly used move-set types, mutation and recombination.

2.2.1. Mutation. A mutation operator simply assigns a set $N(x)$ of "accessible neighbors" or "elementary mutants" to each configuration x. This allows us to interpret X as a (possibly directed) graph with vertex set X and $N(x)$ the (out)neighbors of $x \in X$. Most commonly the move sets are constructed such that $y \in N(x)$ if and only if $x \in N(y)$, in which case the graph is symmetric, or, equivalently, undirected. A graph is faithfully represented by its adjacency matrix $\mathbf{A}$ which has the entries $\mathbf{A}_{xy} = 1$ if $x \in N(y)$ and $\mathbf{A}_{xy} = 0$ otherwise. Obviously, $\mathbf{A}$ is symmetric if and only if the graph is undirected. With each (directed or undirected) graph there is an associated Markov process on its vertex set [117] defined by the transition matrix

$$\mathbf{T} = \mathbf{A}\mathbf{D}^{-1} \tag{2.4}$$

where $\mathbf{D}$ is the so-called degree matrix, which is diagonal and $\mathbf{D}_{xx} = |N(x)|$ is the number of neighbors of x. This Markov process describes a *random walk* on X which has been suggested as a means to sample information about a landscape by Ed Weinberger [203, 204]. We remark that in the case of undirected and symmetric directed graphs the stationary distribution is given by

$$p(x) = \frac{\mathbf{D}_{xx}}{2E} \tag{2.5}$$

where E is the total number of undirected edges.

2.2.2. Recombination and Cross-Over. 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 with the set of genotypes representing the set of vertices. This leaves two alternatives: One can 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 different

strings. This approach was pioneered by Culberson [31] and Jones [94]. The alternative is to leave the vertices to represent individual genotypes and to make the edges more complex. In Gitchoff and Wagner [67] it was shown that recombination spaces can be represented as hypergraphs (which consist of a vertex set X and a collection $\mathcal{E}$ of (not necessarily) distinct subsets of X called (hyper)edges), where the hyper-edges are the sets of all recombinants that can arise from the recombination of two types. With this approach it is was easy to show that string recombination spaces and point mutations spaces are homomorphic. Hypergraphs are still not completely satisfactory, since they do not indicate which pair of types produces which set of recombinants, i.e., which hyper-edge arises from which mating. This led us to invent *P-structures*, which are mappings of pairs of types to the hyper-edges of the hypergraph [184, 200].

We focus here on homologous recombination on a genome consisting of n loci. For each locus k, there are α_k alleles. The set of all the $\prod_k \alpha_k$ possible genotypes will be denoted by V. For each locus k, we label the alleles using a letter from the alphabet $\mathcal{A}_k = \{0, \ldots, \alpha_k - 1\}$. Thus $V = \prod_k \mathcal{A}_k$. A particular genotype (or sequence) $x \in V$ can be regarded as a vector with components $x_k \in \mathcal{A}_k$. A particular cross-over operator is determined by the list χ of loci that the child inherits from the first parent. Thus the loci in $\overline{\chi} = \{1, \ldots, n\} \setminus \chi$ come from the second parent. More formally, given χ, the offspring $x = \chi(y, z)$ of the two parents y and z has the component-wise representation

$$x_k = \begin{cases} y_k & \text{if} \quad k \in \chi \\ z_k & \text{if} \quad k \in \overline{\chi}. \end{cases} \tag{2.6}$$

It will be convenient in the following to express eqn. (2.6) by means of an "incidence operator"

$$\mathbf{H}^{\chi}_{x,(y,z)} = \begin{cases} 2 & \text{if} \quad x = y = z \\ 1 & \text{if} \quad y \neq z \\ 0 & \text{otherwise}. \end{cases} \qquad \text{and} \quad x = \chi(y, z) \tag{2.7}$$

Here we restrict ourselves to recombination on strings. Crossover operators for permutation, such as Traveling Salesman tours, are reviewed for instance in [111].

A *recombination operator* in the sense of most of the GA literature is then a family $\mathcal{F}$ of cross-over operators that act on $X \times X$ with probability $\pi(\chi)$. The incidence "matrix" associated with a recombination operator is simply

$$\mathbf{H}^{\mathcal{F}} = \sum_{\chi \in \mathcal{F}} \mathbf{H}^{\chi} \tag{2.8}$$

The two most important recombination operators are

- [∞] Uniform recombination contains all 2^n possible crossover operators. In this case it is natural to include the identity $\imath$.
- [1] 1-point recombination contains all cross-over operators χ for which the characteristic set is of the form $\chi = \{1, \ldots, k\}$.

Homologous recombination (of strings) under very general conditions leads to very regular configuration spaces. In particular, one can show that the automorphism group of $\mathbf{H}^{\mathcal{F}}$ is generously transitive [184]. This picture, however, changes radically, if unequal crossover is considered, where the number of genes on a chromosome can change [167].

A *cross-over walk* [87, 88], Figure 2.1, on X is the Markov process based on the following rule: The "father" y is mated with a randomly chosen "mother" z. The

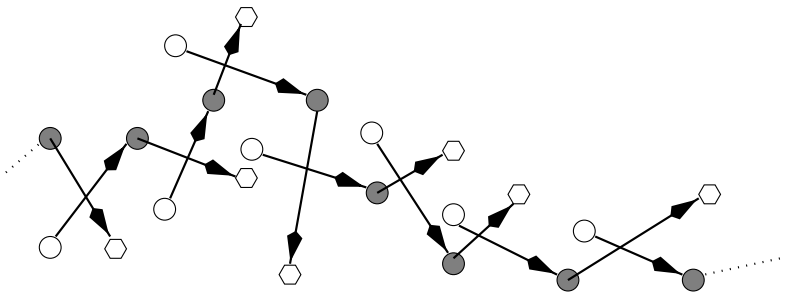


FIG. 2.1. *Crossover walk*

offspring is "son" x which becomes the "father" of the next mating. We regard the sequence of "fathers" as a random walk on X. It is straightforward [182] to derive the transition matrix of this Markov process for homologous recombination from the incidence "matrix" $\mathbf{H}^{\mathcal{F}}$. One obtains

$$\mathbf{S}_{xy}^{\mathcal{F},\vec{\varphi}} = \sum_{\chi\in\mathcal{F}} \pi(\chi)\frac{1}{2}\sum_{z\in X} \mathbf{H}^{\chi}_{x,(y,z)}\wp(z) \tag{2.9}$$

where $\wp(z)$ denotes the frequency distribution of the genotypes in the equilibrium population.

3. Decompositions of Landscapes. Regarding $f : V \to \mathbb{R}$ as a vector in the $|V|$-dimensional Euclidean vector space $\mathbb{R}^{|V|}$ immediately poses the question of whether there are more convenient bases than the standard basis $\{\delta_x\}$, with $\delta_x(y) = 1$ if $y = x$ and 0, otherwise. This is the starting point of what one might call *algebraic landscape theory* or *spectral landscape theory*.

3.1. Fourier Transform of Landscapes. A suitable basis naturally encapsultates information about the regularities of the configuration space. Hence one of the symmetric $V \times V$ matrices introduced in the previous section is the most common starting point.

3.1.1. Discrete Laplace Operators. From the algebraic point of view it appears to be more natural to start with a discrete *Laplace operator*

$$-\mathbf{\Delta} = \mathbf{D_S} - \mathbf{S} \qquad \text{with } (\mathbf{D_S})_{xx} = \sum_{y\in X} \mathbf{S}_{xy} \tag{3.1}$$

since it has number of desirable mathematical properties:
$-\mathbf{\Delta}$ is symmetric and has non-positive off-diagonal entries.
$-\mathbf{\Delta}$ has 0 as an eigenvalue with eigenvector $\mathit{1} = (1,\ldots,1)$. The eigenvalue 0 is unique if and only if the graph associated with the off-diagonal entries is irreducible.
$-\mathbf{\Delta}$ is non-negative definite.
The graph Laplacian $-\mathbf{\Delta} = \mathbf{D} - \mathbf{A}$ arises naturally as the discretization of the Laplacian differential operator for instance in finite element computations. For recent surveys on graph Laplacians see [128, 122, 28, 129].

3.1.2. Coherent Algebras. An alternative, maybe even more appealing starting point is to consider the coherent algebra associated with the configuration space graph or transition operator [105, 183].

A set of complex matrices that is closed under (i) scalar multiplication with complex numbers, (ii) component-wise addition, (iii) ordinary matrix multiplication, (iv) component-wise multiplication, and (v) transposition is called a *coherent algebra* or *cellular algebra*. Equivalently, a matrix algebra $\mathfrak{W} \subseteq \mathbb{C}^{|V|\times|V|}$ is coherent if and only if it satisfies the following axioms:
(i) As a linear space over $\mathbb{C}$, $\mathfrak{W}$ has a basis of $\{\mathbf{R}^{(1)}, \ldots, \mathbf{R}^{(r)}\}$ of 0-1 matrices.
(ii) $\sum_{j=1}^{n} \mathbf{R}^{(j)} = \mathbf{J}$, the all-1 matrix.
(iii) For every $i \in \{1, \ldots, r\}$ there an i' such that $\mathbf{R}^{(i)\mathsf{T}} = \mathbf{R}^{(i')}$.
(iv) $\mathbf{I} \in \mathfrak{W}$.
Axiom (ii) above implies that the relations associated with the basis matrices $\mathbf{R}^{(j)}$ form a partition of $V \times V$. Such partitions are known as *coherent configurations* [81, 82, 83].

For each collection $\mathcal{M} = \{\mathbf{M}_1, \ldots, \mathbf{M}_k\}$ of $|V| \times |V|$ matrices there is a smallest coherent algebra $\langle\langle \mathcal{M} \rangle\rangle$ which is the defined as the intersection of all coherent algebras that contain $\{\mathbf{M}_1, \ldots, \mathbf{M}_k\}$. Since the centralizer algebra is coherent we have

$$\langle\langle \mathcal{M} \rangle\rangle \subseteq \mathfrak{V}_{\mathbb{C}}(\mathsf{Aut}[\mathcal{M}], V) \tag{3.2}$$

Equality hold if and only if there is a permutation group that has $\langle\langle \mathcal{M} \rangle\rangle$ as its centralizer algebra [106]. The coherent algebra $\langle\langle \mathcal{M} \rangle\rangle$ can therefore be regarded as a "combinatorial approximation" of the centralizer algebra [45, 105]. This is of particular importance in the graph case: given the adjacency matrix $\mathbf{A}$ of Γ, there is polynomial time algorithm that determines the coherent algebra $\mathfrak{W}(\Gamma) = \langle\langle \mathbf{A} \rangle\rangle$, see [206, 9, 8]. It is straightforward to check that the degree matrix $\mathbf{D}$, and hence also the transition operator $\mathbf{T} = \mathbf{A}\mathbf{D}^{-1}$ and the associated Laplace operators are also contained in $\langle\langle \mathbf{A} \rangle\rangle$.

Let $\mathcal{R} = \{\mathbf{R}^{(1)}, \ldots, \mathbf{R}^{(r)}\}$ be the standard basis of a coherent algebra $\mathfrak{W}$. We have $\mathbf{R}^{(\mu)}\mathbf{R}^{(\nu)} = \sum_\kappa p^\kappa_{\mu,\nu} \mathbf{R}^{(\kappa)}$ where the *intersection numbers*

$$p^\kappa_{\mu,\nu} = \left|\left\{ z \in V \,\middle|\, (x,z) \in \mu \ (z,y) \in \nu \right\}\right| \ \in \mathbb{N}_0 \tag{3.3}$$

are the same for all pairs $(x, y) \in \kappa$. The $r \times r$ matrices $\hat{\mathbf{R}}^\kappa$ with entries $\hat{\mathbf{R}}^{(\nu)}_{\mu,\kappa} = p^\kappa_{\mu,\nu}$ generate a matrix algebra $\hat{\mathfrak{W}}$ that is isomorphic to $\mathfrak{W}$ [81]. This observation makes coherent algebras appealing objects for our purposes because $\hat{\mathfrak{W}}$ is small enough in many cases to allows for explicit computations of eigenvalues and eigenvectors [183]. This is of particular interest in the case of association schemes (symmetric coherent algebras), in which case all members of $\hat{\mathfrak{W}}$ share a common orthonormal basis of eigenvectors [20]. We remark that, in the case of Hamming graphs, the eigenvectors are the well-known Walsh functions [49].

3.1.3. Graph-Theoretical Fourier Decomposition. In the following let $\{\varphi_k | V \to \mathbb{C}\}$ be an orthonormal basis of eigenfunctions of the desired operator taken from $\mathfrak{W}$. It is natural then to expand the fitness function f in terms of this basis:

$$f(x) = \sum_k a_k \varphi_k(x) \tag{3.4}$$

We shall use the following convention: (i) The index 0 is reserved for the "ground state". If the basis is derived from a Laplacian, for instance, then φ_0 is constant, the associated eigenvalue is zero, and

$$a_0 = \sum_x \varphi_0(x) f(x) = |V|^{-1} \sum_{x \in V} f(x) \tag{3.5}$$

(ii) The distinct eigenvalues of $-\mathbf{\Delta}$ will be denoted by Λ_p and in the Markov chain case we write λ_p. It will be convenient to define the index sets $J_p = \{k| - \mathbf{\Delta}\varphi_k = \Lambda_p\varphi_k\}$ that collect all eigenfunctions belonging to the same (Laplacian) eigenvalue. (iii) We write $\tilde{f}(x) = f(x) - a_0$. This is the "non-flat" part of the fitness function.

3.1.4. Group-Theoretical Fourier Transformation. Let G be a finite group and let S be a symmetric set of generators of G, i.e., $\langle S\rangle = \mathsf{G}$, $S = S^{-1}$, and $\imath \notin S$, where $\imath$ is the identity of G. A graph $\Gamma(\mathsf{G}, S)$ with vertex set G and edges $\{s, t\}$ if and only if $t^{-1}s \in S$ is called a *Cayley graph*. Cayley graphs are vertex transitive and hence regular.

DEFINITION 3.1. *A Cayley graph $\Gamma(\mathsf{G}, S)$ is called* quasi-Abelian *if S is the union of some conjugacy classes of G.*

Clearly, a Cayley graph on a commutative group is quasi-Abelian, since each group element forms its own conjugacy class in this case. Some interesting properties of quasi-Abelian Cayley graphs are discussed in [201, 212]. Below we shall see that certain algebraic properties of Cayley graphs with Abelian groups generalize to quasi-Abelian Cayley graphs.

