

Chapter 3

Rugged and Elementary Landscapes

Konstantin Klemm and Peter F. Stadler

Abstract The landscape of an optimization problem combines the fitness (or cost) function f on the candidate set X with a notion of neighborhood on X , typically represented as a simple sparse graph. A landscape forms the substrate for local search heuristics including evolutionary algorithms. Understanding such optimization techniques thus requires insight into the connection between the graph structure and properties of the fitness function.

Local minima and their gradient basins form the basis for a decomposition of landscapes. The local minima are nodes of a labeled graph with edges providing information on the reachability between the minima and/or the adjacency of their basins. Barrier trees, inherent structure networks, and funnel digraphs are such decompositions producing “coarse-grained” pictures of a landscape.

A particularly fruitful approach is a spectral decomposition of the fitness function into eigenvectors of the graph Laplacian, akin to a Fourier transformation of a real

K. Klemm (✉)

Bioinformatics Group, Department of Computer Science, Interdisciplinary Center for Bioinformatics, University of Leipzig, D-04107 Leipzig, Germany
e-mail: klemm@bioinf.uni-leipzig.de

P.F. Stadler

Bioinformatics Group, Department of Computer Science, Interdisciplinary Center for Bioinformatics, University of Leipzig, D-04107 Leipzig, Germany

Max Planck Institute for Mathematics in the Sciences, Inselstraße 22, D-04103 Leipzig, Germany

Fraunhofer Institut für Zelltherapie und Immunologie – IZI Perlickstraße 1, D-04103 Leipzig, Germany

Department of Theoretical Chemistry, University of Vienna, Währingerstraße 17, A-1090 Wien, Austria

Santa Fe Institute, 1399 Hyde Park Rd., Santa Fe, NM 87501, USA
e-mail: peter.stadler@bioinf.uni-leipzig.de

function into the elementary waves on its domain. Many landscapes of practical and theoretical interest, including the Traveling Salesman Problem with transpositions and reversals, are elementary: Their spectral decomposition has a single non-zero coefficient. Other classes of landscapes, including k -satisfiability (K-SAT), are superpositions of the first few Laplacian eigenvectors. Furthermore, the ruggedness of a landscape, as measured by the correlation length of the fitness function, and its neutrality, the expected fraction of a candidate's neighbors having the same fitness, can be expressed by the spectrum. Ruggedness and neutrality are found to be independently variable measures of a landscape. Beyond single instances of landscapes, models with random parameters, such as spin glasses, are amenable to this algebraic approach.

This chapter provides an introduction into the structural features of discrete landscapes from both the geometric and the algebraic perspective.

3.1 Introduction

The concept of a *fitness landscape* originated in the 1930s in theoretical biology [75, 76] as a means of conceptualizing evolutionary adaptation: A fitness landscape is a kind of potential function on which a population moves uphill due to the combined effects of mutation and selection. Thus, natural selection acts like hill climbing on the topography implied by the fitness function.

From a mathematical point of view, a landscape consists of three ingredients: a set X of configurations that are to be searched, a topological structure \mathcal{T} on X that describes how X can be traversed, and a fitness or cost function $f : X \rightarrow \mathbb{R}$ that evaluates the individual points $x \in X$. This generic structure is common to many formal models, from evolutionary biology to statistical physics and operations research [5, 26, 40, 41]. The topological structure \mathcal{T} is often specified as a move set, that is, as a function $N : X \rightarrow \mathfrak{P}(X)$ specifying for each configuration $x \in X$ the subset $N(x) \subseteq X$ of configurations that are reachable from x . Usually, the move set is constructed in a symmetric way, satisfying $x \in N(y) \iff y \in N(x)$. The configuration space or *search space* (X, \mathcal{T}) becomes an undirected finite graph G in this case. Then for each $x \in X$, the degree of x is given by $\deg(x) = |N(x)|$. We say that G is d -regular for non-negative integer d if $\deg(x) = d$ for all $x \in X$.

Without losing generality we assume that optimization strives to find those $x \in X$ for which $f(x)$ is *small*. Thus, f is interpreted as energy (or fitness with negative sign), and we are particularly interested in the minima of f . A configuration $x \in X$ is a *local minimum* if $f(x) \leq f(y)$ for all $y \in N(x)$. By M we denote the set of all local minima of the landscape. A local minimum $\hat{x} \in M$ is global if, for all $y \in X$, $f(\hat{x}) \leq f(y)$.