DEFINITION 3.2. *For any function $f : \mathsf{G} \to \mathbb{C}$ and any matrix representation $\varrho = \{\rho(s)\}_{s\in\mathsf{G}}$ of G we call the matrix sum*

$$\widehat{f}(\varrho) = \sum_{x\in\mathsf{G}} f(x)\rho(x) \tag{3.6}$$

the (group theoretic) Fourier Transform *of f at ϱ.*

In the case of Cayley graphs we have therefore to distinguish between the "Fourier series expansion" with respect to the graph $\Gamma(\mathsf{G}, S)$, eqn.(3.4), and the representation theoretical Fourier transformation on the group G itself. It will not come as a surprise that there is an intimate connection between the two.

THEOREM 3.3. [158] *Let $\Gamma(\mathsf{G}, S)$ be a quasi-Abelian Cayley graph with a finite group G.*

(1) The function $\varepsilon_{ij}^k : \mathsf{G} \to \mathbb{C}$ defined as

$$\varepsilon_{ij}^k(u) = \sqrt{\frac{d_k}{|\mathsf{G}|}}\rho_{ij}^k(u^{-1}) \tag{3.7}$$

is an eigenvector of $\mathbf{A}(\Gamma)$ with eigenvalue $\Lambda_k = \frac{1}{d_k}\sum_{s\in S}\chi_k(s)$ where $\chi_k(s) = \mathrm{Tr}\rho^k(s)$ is the character of ϱ^k at s; its dimension is d_k.

(2) All quasi-Abelian Cayley graphs on G have a common basis of eigenvectors and hence their adjacency matrices commute.

(3) A function $f : \mathsf{G} \to \mathbb{R}$ can be expanded in the form

$$f(s) = \sum_{ijk} a_{ij}^k \varepsilon_{ij}^k(s) \qquad \text{with} \qquad a_{ij}^k = \sqrt{\frac{d_k}{|\mathsf{G}|}}\widehat{f}_{ji}(\rho^k) \tag{3.8}$$

Fast Fourier Transform algorithms are known for a variety of finite groups. For a recent overview see e.g. [121, 157].

3.1.5. Elementary Landscapes. Lov Grover and others [29, 74, 174] observed that $\tilde{f}$ is in many cases an eigenfunction of the graph Laplacian $-\mathbf{\Delta}$, see Table 3.1 for a list of examples. We say that f is *elementary* w.r.t. $-\mathbf{\Delta}$ if $\tilde{f}$ is an eigenfunction of

TABLE 3.1
Elementary Landscapes.

Problem	Graph	D	λ	Order	Reference
p-spin glass	$\mathcal{Q}_2^n$	n	$2p$	p	definition
NAES	$\mathcal{Q}_2^n$	n	4	2	[74]
Weight Partitioning	$\mathcal{Q}_2^n$	n	4	2	[74, 174]
GBP (constrained)	$\mathcal{Q}_2^n$	n	4	2	[5]
Max Cut	$\mathcal{Q}_2^n$	n	4	2	[5]
Graph α-Coloring	$\mathcal{Q}_2^\alpha$	$(\alpha-1)n$	2α	2	[174]
XY-spin glass	$\mathcal{Q}_\alpha^n$	$(\alpha-1)n$	2α	2	[63]
for $\alpha > 2$:	$\mathcal{C}_\alpha^n$	2	$8\sin^2(\pi/\alpha)$	2	[63]
Linear Assignment	$\Gamma(\mathcal{S}_n, \mathcal{T})$	n		1	[158]
TSP symmetric	$\Gamma(\mathcal{S}_n, \mathcal{T})$	$n(n-1)/2$	$2(n-1)$	2	[29, 74]
	$\Gamma(\mathcal{S}_n, \mathcal{J})$	$n(n-1)/2$	n	2	[29, 74]
	$\Gamma(\mathcal{A}_n, \mathcal{C}_3)$	$n(n-1)(n-2)/6$	$(n-1)(n-2)$	?	[29]
antisymmetric	$\Gamma(\mathcal{S}_n, \mathcal{T})$	$n(n-1)/2$	$2n$	3	[174]
	$\Gamma(\mathcal{S}_n, \mathcal{J})$	$n(n-1)/2$	$n(n+1)/2$	$\mathcal{O}(n)$	[174]
Graph Matching	$\Gamma(\mathcal{S}_n, \mathcal{T})$	$n(n-1)/2$	$2(n-1)$	2	[174]
Graph Bipartitioning	$J(n, n/2)$	$n^2/4$	$2(n-1)$	2	[74, 178, 180]

$-\mathbf{\Delta}$ with an eigenvalue $\lambda_p > 0$. In [175] this notion is extended to calling f elementary w.r.t. a random walk transition operator iff $\mathbf{S}\tilde{f} = \lambda_p \tilde{f}$ with an eigenvalue $\lambda_p < 1$.

If f is elementary, then $\tilde{f}$ satisfies the conditions of Courant's nodal domain theorem, see 3.1.6. Elementary landscapes can thus be expected to have few nodal domains if they belong to a small Laplacian eigenvalue (or to an eigenvalue of a Markov transition matrix close to 1), while landscapes that are far away from the ground state will in general have many nodal domains. Such landscapes will appear "rugged". Grover [74] showed that

$$f(\hat{x}_{\min}) \le a_0 \le f(\hat{x}_{\max}) \tag{3.9}$$

where $\hat{x}_{\min}$ and $x_{\max}$ are arbitrary local minima and maxima, respectively. This *maximum principle* shows that elementary landscapes are well-behaved: There are no local optima with worse than average fitness. We shall return to local optima as a measure of ruggedness in section 4.2.1.

3.1.6. The Nodal Domain Theorem. Discrete Schrödinger operators are defined as

$$\mathbf{H}f(x) = \sum_{y \sim x} b(x,y)\,[f(x) - f(y)] + v(x)f(x)\,. \tag{3.10}$$

where $b(x,y) = b(y,x) > 0$ if and only if $\{x,y\}$ is an edge of the graph Γ; $v(x)$ is an arbitrary "potential function". Of course, the graph Laplacian $-\mathbf{\Delta}$ is a special case.

A well-known feature of Schrödinger operators on Riemannian manifolds M is that the nodal domains of any of its eigenfunctions, that is, the connected components of $M \setminus f^{-1}(0)$, of their eigenfunctions are severely constrained. In order to formulate *Courant's theorem* for graphs, we define for any function $f : V \to \mathbb{R}$ on Γ: $\mathrm{supp}_+(f) = \{x \in V | f(x) > 0\}$, $\mathrm{supp}_-(f) = \{x \in V | f(x) > 0\}$, $\mathrm{zero}(f) = \{x \in V | f(x) > 0\}$,

$\mathrm{supp}^0_+(f) = \mathrm{supp}_+(f) \cup \mathrm{zero}(f)$, and $\mathrm{supp}^0_-(f) = \mathrm{supp}_-(f) \cup \mathrm{zero}(f)$. A (strong) *nodal domain* of f is a maximal connected component of either $\mathrm{supp}_+(f)$ or $\mathrm{supp}_-(f)$. A *weak nodal domain* is a maximal connected component of $\mathrm{supp}_+(f) \cup \mathrm{zero}(f)$ or $\mathrm{supp}_-(f) \cup \mathrm{zero}(f)$, respectively.

Let $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{|V|}$ be the eigenvalues of a Schrödinger operator on Γ with corresponding eigenvectors φ_i. Define $M(i) = \max\{k|\lambda_k = \lambda_i\}$ and $m(i) = \min\{k\colon \lambda_k = \lambda_i\}$. Hence, $m(i) \leq i \leq M(i)$, $M(i) = m(i) + \mathrm{mult}(\lambda_i) - 1$, and $m(i) = M(i) = i$ if and only if λ_i is a simple eigenvalue of $\mathbf{H}$. With this notation we have

THEOREM 3.4. [Nodal Domain Theorem] *Let f be an eigenvector of $\mathbf{H}$ with eigenvalue λ_i. Then:*
(i) there are at most $M(i)$ (strong) nodal domains of f and
(ii) there are at most $m(i)$ weak nodal domains of f.

Various discrete versions of the Nodal Domain theorem have been discussed in the literature [35, 62, 193, 39], however, sometimes with ambiguous statements and incomplete or flawed proofs. An elementary proof can be found in [33]. The interest in nodal domain properties of graph eigenvectors goes back to M. Fiedler [47] who showed that the number of components of $\mathrm{supp}^0_+(f)$ is at most $M(i)$. Some closely related results on the component structure of $\mathrm{supp}_+(f) \cup \mathrm{supp}_-(f)$ can be found in [144].

3.2. Random Landscapes. In many cases, for instance in applications to spin glasses, the definition of the landscape contains a number of random parameters. We therefore define landscapes here as elements of an appropriate probability space.

DEFINITION 3.5. *Let V be a finite set and let W be a predicate of landscapes $f : V \to \mathbb{R}$. A* random W-landscape *$\mathcal{F}$ over V is the probability space*

$$\Omega = (\{f : V \to \mathbb{R} \mid f \ \textit{has property } W\}, \mathcal{A}, \mu) \ , \tag{3.11}$$

where $\mathcal{A}$ is a σ-field and $\mu : \mathcal{A} \to [0,1]$ a measure. Let $\xi : \Omega \to \mathbb{R}$ be a Ω-random variable; we denote expectation value and variance of ξ by $\mathbb{E}[\xi]$ and $\mathbb{V}[\xi]$, respectively. In particular we will consider the family

$$\forall\, x \in V; \quad \mathrm{eval}_x : \Omega \to \mathbb{R}, \quad \mathrm{eval}_x(f) = f(x)\,. \tag{3.12}$$

By abuse of notation we shall write $\mathbb{E}[f(x)]$ for $\mathbb{E}[\mathrm{eval}_x]$, the expectation of f evaluated at $x \in V$. The *covariance matrix* of the random landscape Ω is given by

$$\mathbf{C}_{xy} = \mathrm{Cov}[\mathrm{eval}_x, \mathrm{eval}_y] = \mathbb{E}[f(x)f(y)] - \mathbb{E}[f(x)]\mathbb{E}[f(y)]\,. \tag{3.13}$$

The matrix $\mathbf{C}$ is obviously symmetric and non-negative definite. Taking the set of all maps $\{f : V \to \mathbb{R}\}$ as base space of the probability space Ω, a basis is formed by the set of orthonormal eigenvectors $\{\psi_k\}$ of the covariance matrix $\mathbf{C}$. An expansion of the form

$$f(x) \doteq \sum_k b_k \psi_k(x) \qquad \text{a.s.} \qquad\qquad x \in V \tag{3.14}$$

is known as the *Karhunen-Loève series* or the *principal component decomposition* of f. A crucial result is:

THEOREM 3.6. [90, 97, 116] *Let σ_k^2 denote the eigenvalue of $\mathbf{C}$ belonging to the eigenvector ψ_k. Then the coefficient of the Karhunen-Loève series (3.14) are uncorrelated random variables satisfying*

$$\mathrm{Cov}[b_k, b_j] = \sigma_k^2 \delta_{kj} \qquad 1 \leq k, l \leq |V|. \tag{3.15}$$

TABLE 3.2

Examples of Additive Random Landscapes.
The component landscapes ϑ_I and the index set M, eqn.(3.16), are listed together with information on whether the models are uniform (U), strictly uniform (S), or pseudo-isotropic (P). Properties that are implied by stronger ones are shown as ∘. Adapted from [154].

Model	Component Landscapes and Index set	U	S	P
Ising spin glass	$\vartheta_I(x) = \prod_{k\in I} x_k \qquad I \subseteq \{1,\ldots,n\}$	•		•
SK model	as above with $\lvert I\rvert = 2$	•		•
Nk Landscapes	see [154]	∘	•	∘
Graph Bipartitioning	$\vartheta_{ij}([A,B]) = \begin{cases} 1 & \text{if } \{i,j\} \not\subseteq A, B \\ 0 & \text{otherwise} \end{cases} \qquad i<j$	∘	•	∘
Asymmetric TSP	$\vartheta_{kl}(\tau) = \sum_i \delta_{k,\tau(i)}\delta_{l,\tau(i-1)} \qquad k \neq l$	∘	•	∘

Thus $\sigma_k^2 = \mathbb{V}[b_k]$. Furthermore we have $\sigma^2 = \operatorname{Tr}\mathbf{C} = \sum_k \sigma_k^2$.

Random landscapes of practical importance often exhibit strong regularities.

DEFINITION 3.7. *A random landscape $\mathcal{F}$ is pseudo-isotropic if there are constants a_0, v, and w such that for all $x \in V$*
(i) $\mathbb{E}[f(x)] = a_0$,
(ii) $\mathbb{V}[f(x)] = v^2$, and
(iii) $\lvert V\rvert^{-1}\sum_{y\in V}\mathbf{C}_{xy} = w$.

3.2.1. Additive Landscapes. Many important random landscapes can be written as a sum of components with random coefficients. More precisely, let M be finite index set, let c_j, $j \in M$ be independent, real valued random variables over appropriate probability spaces $\Omega_j = (\mathbb{R}, \mathcal{A}_j, \mu_j)$, and let $\Theta = \{\vartheta_j : V \to \mathbb{R} \,|\, j \in M\}$ be a family of real valued functions on V. An *additive random landscape* (arl) is the probability space $(\mathbf{\Omega}_V, \otimes_j \mathcal{A}_j, \otimes_j, \mu_j)$ with

$$\mathbf{\Omega}_V = \left\{ f : V \longrightarrow \mathbb{R} \mid f(x) = \sum_{j=1}^{M} c_j \vartheta_j(x) \right\} . \tag{3.16}$$

In other words, the random landscape is constructed as a linear combination of non-random landscapes ϑ_j with independent random coefficients c_j.

Using the Karhunen-Loève decomposition, (3.14), any random landscape can be written as a linear combination with uncorrelated random coefficients. Since uncorrelated Gaussian random variables are independent we have

LEMMA 3.8. [154] *Every Gaussian random landscape is additive.*

The most important additive random landscapes exhibit additional regularities:

DEFINITION 3.9. *An arl is* uniform *if and only if*
(i) the random variables c_i, $i \in M$, are i.i.d. and
(ii) there exist constants $a, b \in \mathbb{R}$ such that $\sum_{x\in V}\vartheta_i(x) = \lvert V\rvert a$ and $\sum_{x\in V}\vartheta_i^2(x) = \lvert V\rvert b$ holds.
A uniform random landscape is strictly uniform *if there exist for any $x \in V$ constants $d, e \in \mathbb{R}$ with $\sum_j \vartheta_i(x) = d$ and $\sum_j \vartheta_i^2(x) = e$.*

THEOREM 3.10. [154] *A uniform random landscape is pseudo-isotropic if and only if: (i) $\mathcal{F}$ is strictly uniform, or (ii) $a = 0$, $\mathbb{E}[c_i] = 0$, and there is a constant $e \in \mathbb{R}$ such $\sum_i \vartheta_i^2(x) = e$ for all $x \in V$.*

3.2.2. Isotropy. Uniformity and pseudo-isotropy are still rather weak properties. In [173, 179] the notion of an *isotropic* random landscape was introduced as a "statistically symmetric model", that is, as a random landscape with a covariance matrix that shares the symmetries of the underlying configuration space.

DEFINITION 3.11. *A random landscape is* isotropic w.r.t. a partition $\mathcal{R}$ *of* $V \times V$ *if there are constants* a_0 *and* s *and a function* $c : \mathcal{R} \to \mathbb{R}$ *such that*
(i) $\mathbb{E}[f(x)] = a_0$ *and* $\mathbb{V}[f(x)] = s^2$ *for all* $x \in V$*, and*
(ii) $\mathbf{C}_{xy} = c(\mu)$ *for all* $(x, y) \in \mu$*, i.e., the covariance matrix* $\mathbf{C}$ *is constant on the classes* $\mu \in \mathcal{R}$*.*

The notion of isotropy for random landscapes is the analogue of *stationarity* for stochastic processes. Following the conventions of Karlin and Taylor [98] our notion of isotropy would be called "covariance isotropic", "weakly isotropic", or "wide sense isotropic". For a Gaussian random landscape the notions of (weak) isotropy and strict isotropy coincide of course.

A partition $\mathcal{R}$ of $V \times V$ is *homogeneous* if the diagonal $\{(x, x)|x \in V\}$ is a class of $\mathcal{R}$. It is *class degree regular* if for a given class $\mathcal{X} \in \mathcal{R}$ the number $|\{y \in V|(x, y) \in \mathcal{X}\}|$ is independent of $x \in V$.

THEOREM 3.12. [179]
(i) If $\mathcal{F}$ *is isotropic w.r.t. a homogeneous class degree regular partition of* $V \times V$ *then* $\mathcal{F}$ *is pseudo-isotropic. (ii) If* $\mathcal{F}$ *is isotropic w.r.t. a homogeneous class degree regular partition of* $V \times V$ *and* $\mathbb{E}[f(x)] = a_0$ *for all* $x \in V$*, then* $\mathcal{F}$ *is isotropic w.r.t. a homogeneous coherent configuration if and only if* $\mathbf{C} \in \langle\langle \mathcal{R} \rangle\rangle$*.*

If $\mathbf{A}$ is the adjacency matrix of an undirected graph (or more generally, the symmetric transition matrix of a Markov process on V then we say that a random landscape is **-isotropic w.r.t.* $\mathbf{A}$ if $\mathbb{E}[f(x)] = a_0$ and $\mathbf{C} \in \langle \mathbf{A} \rangle$, i.e., if $\mathbf{C}$ can be written as a polynomial of $\mathbf{A}$. For association schemes (such as those arising from distance regular graphs including the hypercube) isotropy and *-isotropy are equivalent.

THEOREM 3.13. [179] *An arl is *-isotropic if and only the Fourier coefficients (w.r.t. an orthonormal basis of eigenvectors of* $\mathbf{A}$*) satisfy:*
(i) $\mathbb{E}[a_k] = 0$ *for* $k \neq 0$*,*
(ii) $\mathrm{Cov}[a_k, a_j] = \delta_{kj}\mathbb{V}[a_k]$*, and*
(iii) $\mathbb{V}[a_k] = \mathbb{V}[a_j]$ *if* φ_j *and* φ_k *belong to the same eigenspace.*

These conditions mean that the Fourier coefficients are uncorrelated and that they have the same mean and variance whenever they belong to the same mode (eigenspace of $\mathbf{A}$). One might also say that Fourier and Karhunen-Loève series coincide for *-isotropic landscapes.

The class of *-isotropic models (on their natural configuration spaces) includes among others Derrida's p-spin Hamiltonians, the graph-bipartitioning problem, and the TSP. On the other hand, most variants of Kauffman's Nk-model, the XY-Hamiltonians, short-range Ising models, or the Graph-Matching Problem are not isotropic. This has important implications for the structure of these landscapes, as we shall see below.

3.2.3. Entropy. For a random landscape with measure μ we define the *entropy*

$$S = -\int \ln \mu(f) d\mu(f) \tag{3.17}$$

It is well known the Gaussian distributions maximize entropy. The proof for the one-dimensional case can be found e.g. in [80, prop. 1.15]. A proof of the general case is

provided in [177] together with a more detailed discussion of the relationships between isotropy and entropy. The main result is

THEOREM 3.14. *Let $\mathcal{F}$ be a random landscape with positive definite covariance matrix $\mathbf{C}$ with eigenvalues $\sigma_k^2 > 0$. Then the entropy satisfies*

$$S \leq S_{\mathbf{C}} = \frac{1}{2}|V| \ln \frac{2\pi e}{|V|} + \frac{1}{2} \sum_k \ln \frac{\Lambda_k |V|}{\sigma^2} \tag{3.18}$$

It is easy to verify that $S_{\mathbf{C}}$ is the entropy of a Gaussian distribution with covariance matrix $\mathbf{C}$.

The two terms in eqn.(3.18) allow for a direct interpretation. The Gaussian entropy $S_{\mathbf{C}}$ attains its maximum subject to a given variance σ^2 if and only if $\Lambda_k = \sigma^2/|V|$, in which case the second term vanishes. We therefore split the entropy of a random landscape into three contributions

$$S = S_{\sigma^2} + \Delta S_{\mathbf{C}} + \Delta S_{ng} \tag{3.19}$$

where $\Delta S_{ng} = S - S_{\mathbf{C}}$ is the entropy loss due to deviations from a Gaussian distribution, S_{σ^2} is the maximal entropy with given variance σ^2, and $\Delta S_{\mathbf{C}}$, the second term in eqn.(3.18), measures the entropy loss due to variations in the spectrum of $\mathbf{C}$. In particular, whenever there are correlations between different vertices, then $\mathbf{C}$ is non-diagonal and hence $\Delta S_{\mathbf{C}} < 0$. More precisely, $\Delta S_{\mathbf{C}} = 0$ if and only if the corresponding Gaussian random landscape is i.i.d.

3.3. Amplitude Spectra. Eqn.(3.4) decomposes non-elementary landscapes in a natural way into a superposition of elementary ones. A natural way of quantifying this decomposition is to consider the projection f_Λ of the landscape f onto the eigenspace of $-\mathbf{\Delta}$ with eigenvalue Λ. The relative importance of the Λ eigenspace is quantified in a natural way the ratio of the landscape variances of f_Λ and f.

$$B(\Lambda) = \frac{\langle \tilde{f}_\Lambda, \tilde{f}_\Lambda \rangle}{\langle \tilde{f}, \tilde{f} \rangle} \tag{3.20}$$

where, as usual, $\tilde{f}(x) = f(x) - \overline{f}$. We call $B(\Lambda)$ the *amplitude* of (the eigenspace associated with) Λ. In terms of the Fourier decomposition we obtain immediately [174]

$$B(\Lambda) = \sum_{k: -\mathbf{\Delta}\varphi_k = \Lambda \varphi_k} |a_k|^2 \Big/ \sum_{k: -\mathbf{\Delta}\varphi_k \neq 0} |a_k|^2 \tag{3.21}$$

For convenience of notation we set $B(0) = 0$. Thus $B(\Lambda) \geq 0$ and $\sum_\Lambda B(\Lambda) = 1$.

In many cases, in particular for landscapes on Hamming graphs, it is more convenient to refer to an amplitude by the interaction order (number of the eigenvalue when eigenvalues are arranged in ascending order *without* counting multiplicities). Hence one typically finds B_p instead of $B(p\alpha)$ for the p-th eigenspace of an α-letter Hamming graph. Obviously, the Laplacian $-\Delta$ can be replaced for instance by a transition operator if desired. In the case of random landscapes one naturally considers the expectation values $\mathbb{E}[B(\Lambda)]$.

Amplitude spectra are a very useful way of classifying non-elementary landscapes. We mention just a few examples here.

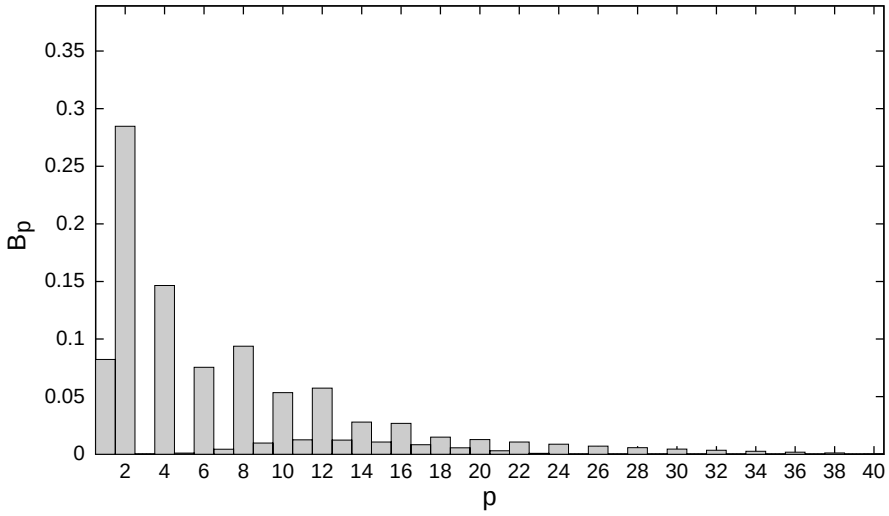


FIG. 3.1. *The estimated amplitude spectrum for a GC landscape with $n = 100$ under mutation [89]. The configuration space is the Hamming graph $\mathcal{Q}_2^{100}$ of sequences taken from the 2-letter alphabet $\{G,C\}$.*
The most striking feature of the amplitude spectrum of RNA landscapes is a strong difference between even and odd modes. This can easily be explained in terms of the physics underlying RNA folding: The major contribution of the folding energy comes from stacking of base pairs. Hence the major changes in free energy caused by a point mutation will arise from these contributions. Since stacking energies are influenced by an even number of nucleotides depending on the location of the affected base pair within a stack. A recent comparison of amplitude spectra for different landscapes based on folding short RNA chains indicates that the amplitude spectra of the free energy landscapes are typical [175].

- Asymmetric TSPs are superpositions of symmetric and anti-symmetric TSPs with equal weights [174]. Together with Table 3.1 this observation explains the behavior of the TSP mentioned in the introduction: with transpositions the symmetric and the anti-symmetric version of the TSP have very similar Laplacian eigenvalues and hence essentially the same correlation structure. In the case of reversals, however, we have a smooth landscape belonging to the 3rd eigenvalue for symmetric C, and an essentially uncorrelated landscape corresponding to a highly "excited state" for the anti-symmetric component.
- The landscape of the *Low Autocorrelated Binary String Problem* consists of a dominating 4-spin contribution and an asymptotically vanishing 2nd order component [174].
- The quadratic assignment problem consists in general of three contributions corresponding to the 3 smallest non-zero eigenvalues of the Laplacian of the Cayley graph $\Gamma(\mathsf{S}_n, \mathcal{T})$ [158].
- The free energy landscapes of two-letter RNA sequences consist predominantly of the small even modes $p = 2, 4, 6, 8$ [89], while the biophysically more relevant 4-letter alphabet AUGC has an additional large $p = 1$ component, Figure 3.1. See section 5.1.1 for an explanation of the RNA model.

Amplitude spectra of landscapes arising from more complicated models, such as evolving cellular automata [32], RNA folding, or electronic circuit design have been computed as well [89, 158, 195]. A Gaussian random landscape is *-isotropic if and only

if ΔS_C is maximal subject to given values of $\mathbb{V}[a_k]$ in Theorem 3.13. In this sense we can regard *-isotropy as a "maximum entropy" condition.

4. Ruggedness and Neutrality. Ruggedness intuitively is just the opposite of smoothness. Neutrality, i.e., the existence of neighboring configurations with the same fitness, appears to be just a way of achieving a "smooth" landscape. It comes as a surprise therefore, that ruggedness and neutrality will turn out to be independently tunable parameters.

4.1. Ruggedness and Autocorrelation Functions. The ruggedness of a landscape is most easily quantified by measuring the correlation of fitness values in "neighboring" positions. Weinberger [203, 204] suggested the following procedure. Given a Markov process on V, we sample the fitness values $f(x^{(t)})$, interpret them as a time series, and compute the autocorrelation function of this time series. Let $\mathbf{T}$ be the transition matrix of such a reversible Markov process with stationary distribution φ_0. The (expected) autocorrelation function along a $\mathbf{T}$-random walk on V is then

$$r(t) = \left(\sum_{x \in V} |\tilde{f}^2(x)| \varphi_0(x) \right)^{-1} \sum_{y \in V} \tilde{f}(x) (\mathbf{T}^t)_{xy} \tilde{f}^*(y) \varphi_0(y) = \frac{\langle \tilde{f}, \mathbf{T}^t \tilde{f} \rangle_{\varphi_0}}{\langle \tilde{f}, \tilde{f} \rangle_{\varphi_0}} \ . \tag{4.1}$$

By expanding f w.r.t. eigenvectors of $\mathbf{T}$ it can be shown [174] that

$$r(t) = \sum_{\lambda \neq 1} B_{\mathbf{T}}(\lambda) \lambda^t \tag{4.2}$$

where $B_{\mathbf{T}}(\lambda)$ are the amplitudes of f w.r.t. the eigenspaces of $\mathbf{T}$. Thus a landscape f is elementary w.r.t. a transition operator $\mathbf{T}$ if and only if the "random walk" autocorrelation function is exponential, $r(t) = \lambda_p^t$.