The Traveling Salesman Problem (TSP) [22], see Fig. 3.1, may serve as an example. Given a set of n vertices (cities, locations) $\{1, \dots, n\}$ and a (not necessarily

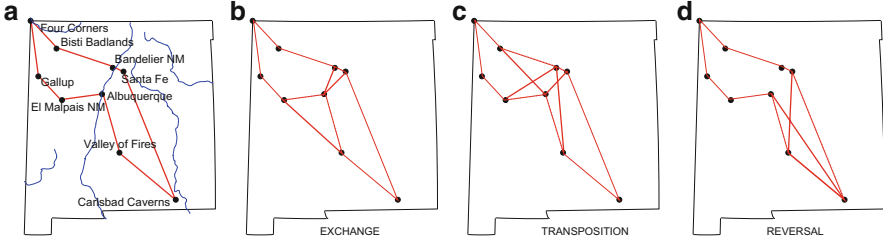


Fig. 3.1 A small instance (a) of the Traveling Salesman Problem with illustration of three different move types (b)–(d) described in the main text

symmetric) matrix of distances or travel costs d_{ij} , the task is to find the permutation (tour) π that minimizes the total travel cost

$$f(\pi) = \sum_{i=1}^n d_{\pi(i), \pi(i+1)} \quad (3.1)$$

where indices are interpreted modulo n . A landscape arises by imposing a topological structure on the set S_n of permutations, i.e., by specifying a move set that determines which tours are adjacent. Often the structure of the problem suggests one particular move set as natural, while others might look quite far-fetched. In principle, however, the choice of the move set is independent of the function f . For the TSP, for instance, three choices come to mind:

1. *Exchange (Displacement)* moves relocate a single city to another position in the tour

$$(1, \dots, i, i+1, i+2, \dots, j, j+1, \dots, n) \\ \mapsto (1, \dots, i, i+2, \dots, j, i+1, j+1, \dots, n).$$

See Fig. 3.1b.

2. *Reversals* cut the tour in two pieces and invert the order in which one half is transversed.

$$(1, \dots, i, i+1, i+2, \dots, k-2, k-1, k, \dots, n) \\ \mapsto (1, \dots, i, k-1, k-2, \dots, i+2, i+1, k, \dots, n).$$

See Fig. 3.1c.

3. *Transpositions* exchange the location of a single city

$$(1, \dots, i-1, i, i+1, \dots, k-1, k, k+1, \dots, n) \\ \mapsto (1, \dots, i-1, k, i+1, \dots, k-1, i, k+1, \dots, n).$$

See Fig. 3.1d.

3.2 Ruggedness

The notion of *rugged landscapes* dates back to the 1980s, when Stuart Kauffman began to investigate these structures in some detail [32]. The intuition is simple. Once the landscape is fixed by virtue of the move set, optimization algorithms making local moves w.r.t. this move set will “see” a complex topography of mountain ranges, local optima, and saddles that influences their behavior. The more “rugged” this topography, the harder it becomes for an optimization algorithm based on local search to find the global optimum or even a good solution. Ruggedness can be quantified in many ways, however [29]:

1. The length distribution of down-hill walks, either gradient descent or so-called *adaptive walks*, is easily measured in computer simulations but is hard to deal with rigorously, see, e.g., [37].
2. Richard Palmer [45] proposed to call a landscape f rugged if the number of local optima scales exponentially with some measure of system size, e.g., the number of cities of a TSP. The distribution of local optima is in several cases accessible by the toolkit of statistical mechanics, see e.g. [50].
3. Barrier trees give a much more detailed view compared to local optima alone. Gradient walks are implicitly included in barrier tree computations. Section 3.3 of this chapter reviews barrier trees and other concise representations of landscapes.
4. Correlation measures capture landscape structure in terms of the time scales on which the cost varies under a random walk. These involve algebraic approaches with spectral decomposition, which are the topic of Sects. 3.4 and 3.5.

3.3 Barriers

Optimization by local search or gradient walks is guaranteed to be successful in a landscape with a unique cost minimum. In all other cases, variations of local search are more suitable [14,33] when they accept inferior solutions to some extent. Then the walk eventually overcomes a barrier to pass over a saddle and enters the basin of an adjacent – possibly lower – local minimum. In this section we formalize the notions of walks, barriers, saddles, basins, and their adjacency. They form the basis of coarse-grained representations of landscapes. These representations “live” on the set of local minima M which is typically much smaller than the set of configurations X .