For regular graphs $\mathbf{T}$, $\mathbf{A}$ and $-\mathbf{\Delta}$ have the same eigenspaces and the eigenvalues of the transition matrix can be expressed in terms of the Laplacian eigenvalues as $\lambda = 1 - \Lambda/D$, where D is the vertex degree of the graph. Thus eqn.(4.2) becomes

$$r(t) = \sum_{\Lambda \neq 0} B(\Lambda) \left(1 - \Lambda/D\right)^t \ . \tag{4.3}$$

The information contained in $r(s)$ is therefore equivalent to the amplitude spectrum. A landscape is highly correlated if $r(s)$ decays slowly, i.e., if $B(\Lambda)$ is large for small eigenvalues Λ. The *correlation length*

$$\ell = \sum_{t=0}^{\infty} r(t) = D \sum_{\Lambda \neq 0} \frac{B(\Lambda)}{\Lambda} \tag{4.4}$$

may be used to condense the correlation information into a single measure of ruggedness.

Most early work on RNA landscapes, e.g. [59, 188] uses a different type of correlation measure based on the Hamming distance. In [174, 179] this approach is generalized to relations on $\mathcal{R}$ on $V \times V$.

DEFINITION 4.1. *Given a relation $\mathcal{R}$ on $V \times V$, the autocorrelation of f w.r.t. $\mathcal{R}$ is*

$$\varrho(\mathcal{R}) = \frac{|V|^2}{|\mathcal{R}|} \frac{\sum_{(x,y) \in \mathcal{R}} (f(x) - \overline{f})(f(y) - \overline{f})}{\sum_{x,y \in V} (f(x) - \overline{f})(f(y) - \overline{f})} \tag{4.5}$$

On Hamming graphs, for instance, it is natural to consider the distance classes, i.e., $(x,y) \in \mathcal{R}_d$ if and only if $d_H(x,y) = d$. Such distance-dependent correlation functions have been considered also for some combinatorial optimization problems [3, 4, 168, 178]. Given a partition of $V \times V$, we may of course regard ϱ as a function of the classes of this partition. Furthermore, if this partition is sufficiently "nice", then the correlation function ϱ itself also has useful algebraic properties. An example is the following:

THEOREM 4.2. [172] *Let f be landscape on a graph Γ that has a homogeneous coherent algebra $\mathfrak{W}[\Gamma]$. Then $r(s)$ is exponential if and only if ϱ is a left eigenvector of the collapsed adjacency matrix $\hat{\mathbf{A}}$.*

4.2. Ruggedness and Local Optima.

4.2.1. The number of local optima. Local optima play an important role since they might be obstacles on the way to the optimal solution. In the theory of disordered systems, local minima of the energy function are usually called metastable states. For the sake of definiteness we shall consider *local minima*, i.e., configurations $\hat{x} \in V$ satisfying

$$f(x) \le f(y) \quad \text{for all } y \in N(x)\,. \tag{4.6}$$

Analogous expressions for local maxima can be obtained by replacing f with $-f$. The number and distribution of local minima provides an alternative approach to landscape ruggedness.

In [141] Richard Palmer proposed to call a landscape f *rugged* if the number M_f of local optima scales exponentially with some measure of "system size" such as the number of cities in a TSP or the number of spins in spin glass. Unfortunately, there is in general no simply way of computing M_f without exhaustively generating the landscape. Alternatively, one can of course estimate M_f by checking whether a randomly generated $x \in X$ is a local minimum. Numerical data of this kind are reported e.g. in [181, 180, 63]. Methods from statistical mechanics can be used, however, to obtain the scaling of the expected value $\mathbb{E}[\mathsf{M}]$ with the system size for a variety of disordered systems, see e.g. [191, 189, 19, 73, 36, 156, 34, 46].

A non-rigorous result is particular interest in this context. The *correlation length conjecture* [181] suggests that the number of local optima of a "typical" landscape can be estimated from its correlation length ℓ, eqn.(4.4). More precisely, one expects on the order of one local optimum on a mountain with a radius that is determined by the correlation length ℓ. Numerical surveys provided good evidence that the correlation length conjecture yields a fairly accurate prediction of the number of local optima (meta-stable states) of isotropic elementary random landscape, see [63] for a summary of the numerical data.

4.2.2. Basins. To each local minimum $\hat{x}$ there is an associated *basin* $\mathcal{B}(\hat{x})$ defined by means of the steepest descent algorithm: Starting with $z_0 = y$ we choose at each step the neighbor $z_{k+1} \in N(z_k)$, $f(z_{k+1}) < f(z_k)$ with the smallest fitness value and repeat the procedure until it terminates when $z_{k+1} = \hat{x}$ is a local minimum. The notion of a basin hence may become ambiguous when there is "local neutrality" in $N(x)$, i.e., if there are $x \in X$ and $y, y' \in N(x)$ with $f(y) = f(y')$. It is an open question how the basin should be defined in full generality. It is not surprising that the distribution of basin sizes is crucial for the performance of simple optimization heuristics.

Probably the simplest approach is to generate an initial configuration at random and then to use steepest descent to reach the minimum of the basin. The question then becomes how likely it is to hit the basin of the global optimimum by chance. Let α_j, $j = 1 \ldots \mathsf{M}_f$, denote the sequence of relative basin sizes $|\mathcal{B}(\hat{x})|/|E|$.

THEOREM 4.3. [65] *The probability $p(m)$ that in a sample of m randomly chosen configurations we find at least one configuration in each basin is*

$$p(m) = \sum_{k=0}^{\mathsf{M}_f} (-1)^{\mathsf{M}_f - k} \sum_{1 \le j_1 \le \ldots \le j_k \le \mathsf{M}_f} (\alpha_{j_1} + \ldots + \alpha_{j_k})^m \tag{4.7}$$

From this rather complicated expression one can deduce, for instance

COROLLARY 4.4. [65] *Suppose $\mathsf{M}_f \gg 1$, $m = a^2 \mathsf{M}_f$ for some $a > 0$ and the relative basin sizes are uniformly distributed. Then $p(m) = \exp(-1/a)$.*

In other words, sampling $\mathcal{O}(\mathsf{M}_f^2)$ points at random provides a finite chance to find the basin of the global optimum.

However, so far there does not appear to be a good method for estimating basin sizes beyond exhaustive enumeration or random sampling. An important aspect is the correlation between basin size and fitness of the minimum: In highly correlated landscapes, i.e., in landscapes in which the amplitude spectrum shows large values of $B(\Lambda)$ for small values of Λ only, it appears that deeper minima have larger basins [46, 176].

4.2.3. Barriers and Depth. The basins of local minima are separated by saddle points and fitness barriers. Let $\hat{x}$ and $\hat{y}$ be two local minima and let $\mathbf{p}$ be a path in X from $\hat{x}$ to $\hat{y}$. Then the fitness barrier separating $\hat{x}$ from $\hat{y}$ is

$$f[\hat{x}, \hat{y}] = \min \left\{ \max \left[f(z) \middle| z \in \mathbf{p} \right] \;\middle|\; \mathbf{p} : \text{path from } \hat{x} \text{ to } \hat{y} \right\}, \tag{4.8}$$

A point $\hat{z} \in X$ satisfying the minimax condition in eqn.(4.8) is a *saddle point* of the landscape. The saddle-point energies $f[\hat{x}, \hat{y}]$ form an ultra-metric distance measure on the set of local minima, see e.g. [145, 196, 131]. This hierarchical structure can be represented by the *barrier tree* of the landscape, Figure 4.1. Its leaves are the local minima and its internal nodes correspond to saddle points.

The *barrier* enclosing a local minimum is the height of the lowest saddle point that gives access to a more favorable minimum. In symbols:

$$B(\hat{x}) = \min \left\{ f[\hat{x}, \hat{y}] - f(\hat{x}) \middle| \hat{y} : f(\hat{y}) < f(\hat{x}) \right\} \ . \tag{4.9}$$

If $B(\hat{x}) = 0$ then the local minimum $\hat{x}$ is degenerate. It is easy to check that eqn.(4.9) is equivalent to the definition of the depth of a local minimum in [103]. For metastable states it agrees with the more general definition of the depth of a "cycle" in the literature on inhomogeneous Markov chains [7, 22, 23]. The information contained in the energy barriers is conveniently summarized by two global parameters. Let Ω_f be the set of all global minima of f and let $\hat{x} \in \Omega_f$.

$$\mathsf{D} = \max \left\{ B(s) \middle| s \notin \Omega_f \right\} \tag{4.10}$$

$$\psi = \max \left\{ \frac{B(s)}{f(s) - f(\min)} \middle| s \notin \Omega_f \right\} \tag{4.11}$$

Both parameters are easily obtained from the barrier tree. The *depth* D and *difficulty* ψ [77, 22, 103, 160, 23] play a crucial role in theory of Simulated Annealing, see section 6.1.

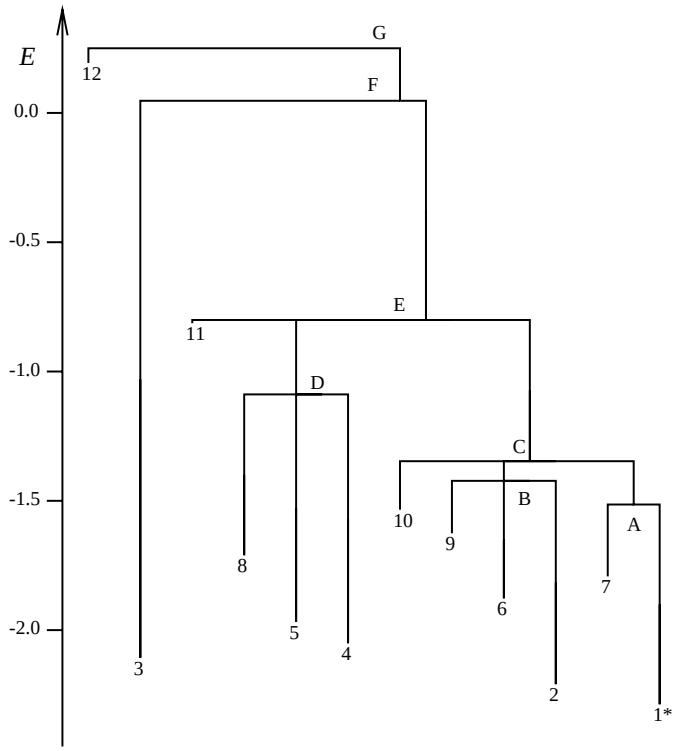


FIG. 4.1. *Example of a barrier tree of a landscape. Data are Gaussian random numbers on a* $\mathcal{Q}_2^7$. *The leaves 1-12 denote the local minima. The global minimum 1 is marked with an asterisk. Saddle points are labeled with capital letters from A to G. The saddle points* B, C, D, E *are "degenerate" indicating that the lowest energy paths leaving e.g. 4,5,8 run through a common exit point. Note that all* $2^7 = 128$ *configurations have pairwise distinct energies, hence there are no two distinct saddle points with the same energy, which may exist in general. The Barrier of* 5 *is* $B(5) = E(\mathsf{D}) - E(5)$, *along the lowest path from* 5 *to* 4, *while* $B(4) = E(\mathsf{E}) - E(4)$, *along the lowest path from* 4 *to* 1^*.

4.3. Neutrality. In this section we consider exclusively landscapes on finite simple undirected graphs with vertex set V and edge-set E. The number of neutral neighbors of $x \in V$ is

$$\nu(x) = \sum_{y \in N(x)} \delta\big(f(x), f(y)\big) \tag{4.12}$$

which can again be regarded as a landscape on Γ. Empirically, it turns out the important classes of landscapes arising in evolutionary biology and the theory of computer simulations exhibit a large degree of neutrality. We postpone a discussion of these cases to section 5. Below we briefly discuss two mechanisms for generating neutrality in simple models.

4.3.1. Neutrality from Symmetry. A rather trivial course of neutrality are symmetries in the fitness function. In some cases these symmetries arise from embedding a combinatorial optimization problem in a state space that is too large. We briefly outline one example.

Given a weighted graph with an even number n of vertices and a symmetric weight

matrix $\mathbf{W}$, the task of the *graph matching problem* (GMP) is to determine a set ξ of $n/2$ edges (i_k, j_k) with distinct incident vertices (a matching) such that

$$f(\xi) = \sum_{k=1}^{n/2} \mathbf{W}_{i_k, j_k} \tag{4.13}$$

is maximized. A matching ξ is conveniently encoded as a permutation π such that $\{\pi(2k-1), \pi(2k)\}$ is an edge of the matching. The resulting landscape is elementary on the Cayley graph $\Gamma(\mathsf{S}_n, \mathcal{T})$ with the transpositions as generators. Obviously, canonical transpositions of the form $\tau_{2k-1,2k}$ leave $f(\xi)$ unchanged since they merely exchange the endpoints of the same edge, and hence lead to the same matching.

4.3.2. Neutrality in Additive Random Landscapes. At present the most interesting approaches to neutrality focus on random landscapes. Hence we shall consider the random variable version of eqn.(4.12):

DEFINITION 4.5. *Let $\mathcal{F}$ be a random landscape. The random variable*

$$\nu_x : \mathcal{F} \longrightarrow \mathbb{Z}, \quad \nu_x(f) = \sum_{x' \in N(x)} \delta\big(f(x), f(x')\big) \ . \tag{4.14}$$

is called the neutrality of $\mathcal{F}$ in x. It is convenient to define the following parameters for all $y, y', y'' \in N(x)$:

$$c_x(y) = \big|\{j \in \Phi \mid \vartheta_j(x) \neq \vartheta_j(y)\}\big| \tag{4.15}$$

$$w_x(y', y'') = \big|\{j \in \Phi \mid \vartheta_j(x) \neq \vartheta_j(y') \ \wedge \vartheta_j(x) \neq \vartheta_j(y'')\}\big| \tag{4.16}$$

$$\Xi = \mathbb{E}\left[\frac{1}{|V|}\sum_x \left(\nu_x - \frac{1}{|V|}\sum_{x'} \nu_{x'}\right)^2\right] \ , \tag{4.17}$$

where $x \in V$ is an arbitrary vertex. The quantity Ξ is the expected variance of the family ν_x across a given landscape.

Theorem 4.6 below describes quite completely how additive random landscapes behave when their coefficients c_j vanish with a non-zero probability. This class of random landscapes, so far, the only one for which a detailed analysis of neutrality is available. Newman and Engelhardt [134] and [11] consider variations of Kauffman's Nk Landscape with integer coefficients, which also leads to non-vanishing neutrality in general.

THEOREM 4.6. [154] *Let $\mathcal{F}$ be an arl with coefficients c_i satisfying*

$$\mu\{c_j = \xi\} = \begin{cases} \mu_0 > 0 & \text{if } \xi = 0 \\ 0 & \text{otherwise.} \end{cases} \tag{4.18}$$

Then we have

$$\mathbb{E}[\nu_x] = \sum_{y \in N(x)} \mu_0^{c_x(y)} \tag{4.19}$$

$$\mathbb{V}[\nu_x] = \sum_{y', y''} \mu_0^{c_x(y') + c_x(y'')} \left[\mu_0^{-w_x(y', y'')} - 1\right] \tag{4.20}$$

$$\Xi = \frac{1}{|V|}\left[\sum_y \mathbb{V}(\nu_y) - \frac{1}{|V|}\sum_{y,y'} \mathrm{Cov}(\nu_y, \nu_{y'})\right] \tag{4.21}$$

$$+\frac{1}{|V|}\sum_y \mathbb{E}[\nu_y]^2 - \left(\frac{1}{|V|}\sum_y \mathbb{E}[\nu_y]\right)^2 ,$$

where $\frac{1}{|V|}\sum_{y,y'} \mathrm{Cov}(\nu_y, \nu_{y'}) \geq 0$.

In [154] a number of applications of Theorem 4.6 are discussed. Here we restrict ourselves to the simplest one:

COROLLARY 4.7. *For a p-spin model with coefficients c_i satisfying eqn.(4.18) we have*

$$\mathbb{E}[\nu] = n\,\mu_0^{\binom{n-1}{p-1}} \tag{4.22}$$

$$\mathbb{V}[\nu] = n(n-1)\mu_0^{2\binom{n-1}{p-1}}\left[\mu_0^{-\binom{n-2}{p-2}} - 1\right] + n\,\mu_0^{\binom{n-1}{p-1}}\left[1 - \mu_0^{\binom{n-1}{p-1}}\right] \tag{4.23}$$

$$\Xi = 0\ . \tag{4.24}$$

Consider a spin-glass model where the spins are arranged on a finite-dimensional lattice. That is, independent of the size of the system, there is only a finite number of lattice neighbors for each spin. In *short range spin glasses*, the only non-zero interaction coefficients link lattice neighbors, i.e., all but $\mathcal{O}(n)$ coefficients vanish. A short range spin glass is therefore characterized by $\mu_0 = 1 - \frac{z}{n^{p-1}}$, where $z > 0$ is a parameter determined by the connectivity of the lattice. As a consequence we have for every short range spin glass

$$\lim_{n\to\infty} \mathbb{E}[\nu/n] = \mathrm{e}^{-z} \quad \text{and} \quad \lim_{n\to\infty} \mathbb{V}[\nu/n] = 0\ . \tag{4.25}$$

The p-spin models are elementary w.r.t. spin-flip moves, see Table 3.1. On the other hand, we may use μ_0 to tune the degree of neutrality to any desired value. Conversely, given a value of $\mathbb{E}[\nu]$, we may choose p arbitrarily, thereby prescribing any desired degree of ruggedness. Thus we have established that *ruggedness and neutrality are independent features of (random) landscapes*.

5. Landscapes and Genotype Phenotype Maps.

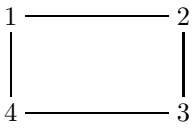
5.1. General Considerations. In the context of RNA sequences, fitness oftentimes does not depend on the particular sequence of nucleotides but its actual (spatial) structure. That is, there exists a generic partition on the configuration space by whose elements will be called phenotypes, representing classes of genotypes. However, note that two phenotypes do not necessarily have different fitness values. Accordingly, when some notion of phenotype representing an ensemble of genotypes of equal fitness exists, we can decompose the landscape as follows:

$$\textbf{Genotypes} \longrightarrow \textbf{Phenotypes} \longrightarrow \textbf{Fitness}\ . \tag{5.1}$$

Obviously, many properties of f are closely related to properties of the genotype-phenotype mapping which we will study in the following using Ribonuclein amino acids (RNA) and sequential dynamical systems (SDS) as paradigms. We will call the preimage of a fixed phenotype its *neutral network* and we will discuss the properties and role of neutral networks. In the following we will provide some background on RNA and SDS.

5.1.1. RNA. RNA acts in viruses and cells as messenger (mRNA), carrying the genetic information from the DNA to the translation apparatus, as transfer RNA, or tRNA for short, it plays the role of an adapter for the synthesis of proteins and finally as ribosomal RNAs (rRNA) being integral parts of the ribosome and exhibiting catalytic activities in natural polypeptide synthesis [25, 26, 207]. RNA thus serves two purposes: (i) storage of genetic information based on a one-dimensional template that can be read and copied on request, and (ii) catalytic properties as ribozymes which require three-dimensional structures in order to gain efficiency and specificity in processing specific substrates. As demonstrated by Spiegelman, *in vitro* evolution experiments can be performed to select RNA molecules that are capable of fast replication [125]. Indeed, replication rates are optimized in serial transfer experiments [44, 96, 161]. In case one wants to optimize other properties than replication, intervention is required making use of special techniques, which interfere with *natural selection*. A well known example is represented by the SELEX method – an acronym for *systematic evolution of ligands by exponential enrichment* – which allows one, for example, to create molecules with optimal binding constants [192]. The SELEX procedure is a protocol which isolates high-affinity nucleic acid ligands for a target, for example a protein, from a pool of variant sequences. Multiple rounds of replication and selection exponentially enrich the population of species which exhibits the highest affinity, i.e. which fulfill the required task. This procedure thus allows for simultaneous screening of highly diverse pools of nucleic acid molecules for different functionalities (for a review see, e.g. [43, 107]). Results from those experiments clearly demonstrate the essential property of RNA molecules, that genotype, i.e. the RNA sequence, and phenotype, associated to the structure, are combined in one molecule. Computer models of an RNA toy world were pioneered by the Vienna group [53, 155, 163, 164, 165, 93, 58] and lead to first realistic models of biological landscapes, see section 5.2.

5.1.2. Sequential Dynamical Systems. SDS are discrete dynamical systems that were introduced to capture basic features of computer simulations [12, 14, 132, 13]. An SDS consists of: (a) an undirected graph Y (with vertex set $\{1,\ldots,n\}$), (b) a collection of Boolean functions (F_i) that update the state of each vertex i as a function of its neighbors while leaving all other vertex states unchanged, and (c) an *update schedule* π, defining the order in which the vertices are updated. The composition of the maps F_i in the order prescribed by the update schedule π yields the SDS $[\mathfrak{F},\pi]=\prod_{i=1}^{n} F_{\pi(i)} : \mathbb{F}_2^n \longrightarrow \mathbb{F}_2^n$.
Example. Let $Y=\mathrm{Circ}_4$, be the circle graph on 4 vertices.



Suppose we have the parity function, $p_3 : \mathbb{F}_2^3 \to \mathbb{F}_2$, $p_3(x_1,x_2,x_3)=\sum_i x_i \mod 2$ for each vertex. Then we obtain for the update schedule $(1,2,3,4)$ with initial state $(1,1,0,0)$

$$\begin{aligned} F_1(1,1,0,0) &= (0,1,0,0),\\ F_2\circ F_1(1,1,0,0) &= (0,1,0,0),\\ F_3\circ F_2\circ F_1(1,1,0,0) &= (0,1,1,0),\\ F_4\circ F_3\circ F_2\circ F_1(1,1,0,0) &= (0,1,1,1)\ , \end{aligned}$$

FIG. 5.1. *A particular class of SDS are sequential cellular automata (sCA). Here we display the space time evolution of* 4 *different sCA over* Circ_{75} *with underlying rule* 90 *(applied for each vertex) and fixed initial condition. The sequential updates monitored are:* (a) $(1, 2, \ldots, n)$ *(natural order)* (b) $(1, 3, \ldots, 75, 2, 4, \ldots, 74)$ *(odd-even)* (c) $(2, 4, \ldots, 74, 1, 3, \ldots, 75)$ *(even-odd).*

and consequently we have $[F_{\mathrm{Circ}_4}, (1, 2, 3, 4)](1, 1, 0, 0) = (0, 1, 1, 1)$.

One important question is to analyze the set of all schedules π' that lead to the same dynamical system. In Fig. 5.1 we present examples on how the update schedule affects the dynamics of an SDS.

5.2. RNA Secondary Structure Folding.

5.2.1. Genotypes and Phenotypes for RNA. In the following we will consider RNA sequences of constant length, represented by n-tuples, $(x_1, \ldots, x_n)$, with $x_i \in \mathcal{A}$, $\mathcal{A}$ being a finite alphabet formed by the nucleotides. The basic mutational mechanism are random point mutations that occur with independent probability. This motivates us to call two sequences adjacent if they differ in exactly one nucleotide. Sequence space with this adjacency relation is referred to as $\mathcal{Q}_\alpha^n$ (the generalized n-cube), where $\alpha = |\mathcal{A}|$. In $\mathcal{Q}_\alpha^n$ each sequence has $(\alpha - 1)n$ neighbors and the maximal distance between two sequences is n.

RNA phenotypes are in general molecular structures of various resolutions. Here we will consider the following class of RNA secondary structures [202]:

DEFINITION 5.1. *A* secondary structure *over* n *vertices* $\{1, \ldots, n\}$, s_n, *is a vertex-labeled graph with an adjacency matrix* $A(s_n) = (a_{i,k})_{1 \le i,k \le n}$ *such that*

- $a_{i,i+1} = 1$ *for* $1 \le i \le n - 1$
- *for each* i *there is at most a single* $k \neq i - 1, i + 1$ *such that* $a_{i,k} = 1$
- *if* $a_{i,j} = a_{k,l} = 1$ *and* $i < k < j$ *then* $i < l < j$.

We call an edge $\{i, k\}$, $|i - k| \neq 1$ *a base pair. A vertex* i *connected only to* $i - 1$ *and* $i + 1$ *is called unpaired.*

The combinatorics of secondary structures viewed as abstract graphs has been studied in detail in Waterman *et.al.*[91, 162]. A particular result from asymptotic combinatorics on secondary structures – with certain restrictions such as minimum helix length – is that their number asymptotically becomes $O(a^n)$ with $a < 2$ [84]. This result immediately implies that there are structures having preimages of exponential size. Moreover, the RNA model allows for several generic choices of the fitness assignment, as for example using the thermodynamic stability and the degradation constant of the corresponding secondary structure.

5.2.2. The Intersection Theorem. We call a nucleotide sequence (x_i) compatible w.r.t. a secondary structure s_n iff for all $a_{i,k}$ with $a_{i,k} = 1$ and $k \neq i - 1, i + 1$ the nucleotides x_i and x_k *could in principle* form a Watson-Crick base pair. We de-

note the set of compatible sequences w.r.t. some secondary structure s_n by $\mathrm{C}(s_n)$. Note that we have

$$\mathrm{C}(s_n) \cong \mathcal{Q}_\alpha^{n_1} \times \mathcal{Q}_\beta^{n_2}$$

where n_1, n_2 are the numbers of unpaired and paired bases respectively and β is the size of the alphabet formed by the base pairs i.e. all pairs of nucleotides that can actually establish a chemical bond.

In terms of combinatorics, the uniqueness property of the Watson-Crick base pairs of an RNA secondary structure corresponds to an involution (viewing the base pairs as transpositions within the symmetric group, S_n [153, 155]).

THEOREM 5.2. *[155] Let s_n^1, s_n^2 be two secondary structures with the sets of compatible sequences $C(s_n^1)$, $C(s_n^2)$. Then*

$$C(s_n^1) \cap C(s_n^2) \neq \varnothing \ . \tag{5.2}$$

Accordingly, for any two secondary structures there exists a sequence that *could* in principle realize both from which we can conclude that the corresponding neutral networks come relatively close in sequence space. This in not true for more than two sequences. A necessary and sufficient condition for the intersection of the compatible sets of an arbitrary number of secondary structures to be non-empty can be found in [52].

5.2.3. Connectivity of Neutral Networks. In the following, we will denote a probability measure by μ_n where n refers to some index of the corresponding probability space Ω_n (here: a random graph) over n vertices. Let P_n be some property (event) in Ω_n. Then we write "P_n holds a.s." if and only if we have $\lim_{n\to\infty} \mu_n\{P_n\} = 1$.
The random graph model. Let $\mathcal{Q}_\alpha^n$ be a generalized n-cube over an alphabet of length α. Let Γ_n be a subgraph of $\mathcal{Q}_\alpha^n$ and $\mu_n\{\Gamma_n\} = \lambda_n^{|\Gamma_n|}(1-\lambda_n)^{\alpha^n - |\Gamma_n|}$. Then we call $\mathcal{Q}_{\alpha,\lambda_n}^n$ the random induced subgraph model.
For RNA folding landscapes we can interpret the probability λ as the neutrality degree i.e. the number of neutral neighbors, ν divided by the total number of neighbors, $(\alpha-1)n$.

THEOREM 5.3. [147] *In $\mathcal{Q}_{\alpha,\lambda_n}^n$, let $C_n^{(1)}$ be the largest component of a $\mathcal{Q}_\alpha^n$-subgraph Γ_n. Then there exists a constant $c > 0$ such that for $\lambda_n \geq \frac{c\ln(n)}{n}$*

$$|C_n^{(1)}| \sim |\Gamma_n| \qquad a.s.$$

holds.

It may be of interest to note that theorem 5.3 establishes the existence of the giant component *indirectly*. The proof gives no clue on how to construct a path between two vertices and moreover on how long such a path might be. The explicit construction of (short) paths between vertices of neutral networks would therefore be of particular interest and leads to a deeper understanding on how likely such a path would be realized in an evolutionary search. In fact the next result provides such a *constructive* proof, although we will need the higher probability $\lambda_n \geq n^{-a}$ with $0 \leq a < 1/2$.

THEOREM 5.4. [150] *Let $0 \leq a < 1/2$ and let $k \in \mathbb{N}$ with $k > \frac{1+3a}{1-2a}$. In $\mathcal{Q}_{\alpha,\lambda_n}^n$ let λ_n be such that $\exists n_0 \in \mathbb{N}$; $\forall n \geq n_0$ $\lambda_n \geq n^{-a}$ holds. Finally, let $d_{\mathcal{Q}_\alpha^n}$ and d_{Γ_n} denote the distances in the graphs $\mathcal{Q}_\alpha^n$ and Γ_n, respectively. Then*

$$\forall\ P, Q \in \mathcal{Q}_\alpha^n; \quad \lim_{n\to\infty} \mu_n\{d_{\Gamma_n}(P,Q) \leq [2k+3]\, d_{\mathcal{Q}_\alpha^n}(P,Q)\} = \lambda_n^2$$

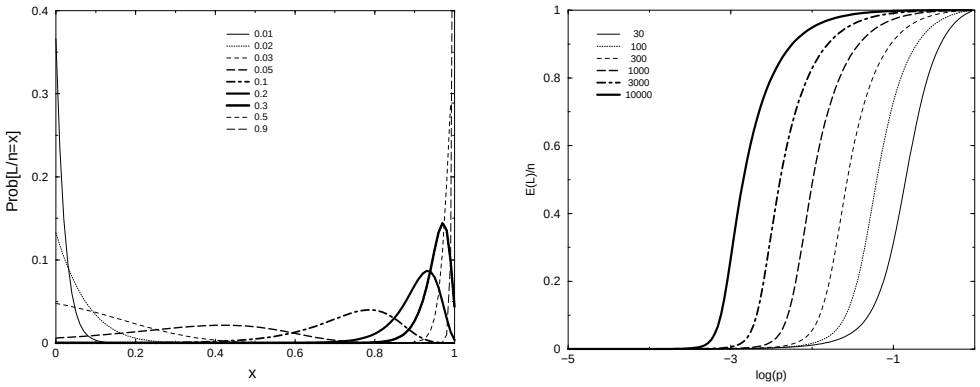


FIG. 5.2. *L.h.s.:Distribution of scaled neutral path lengths L/n on random subgraphs of $\mathcal{Q}_2^{100}$ for different values of p.*
R.h.s.: Average length of neutral path for different sequence length n.

holds. In particular for constant $\lambda_n = \lambda$ we have

$$\forall\, P, Q \in \mathcal{Q}_\alpha^n; \quad \lim_{n\to\infty} \mu_n\{d_{\Gamma_n}(P,Q) \leq 7 d_{\mathcal{Q}_\alpha^n}(P,Q)\} = \lambda^2\,.$$

Let us finally come to the last result on generalized n-cubes. From now on we will assume a constant probability $\lambda > 0$.

THEOREM 5.5. [147] *In the random graph $\mathcal{Q}_{\alpha,\lambda}^n$ the probability $\lambda^* = 1 - \sqrt[\alpha-1]{\alpha^{-1}}$ is the threshold value for connectivity. That is, a.s. no random graph is connected for $\lambda < \lambda^*$ and a.s. every random graph is connected for $\lambda > \lambda^*$.*

The above theorem is in fact well known for binary n-cubes. However the proof in [17] is based on an estimation of some edge boundary and utilizes in this context an isoperimetric inequality from [78].
The proof of 5.5 does in fact explicitly construct "many" independent paths which eventually lead to the desired result. Let P, Q be arbitrary vertices of the random graph. As in Theorem 5.4 we can reduce the case to P, Q having finite Hamming distance. For $\lambda > \lambda^*$, one then shows that any vertex has an arbitrary finite number of neighbors in the random graph. Using these neighboring vertices one proceeds completely analogous to the proof of Theorem 5.4. To prove that λ^* is a threshold value we show that there exist isolated vertices in case of $\lambda < \lambda^*$. This can be proved by considering the random variable counting the isolated vertices, Z. It is obvious that Z has mean $\mu = \lambda\, \alpha^n\, (1-\lambda)^{(\alpha-1)n}$ and for finite μ one can show that Z becomes in the limit of large n Poisson. From this we can conclude that a.s. for $\lambda < \lambda^*$ and arbitrary natural number ℓ, there are at least ℓ isolated vertices in the random graph.

Extensive computational studies on RNA landscapes indeed show that the neutrality $\nu/(\alpha-1)n$ is above the threshold value λ^* for many RNA structures and that there are indeed extensive (almost) connected neutral networks [75, 76].

5.2.4. Neutral Paths. Neutral paths were used to gain information about the structure of the (connected components of) neutral networks in a series of computer experiments on RNA folding landscapes [164, 75, 76]. In each step we attempt to find a neutral neighbor such that the distance from the starting point increases.

In a random subgraph $\Gamma_{n,p}$ of a distance regular graph Γ_n the probability that a neutral path with d steps cannot be elongated any further equals $(1-p)^{\alpha(d)}$ where

$\alpha(d)$ denotes the the number of "forward steps", i.e. the number of adjacent vertices actually increasing the distance to the starting point. For Hamming graphs $\mathcal{Q}_\alpha^n$, for instance, we have $\alpha(d) = (a-1)(n-d)$. The probability that a neutral path of $\Gamma_{n,p}$ terminates after exactly d steps reads [154]:

$$\text{Prob}[\mathcal{L} = d] = (1-p)^{\alpha(d)} \times \prod_{d'=1}^{d} \left[1 - (1-p)^{\alpha(d'-1)}\right] \ . \tag{5.3}$$

Let next $L(n) = \text{diam}\Gamma_n$ and $x = d/L(n)$. We consider a sequence Γ_n of distance transitive graphs such that $L = L(n) \to \infty$ and $\alpha(d)$ can be written in the form $\alpha(d) = D(n)\vartheta(x)$ where $D(n)$ is the vertex degree of Γ_n and $\vartheta : [0,1] \to [0,1]$ is differentiable. Let ω_n tend to infinity arbitrarily slowly and suppose $\zeta = \lim_{n\to\infty} \log D(n)/\log L(n)$ exists. Then $\text{Prob}[\mathcal{L}/\text{diam}\Gamma_n = x]$ has a maximum at

$$x^* = \begin{cases} 1 & \text{if} \quad p = \omega_n \log D(n)/D(n) & \\ 0 < s < 1 & \text{if} \quad p = C \log D(n)/D(n) & C > 1/\zeta \\ 0 & \text{if} \quad p = C \log D(n)/D(n) & C < 1/\zeta \ . \end{cases} \tag{5.4}$$

For an example see Fig. 5.2. Neutral paths provided the first evidence for extended neutral networks in RNA models [164].

5.3. Sequential Dynamical Systems.

5.3.1. Genotypes and Phenotypes of SDS. The schedules are the SDS-genotypes and form the update graph $U(Y)$ whose vertices are permutations, written as n-tuples without repetition: $(i_1, \ldots, i_n)$. In order to understand what adjacency of schedules means let us consider $Y = \text{Circ}_4$:

Now suppose we apply the maps $F_1, \ldots, F_4$ according to the orderings $(1,2,3,4)$ and $(3,2,1,4)$. Since 2 is adjacent to 1 and 3 there exist maps $F_1, \ldots, F_4$ such that $F_1 \circ F_2 \circ F_3 \circ F_4 \neq F_3 \circ F_2 \circ F_1 \circ F_4$ (see Fig. 5.3 for an illustration). That is, in general we cannot transpose vertices 1 and 3 although they are *not* adjacent in Circ_4. Hence, if we want to define an adjacency relation between two permutations $\pi = (i_1, \ldots, i_n)$, $\pi' = (j_1, \ldots, j_n)$ such that for all maps $F_1, \ldots, F_n$ holds $\prod_{r=1}^n F_{\pi(r),Y} = \prod_{r=1}^n F_{\pi'(r),Y}$, we can *at most* allow the transposition of *consecutive* coordinates (being Y-vertices) i_k, i_{k+1} in $(i_1, \ldots, i_n)$. In fact it is straightforward to show that every transposition of consecutive non-adjacent vertices i_k, i_{k+1} leaves the SDS invariant [14]. Hence two schedules $(i_1, \ldots, i_n)$, $(h_1, \ldots, h_n)$ are adjacent (point mutants) if they differ by exactly one flip of two consecutive coordinates that are not Y-neighbors (or equivalently: iff (a) $i_\ell = h_\ell$, $\ell \neq k, k+1$ and (b) $\{i_k, i_{k+1}\}$ is not adjacent in Y). Note that the above definition of adjacency leads to a maximum of $n-1$ neighbors and a maximal distance of $\binom{n}{2}$ between two schedules.

$U(Y)$ induces equivalence classes of schedules by identifying any two vertices that are connected by a path in the update graph, which we will write as $\pi \sim_Y \pi'$. As an illustration see Fig. 5.3, where we draw the update graph of the square, $Y = \text{Circ}_4$. It turns out that there exists an one-to-one correspondence between sets of equivalent schedules and the acyclic orientations of Y, $\psi_Y : \mathsf{S}_n/\sim_Y \longrightarrow \text{Acyc}(Y)$,

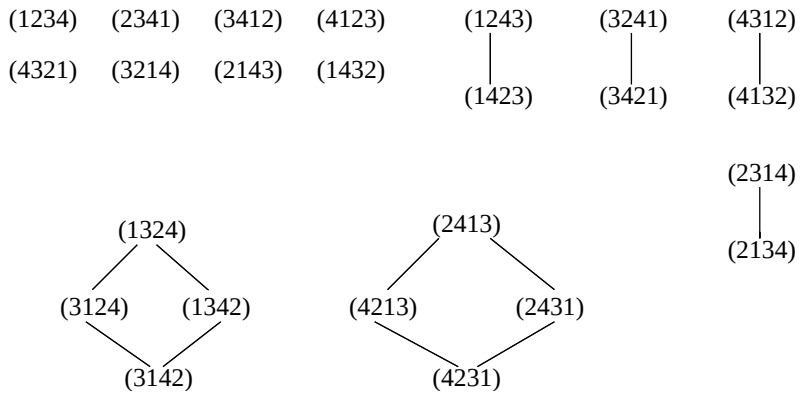


FIG. 5.3. *The update graph of $Circ_4$, $U(Circ_4)$. $U(Circ_4)$ has 24 vertices, 8 of which are isolated points (corresponding to the Hamiltonian paths in $Circ_4$), 4 components of size two and 2 components of size 4.*

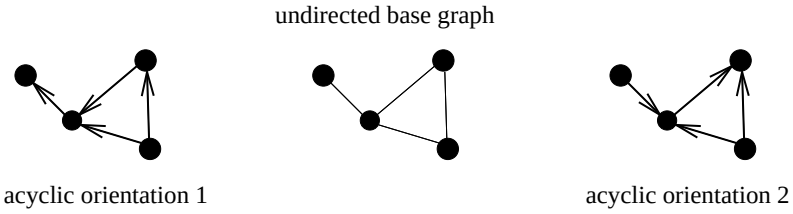


FIG. 5.4. *Acyclic orientations of an undirected graph are obtained by assigning directions to its edges such that the resulting directed graph is cycle-free.*

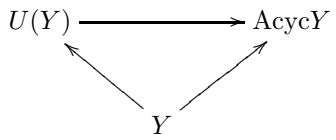
see Fig. 5.4, [148]. An acyclic orientation of an undirected graph Y is obtained by assigning directions on its edges such that the resulting directed graph is a tree. We denote the set of acyclic orientations of Y by $\mathrm{Acyc}(Y)$. The number of acyclic orientations of a graph Y is given by the absolute value of its chromatic polynomial at (-1) [185]. Accordingly, acyclic orientations of Ya can be viewed as the *phenotypes* of the mapping:

$$\lambda_Y : U(Y) \longrightarrow \mathrm{Acyc}(Y) \ . \tag{5.5}$$

It is worth mentioning that λ_Y is highly nontrivial. For example, determining the λ_Y-preimage of an acyclic orientation corresponds to the computation of the number of linear orders that are compatible to a given partial order (which is naturally induced by the acyclic orientation).

Further, it is clear that SDS *by construction* allow for a variety of genotype–phenotype maps. Unlike the RNA case, where we have fixed genotypes and there are only relatively few concepts of phenotypes, like for example secondary structures or tertiary structures, SDS genotype–phenotype maps depend on the choice of the base graph, Y. From this point of view RNA seems to be a particular case since of course the secondary structure notion strongly depends on the linear sequence realizing it. For SDS the graph Y yields both, the update graph $U(Y)$ whose vertices are the

genotypes and the phenotypes that factor through acyclic orientations:



5.3.2. Neutral networks. Now we can ask how well can we search for a specific schedule of a simulation, simply using some analogue of point mutations in the update graph? Of course, this question is motivated by our findings in the RNA case. In fact, straightforward comparison of (generalized) n-cubes $\mathcal{Q}_\alpha^n$ (the search space for RNA) and the update graphs (the search space for SDS) reveals that both are excellent search spaces. We explicitly have $\deg(\mathcal{Q}_\alpha^n) = (\alpha-1)n$, $\deg(U(Y)) \leq n-1$, $\operatorname{diam}(\mathcal{Q}_\alpha^n) = n$ and $\operatorname{diam}(U(Y)) \leq \binom{n}{2}$. Furthermore $|\mathcal{Q}_\alpha^n| = \alpha^n$ and $|U(Y)| = n!$ holds. In view of this similarity, it remains to analyze whether the genotype–phenotype mapping constructed in (5.5) exhibits a significant degree of neutrality.

We will next give a concentration result for the number of acyclic orientations of the random graph $G_{n,p}$ from which we can draw the following two conclusions:
(a) the number of neutral networks is sharply concentrated around its mean
(b) the average size of a neutral network, N is given by

$$p^{-n} \prod_{i=1}^{n} [1-(1-p)^i] \; . \tag{5.6}$$

THEOREM 5.6. [148] *Let $G_{n,p}$ be a random graph i.e. the graph over $\{1,\ldots,n\}$ where each edge is selected with independent probability p and $\log_2(|\mathrm{Acyc}(G_{n,p})|) : G_{n,p} \to \mathbb{N}$ the r.v. counting the number of acyclic orientations of $G_{n,p}$. Then $\log_2(|\mathrm{Acyc}(G_{n,p})|)$ is sharply concentrated around its mean, i.e. $\forall \lambda > 0$;*

$$\mu_{n,p}(\{ \mid \log_2(|\mathrm{Acyc}(G_{n,p})|) - \mathbb{E}[\log_2(|\mathrm{Acyc}(G_{n,p})|)] \mid > \lambda\sqrt{n(n-1)/2}\,\}) < 2e^{-\lambda^2/2} \; ,$$

where $n[\log_2(n) - \log_2 e - \log_2 p - o(1)] \leq \mathbb{E}[\log_2(|\mathrm{Acyc}(G_{n,p})|)]$. In particular on the average there are $p^{-n}\prod_{i=1}^{n}[1-(1-p)^i]$ permutations (schedules) that are mapped by λ_Y into an acyclic orientation.

Note, that the above theorem, however, does not provide information on the distribution of sizes of neutral networks.

6. Dynamics on Landscapes.

6.1. Landscape Structure and Simulated Annealing. Simulated annealing [104, 77, 139] is a very general optimization method based on stochastically simulating the slow cooling of a physical system. The basic idea is that there is a "temperature" T, various ways to change the state of the system, and a probability of accepting a change that depends on the difference in the fitness function. The transition matrix is therefore of the form

$$\mathbf{P}_{yx} = \mathbf{T}_{yx} \times \begin{cases} 1 & \text{if} \quad f(y) \leq f(x) \\ \exp\big(-(f(y)-f(x))/T\big) & \text{if} \quad f(y) > f(x) \end{cases} \tag{6.1}$$

The temperature is slowly decreased at each step. The sequence $\{T_t\}$ is called the *cooling schedule.*

When the temperature is zero, changes are accepted only if f decreases, an algorithm also known as hill-climbing or adaptive walk [66], or more generally, the greedy algorithm or steepest descent. In this case the system soon reaches a state in which none of the proposed changes can decrease the cost function, but this is usually a poor optimum. Little is known about the relationships of adaptive and gradient walks and landscape structure apart from extensive numerical studies mostly on Nk model landscapes [100, 205, 54] and uncorrelated random landscapes [119, 118, 143]. Similar numerical studies have been performed for RNA folding landscapes [59] and in a model of early vascular land plants [135].

Landscape characteristics such as depth and difficulty determine the asymptotic behavior of simulated annealing.

THEOREM 6.1. [77]. *Simulated Annealing converges almost surely to a global minimum if and only if the cooling schedule T_k satisfies $\sum_{k\geq 0}\exp(-\mathsf{D}/T_k)=\infty$.*

A general theory of "Simulated Annealing Algorithms and Markov Chains with Rare Transitions" that emphasizes the importance of depth and difficulty for convergence results and error bounds is reviewed in [23].

6.2. Quasispecies Dynamics. A particular class of dynamics that has been studied in various landscapes is a subclass of genetic algorithms in which only mutation but no crossover is considered. Given some landscape $f : X \to \mathbb{R}$ some configuration, x, is replicated with rate $f(x)$. The replication process is error-prone and produces the mutant configuration y with probability $Q_{x,y}$. We can visualize this process as follows

$$x \xrightarrow{f(x)} \xrightarrow{Q_{x,y}} x+y \tag{6.2}$$

The first class of landscapes in which mutation based dynamics has been investigated were single peak landscapes. In a single peak landscape one particular configuration has the maximum fitness while all other configurations have inferior fitness values. Eigen, Schuster, and collaborators [40, 42, 187, 41] completely analyzed the error-prone replication of haploid organisms (or, equivalently, biopolymer sequences) on a single peak landscape. They discovered the genotypic error threshold phenomenon, i.e. the existence of some critical error rate at which the population becomes unstable and drifts essentially randomly through sequence space.

More complicated landscapes were considered beginning with the double-peak model [166] exhibiting a trade-off between width and height of the peaks that depends on the mutation rate. Error-threshold phenomena on spin-glass type landscape are studied for instance in [190, 18]. The effects of population sizes are discussed in [137, 2, 120, 21]. Inspired by a series of computer simulations based on RNA folding landscapes [57, 56, 59, 93] interest has recently shifted to so-called *single shape landscapes*. These arise from neutral networks by assigning a high fitness value to all sequences belonging to a particular neutral network and a low fitness to all other configurations [152].

It could be shown that RNA mutation dynamics exhibits for single-shape landscapes *phenotypic error thresholds* [93, 152]. The phenotypic error-threshold is a natural generalization of Eigen's genotypic error threshold which corresponds to the absence of neutrality. Accordingly, the error threshold phenomenon does not seem to be an artifact of the particular choice of single peak landscapes, although many types of fitness function do not exhibit the error-threshold phenomenon [199, 209].

In the following we use a single-shape landscape of a SDS of the form

$$f_{a_0} : \mathrm{Acyc}(Y) \to \{1, \sigma\}, \quad f(a) = \begin{cases} \sigma > 1 & \text{for } a = a_0 \\ 1 & \text{else.} \end{cases} \tag{6.3}$$

as an example. We shall see that the landscape

$$\lambda_Y : U(Y) \longrightarrow \mathrm{Acyc}(Y) \to \{1, \sigma\} \ ,$$

exhibits an error threshold phenomenon for mutation based replication of update schedules.

To this end we introduce a replication-deletion process over permutations with acyclic orientations as phenotypes. We refer to a permutation π as a *master* or a *non-master*, respectively, depending on whether or not π is an element of $\lambda_Y(a_0)$. A *population* $V = \{v_i |\ i \in \mathbb{N}_N\}$ is a finite family of vertices. Each element of V has a fitness of 1 if it corresponds to a non master acyclic orientation or σ otherwise. The replication-deletion process consists of two coupled random events: an element of V is selected with some fitness weighted probability and is then subject to replication whereas another randomly chosen one is deleted. This process is the well known Moran model [130]. In detail, the replication-deletion process works as follows [68]: suppose there are $m \in \mathbb{N}_N$ elements having the master–phenotype and let $\overline{\sigma} = (N + (\sigma - 1)m)/N$. We select an ordered pair (v_r, v_d) from V: The first element v_r has then a master-phenotype with probability $p_\mu = \sigma m/(N\overline{\sigma})$ and has a non-master phenotype otherwise. The second element v_d is chosen with uniform probability $1/(N-1)$ from $V \setminus \{v_r\}$. The pair (v_r, v_d) is mapped into the pair (v_r, v^*) where v_r remains (unchanged) in the population and v_d is replaced by v^*. In order to describe the mapping $(v_r, v_d) \mapsto (v_r, v^*)$ we first introduce the maps

$$e_j : \mathsf{S}_n \to \mathsf{S}_n; \qquad e_j((i_1, \ldots, i_n)) = (i_1, \ldots, i_{j+1}, i_j, \ldots, i_n) \ . \tag{6.4}$$

for all $j = 1, \ldots, n$. The maps e_j are the analogue of point mutations in the RNA case. The mapping $(v_r, v_d) \mapsto (v_r, v^*)$ is now obtained as follows: We select each e_j, $j = 1, \ldots, n-1$ independently with probability φ and derive the multi-set $I = (j_1, \ldots, j_s)$ where $j_a < j_b$ for $a < b$ and $j_h \in \{1, \ldots, n-1\}$. Then we set

$$v^* = \left[\prod_{j \in I} e_j \right] (v_r). \tag{6.5}$$

The above mappings are considered as independent events and the time interval Δt which elapses between two such actions is assumed to be exponentially distributed according to $P(\Delta t > \tau) = \exp(-\tau N \overline{\sigma})$.

Let us now turn to the time evolution of a population of permutations. We introduce the following metric on acyclic orientations:

$$\begin{aligned} &d(\ ,\ ) : \mathrm{Acyc}(Y) \times \mathrm{Acyc}(Y) \to \mathbb{N}, \\ &d(a, a') = |\{y \in \mathrm{E}[Y] \mid y \text{ has a different orientation in } a \text{ and } a'\}| \end{aligned}$$

Each element of $v \in V$ has distance $d(v, a_0)$ from the "target" a_0. In the following we focus on the frequency distribution of these distances. Specifically, we generate a random graph $Y \in G_{n,p}$ and choose a random acyclic orientation $a_0 \in \mathrm{Acyc}Y$ to be the master–phenotype and set $\sigma = 10$. The initial population consists of N=1000

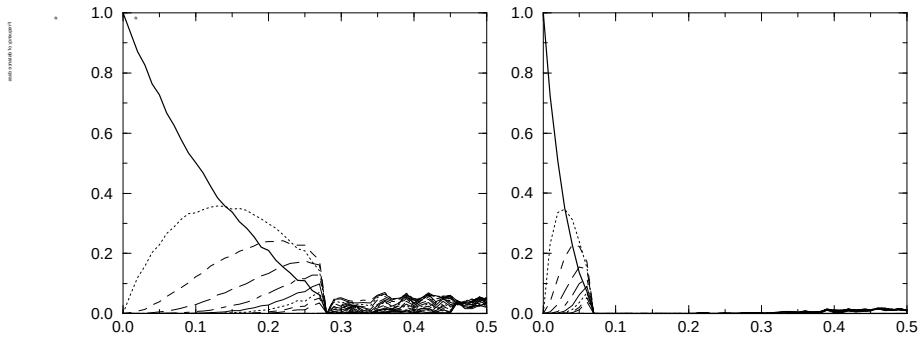


FIG. 6.1. *The error threshold phenomenon for the compositum $f_{a_0} \circ \lambda_{G_{30,p}}$ for probabilities $p = 0.25$ (l.h.s) and $p = 1.0$, respectively. We plot the fraction of a population of size $N = 1000$ in the distance classes $D = 0$ (full line), $D = 1$ (dotted), $D = 2$ (short-dashed), $D = 3$ (long-dashed), $D = 4$ (dash-dotted), etc., as a function of the mutation probability φ.*

permutations corresponding to the master acyclic orientation, see Fig. 6.1 for two examples.

The critical value of the mutation probability φ can be obtained analytically [109]:

$$\varphi^* = 1/p(1 - \sqrt[n-1]{1/\sigma}) \,. \tag{6.6}$$

For error rates below the threshold we have a non-uniform distribution of the population, a quasispecies of schedules and above threshold the population is uniformly distributed. In particular, for $Y = K_n$, i.e., $p = 1$ the mapping λ_Y is bijective and consequently, each phenotype is represented by exactly one genotype. Accordingly, we obtain the classical single peak landscape of [41]. By modulating the edge-picking probability p one obtains a variety of genotype–phenotype mappings. The smaller p becomes the more selective neutrality is exhibited which allows to tolerate more and more replication errors.

Neutrality has a number of important impacts on the dynamical behavior of population replicating according to eqn.(6.2). The diffusive motion of the population's "center of gravity" is described in [37]. The diffusion constant is related to population size N, per digit mutation rate φ and the fraction p of neutral neighbors [93]

$$D \approx \frac{6f(a_0)\varphi}{3 + 4N\varphi} np \tag{6.7}$$

in the case of a 4 letter alphabet. A constant "rate of innovation" is reported in [92] for the landscapes in which all neutral networks come close together, as in the case of RNA. An analytical study of very simple model landscapes shows that crossing entropy barriers is faster by orders of magnitude than the crossing of fitness barrier [194].

6.3. Genetic Algorithms and Genetic Programming. Genetic Algorithms, Evolutionary Strategies, and Genetic Programming [146, 15, 110, 86, 99, 55] can be viewed as dynamical systems defined on a fitness landscape, and the interplay of landscape structure and performance of genetic algorithms is an area of active research. Most of the literature on this topic, however, deals with computer simulations and empirical connections between measures such as fitness distance correlation [95] and

algorithm performance. We deliberately exclude this topic here and refer the reader to recent books including [10, 71, 127, 169].

Much of the mathematical analysis of Genetic Algorithms is concerned with the convergence of the population, see e.g. [136, 159]. Schemata, i.e., hyperplanes in $\mathcal{Q}_a^n$ appear to play an important role here [69, 70, 72, 114, 140, 48, 197, 198].

The fitness function $f : X \to \mathbb{R}$ can be extended in a natural way to arbitrary subsets of X by setting

$$f(A) = \frac{1}{|A|} \sum_{x \in A} f(x) \ . \tag{6.8}$$

A schema is defined in terms of its fixed bits h as

$$\mathcal{H} = H[h] = \{x \in V | \forall i \in H : x_i = h_i\} \ . \tag{6.9}$$

Note that we regard $H \subseteq \{1, \ldots, n\}$ as the index set of fixed positions. The value $f(H[h])$ is called the schema-fitness. For a discussion of the Schema Theorem and the Building Block Hypothesis we refer to the literature [1, 15, 85, 60, 86, 186]. A variety of landscape classes can be defined in terms of schema fitnesses. We restrict ourselves to a simple example here just to give the flavor. In a deceptive landscape an optimal schema of some size is "contradicted" by one of its sub-schemata. Intuitively, this is just the converse of GA-easy [113].

DEFINITION 6.2. [208] *A landscape f is* deceptive *if there are vertices $x, y \in \mathcal{Q}_\alpha^n$ and index sets $H \subset K \subset \{1, \ldots, n\}$ such that*

(i) $K[x] \neq K[y]$,
(ii) $f(H[x]) > f(H[z])$ *for all* z *with* $H[x] \neq H[z]$, *and*
(iii) $f(K[y]) > f(K[z])$ *for all* z *with* $K[y] \neq K[z]$.

A discussion of various notions of deceptive and GA-easy functions and their mutual relationships can be found in [177, 133].

7. Trends in Landscape Theory. In the following we will try to discuss some developments in landscape theory, currently being under investigation, that we think have some relevance for a more complete picture of this subject. As this section is intended to be an outlook in different directions of landscape theory, our representation is not entirely self contained. Explicitly, subsection 7.2 does require some background on basic cohomology theory [126].

7.1. Configuration Space Topologies. Combinatorial ("discrete") landscapes are treated quite differently from their manifold ("continuous") counterparts. The reason is that functions on $\mathbb{R}^n$, or more generally Riemannian manifolds can be analyzed in terms of differential operators such as gradients, while finite sets are usually discussed in terms of graph-theoretical properties. It seems desirable therefore, to find a basic framework that allows to deal with landscapes on arbitrary configurations spaces. A suitably general language is provided by the theory of *pretopological spaces*.

A pretopological space consists of an arbitrary set X and a collection $\mathcal{N}(x)$ of neighborhoods for every point $x \in X$, such that
(P1) $N \in \mathcal{N}(x)$ implies $x \in N$;
(P2) $N \in \mathcal{N}(x)$ and $N \subseteq N'$ implies $N' \in \mathcal{N}(x)$
(P2) $N, N' \in \mathcal{N}(x)$ implies $N \cap N' \in \mathcal{N}(x)$
Pretopologies are more general then the much more familiar topological spaces. In fact, $(X, \mathcal{N})$ is a topological space if and only if

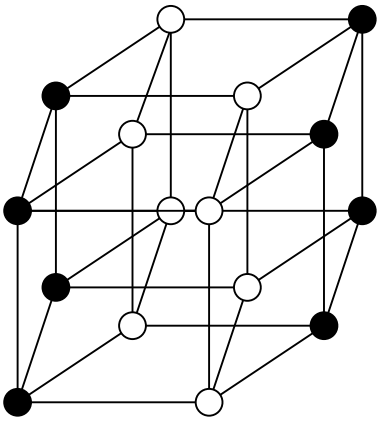


FIG. 7.1. *A 2-neutral landscape $f : \mathcal{Q}_2^4 \to \mathbb{F}_2$ (here all black vertices map into 0 and 1, otherwise. Note that each of the two fitness classes forms two connected subgraphs.*

(T) For each $N \in \mathcal{N}(x)$ there is an $N' \in \mathcal{N}(x)$ such that $N \in \mathcal{N}(y)$ for all $y \in N'$.

Directed graphs are exactly the finite pretopological spaces. Their neighborhood systems consists of all sets N' containing x and all vertices adjacent to x, i.e., $N(x) \cup \{x\} \subseteq N'$. Notions such as minima, maxima, or continuity of a function, connectedness, convergence, limits, etc. can be defined on pretopological spaces [50, 101, 24, 102]. Their usefulness in the context of genotype-phenotype maps and fitness landscapes is discussed in [171].

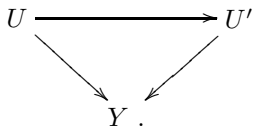
The virtue of the topological approach is that it allows a unified description of combinatorial landscapes and potential surfaces on manifolds alike. For example, basic notions such as local minima, saddle points, and so on can be defined in the same way. For example, $x \in X$ is a *local minimum* if there is a neighborhood $N \in \mathcal{N}(x)$ of x such that $f(x) \leq f(y)$ for all $y \in N$. Similarly, one can use paths to define saddle points analogous to eqn.(4.8).

7.2. An algebraic context for neutral landscapes. From an algebraic point of view it is natural to ask a question like to following: *Given a graph Y, under which conditions is there a specific* class *of landscapes f on Y, and if so, how many landscapes of this* class *can be constructed?* Typically one would be interested in Y-local properties such having a fixed number k of neutral Y-neighbors. Surprisingly, it appears that no such theory has been developed for landscapes, yet. Since we will frequently make explicit references to the underlying graph in the following, we shall write $\mathrm{v}[Y]$ and $\mathrm{e}[Y]$ for its vertex and edge sets, respectively.

Call a landscape k-neutral over Y if for any $j \in \mathrm{v}[Y]$ $|\{\ i \in B_1(j) \mid f(i) = f(j)\ \}| = k$ holds. We are interested in the collection of all k-neutral landscapes over Y. The key idea is to consider the class of *all* induced subgraphs of Y and relate the k-neutral landscapes over these to the k-neutral landscapes over Y. More precisely, we expand k-neutral landscapes over Y-subgraphs to k-neutral landscapes over Y. Clearly, this idea is motivated from analytic continuations of functions.

We begin our analysis by introducing what we consider to be the "local pieces" of Y: To this end we consider the category $C(Y)$ whose objects are all Y-induced subgraphs and morphisms are the inclusion maps. In other words, we have the com-

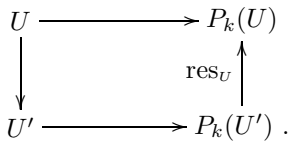
mutative diagram



We call $C(Y)$ the I-topology of Y. A covering of Y in the I-topology is then a multiset of $C(Y)$-morphisms $(U_i \longrightarrow Y)_{i\in I}$ with the property $\cup_I \mathrm{e}[U_i] = \mathrm{e}[Y]$. Next we consider the mapping P_k which assigns to each induced Y-subgraph the free Abelian group generated by its k-neutral maps:

$$P_k(U) = \mathbb{Z}[\{f : Y \to K \mid \forall\, j \in U;\ f \text{ is } k\text{-neutral in j }\}] \ . \tag{7.1}$$

We will denote elements of $P(U)$ by f_U. For any $U, U' \in C(Y)$ let $\mathrm{res}_U(f_{U'}) = f_{U\cap U'} \in P(U \cap U')$ be the mapping $f_{U'} \mapsto f_{U'}$, considered as an element of $P(U \cap U')$, which is naturally induced by the inclusion $U \cap U' \to U'$. Accordingly, any $C(Y)$-morphism induces the commutative diagram



and P_k is a contravariant functor from $C(Y)$ into the Abelian groups **Ab**. Next we introduce the derivation map

$$d^{(s)} : \prod_{\cap_{h=1}^{s} U_{i_h}, i_h < i_{h+1}} P_k(\cap_{h=1}^{s} U_{i_h}) \longrightarrow \prod_{\cap_{h=1}^{s+1} U_{i_h}, i_h < i_{h+1}} P_k(\cap_{h=1}^{s+1} U_{i_h}) \ .$$

$d^{(s)}$ is defined as follows: $d^{(s)}((f_{\cap_{h=1}^{s} U_{i_h}})) = (\beta_{\cap_{h=1}^{s+1} U_{i_h}})$ where

$$\beta_{\cap_{h=1}^{s+1} U_{i_h}} = \sum_{g=1}^{s+1} (-1)^g \mathrm{res}_{U_{i_g}} f_{\cap_{h,h\neq g} U_{i_h}} \ .$$

The key result relating local and global information on k-neutral landscapes can be encoded in the exactness of the following short sequence of Abelian groups:

Lemma 7.1. [149] *Let Y be a connected graph and $(U_i \longrightarrow Y)_{i\in I}$ be a covering of Y in the I-topology. Then we have the short exact sequence*

$$P_k(Y) \longrightarrow^{d^{(1)}} \prod_{i\in I} P_k(U_i) \longrightarrow^{d^{(2)}} \prod_{i<j} P_k(U_i \cap U_j) \ . \tag{7.2}$$

Equivalently, the contravariant functor $P_k : C(Y) \longrightarrow$ Ab is a sheaf.

Basically, Lemma 7.1 allows us to arbitrarily patch together consistent, local k-neutral pieces in order to obtain a k-neutral landscape over Y. One natural algebraic invariant of the sheaf P is its cohomology and since P encodes information on a collection of Y-local k-neutral landscapes its cohomology groups will contain information on the neutral landscapes over Y itself. The following result provides a purely algebraic interpretation of the k-neutral landscapes over Y as some cohomology group of the sheaf P_k.

THEOREM 7.2. [149] *Let Y be a graph. Then we have*

$$\mathbb{Z}[Neut_k(Y)] \cong H^0(Y, P_k) \tag{7.3}$$

where $H^0(Y, P_k)$ is the 0-th derived functor cohomology group of the sheaf P_k.

7.3. Landscape Morphisms. Landscape theory so far is not a *relative* theory in the sense that we would understand how structural changes in the move set (or equivalently base graph over the configurations) affect its properties. Relative Theories, however, are standard in mathematics. For instance, in algebraic geometry one has the concept of base changes of schemes over sites or consider the mappings of (co)homology groups of topological spaces. In the following we will discuss briefly the particular case of morphisms between SDS as introduced in 7.3. Of course, we will try to design SDS-morphisms such that they allow for some "information" transfer from one SDS (viewed as a dynamical system) to another.

DEFINITION 7.3. *Let $[\mathfrak{F}_Y, \pi]$ and $[\mathfrak{F}_Z, \sigma]$ be two SDS. A morphism $\Phi : [\mathfrak{F}_Y, \pi] \longrightarrow [\mathfrak{F}_Z, \sigma]$ is a tuple (φ, ψ), where $\varphi : Y \longrightarrow Z$ and $\psi : \mathbb{G}[\mathfrak{F}_Z, \sigma] \longrightarrow \mathbb{G}[\mathfrak{F}_Y, \pi]$ are graph and digraph morhpisms, respectively.*

Next we show that there are in fact nontrivial SDS-morphisms and study one particular class, naturally induced by locally bijective and locally surjective graph morphisms. Here, we call a graph morphism $\varphi : Y \longrightarrow Z$ locally surjective or locally bijective, respectively, iff

$$\mathrm{res}_{B_{1,Y}(i)}(\varphi) : B_{1,Y}(i) \longrightarrow B_{1,Z}(\varphi(i)) \tag{7.4}$$

is surjective (or bijective) for all $i \in \mathrm{v}[Y]$.

Let $\varphi : Y \longrightarrow Z$ be a graph morphism. Then we call the set

$$\mathrm{Acyc}^{\varphi}(Y) = \{\mathfrak{O} \in \mathrm{Acyc}(Y) \mid \forall\, z \in \mathrm{e}[Z];\ \forall\, y, y' \in \varphi^{-1}(z);\ \mathfrak{O}_Y(y) = \mathfrak{O}_Y(y')\}$$

the set of φ-symmetric acyclic orientations. It is shown in [151] that there exists a one-to-one correspondence $\psi_\varphi : \mathrm{Acyc}Z \longrightarrow \mathrm{Acyc}^{\varphi}(Y)$ for locally surjective φ. From this we obtain a mapping $\eta_\varphi : \mathsf{S}_m \to \mathsf{S}_n$ such that

$$\begin{array}{ccc} \mathsf{S}_m & \xrightarrow{\eta_\varphi} & \mathsf{S}_n \\ \downarrow & & \downarrow \\ \mathrm{Acyc}Z & \xrightarrow{\psi'_\varphi} & \mathrm{Acyc}Y \end{array}$$

is commutative. The following theorem establishes a relation between the phase spaces of SDS that have SDS-morphisms induced by locally bijective and surjective graph morphisms, respectively. Let $[\mathrm{Nor}_Z, \pi]$ denote an SDS over the graph Z, with a Boolean Nor function on each vertex.

THEOREM 7.4. *Let Y, Z be connected loop free graphs, let $\varphi : Y \longrightarrow Z$ be a graph morphism and define*

$$\varphi_* : \mathfrak{F}_2^{|Z|} \longrightarrow \mathfrak{F}_2^{|Y|} \qquad by \quad \varphi_*(x)_k = x_{\varphi(k)}\ .$$

Then the following assertions hold:
(a) If $\varphi : Y \longrightarrow Z$ is locally bijective and $[\mathfrak{F}_Z, \pi]$ and $[\mathfrak{F}_Y, \eta_\varphi(\pi)]$ are induced by the set of local functions $f_{(k)} : \mathbb{F}_2^k \to \mathbb{F}_2$. Then one has the following morphism of SDS

$$\Phi = (\varphi, \varphi_*) : [\mathfrak{F}_Y, \eta_\varphi(\pi)] \longrightarrow [\mathfrak{F}_Z, \pi]\ . \tag{7.5}$$

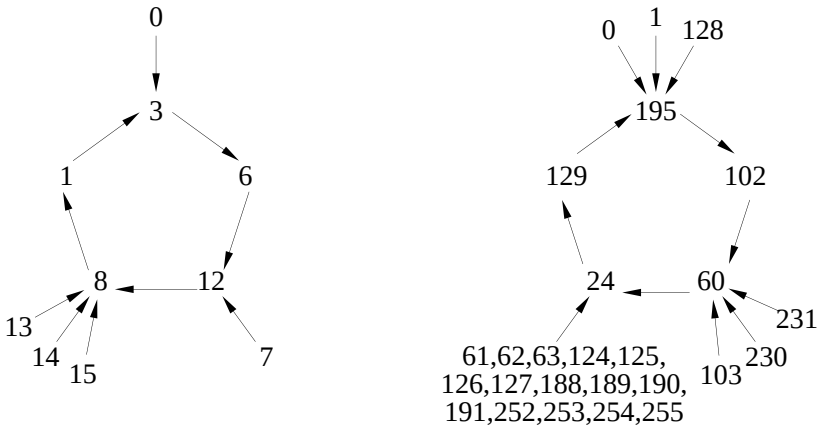


FIG. 7.2. *Illustration of Theorem 7.4 showing a phase space embedding induced by the covering map* $\mathcal{Q}_2^3 \to K_4$. *The l.h.s. shows a limit cycle of an SDS composed by Min-functions (i.e. local, Boolean maps returning the minority value in the corresponding neighborhood and* 0 *in case of an equal number of* 0*'s and* 1*'s) over* K_4 *with the identity as update schedule. The r.h.s. shows the corresponding SDS over* $\mathcal{Q}_2^3$ *with the schedule* $\eta_\varphi(id)$, *as defined in Theorem 7.4. It follows that the digraph of l.h.s. can be embedded into the digraph of the r.h.s.*

(b) Let $\varphi : Y \longrightarrow Z$ *be locally surjective. Then we have the following morphism of SDS:*

$$\Phi = (\varphi, \varphi_*) : [\mathrm{Nor}_Y, \eta_\varphi(\pi)] \longrightarrow [\mathrm{Nor}_Z, \pi] \ . \tag{7.6}$$

In particular, Theorem 7.4 shows how to translate any graph automorphism of Y into a phase space isomorphism of the corresponding SDS, independent of the Y-local functions used, Fig. 7.2. In other words, the symmetries of the base graph induce dynamically equivalent schedules which proves that SDS can in fact be formulated over *unlabelled* graphs.

Theorem 7.4 describes the relationship between two SDS over graphs that are related by locally surjective graph morphism. A similar morphism concept would be a step towards a relative landscape theory. For example, one might try to identify the impact of certain classes of graph morphisms on the corresponding amplitude-spectra.

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