We review four such representations. Inherent structure networks contain complete information about adjacency of the gradient walk basins of the local minima. Barrier trees describe for each pair of local minima the barrier, i.e., the increase in cost to be overcome in order to travel between the minima. The funnel digraph displays the paths taken by an idealized search dynamics that takes the exit at lowest cost from each basin. Valleys were recently introduced to formalize the

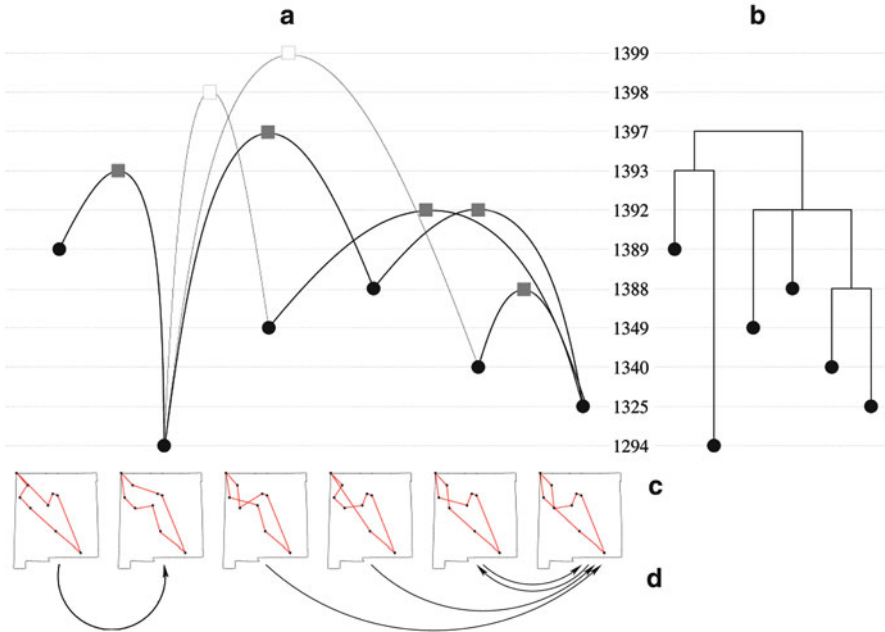


Fig. 3.2 Graphical representations of local minima and saddles for the TSP instance of Fig. 3.1 under transpositions. **(a)** Local minima (*circles*) and direct saddles between their basins (*y*-axis not drawn to scale). The inherent structure network is the complete graph because a direct saddle exists for each pair of minima. In the illustration, however, saddles at a cost above 1,400 have been omitted. **(b)** The barrier tree for the same landscape. An inner node (*vertical line*) of the barrier tree indicates the minimal cost to be overcome in order to travel between all minima in the subtrees of that node. In **(a)**, the direct saddles relevant for the construction of the barrier tree are drawn as *filled rectangles*. **(c)** Local minima are those TSP tours without neighboring tours (configurations) of lower cost. Note that this depends on the move set: Under reversals rather than transpositions, the two rightmost configuration are adjacent. **(d)** In the funnel digraph, an arc $a \rightarrow b$ indicates that the lowest direct saddle from minimum a leads to minimum b

landscape structure implied by adaptive walks. Figure 3.2 serves as a comprehensive illustration throughout this section.

3.3.1 Walk and Accessibility

For configurations $x, y \in X$, a walk from x to y is a finite sequence of configurations $\mathbf{w} = (w_0, w_1, \dots, w_l)$ with $w_0 = x, w_l = y$, and $w_i \in N(w_{i-1})$ for all $i \in \{1, 2, \dots, l\}$. By \mathbb{P}_{xy} we denote the set of all walks from x to y . We say that x and y are *mutually accessible at level $\eta \in \mathbb{R}$* , in symbols

$$x \leftarrow \underline{\rho}^{\eta} \rightarrow y, \tag{3.2}$$

if there is a walk $\mathbf{w} \in \mathbb{P}_{xy}$ such that $f(z) \leq \eta$ for all $z \in \mathbf{w}$. The *saddle height* or *fitness barrier* between two configurations $x, y \in X$ is the smallest level at which x and y are mutually accessible,

$$f[x, y] = \min\{\eta \in \mathbb{R} \mid x \xrightarrow{\rho} \eta \xrightarrow{\rho} y\}. \quad (3.3)$$

The saddle height fulfills the *ultrametric* (strong triangle) inequality. Namely, for all configurations $x, y, z \in X$

$$f[x, z] \leq \max\{f[x, y], f[y, z]\}. \quad (3.4)$$

because the set of walks from x to z passing through y is a subset of \mathbf{P}_{xz} .

3.3.2 Barrier Tree

Equipped with these concepts, let us return to the consideration of local minima. When restricting arguments to elements of M , the saddle height $f : M \times M \rightarrow \mathbb{R}$ still fulfills the ultrametric inequality and thereby induces a hierarchical structure on M [47]. To see this, we use the maximum saddle height

$$m = \max\{f[\hat{x}, \hat{y}] \mid \hat{x}, \hat{y} \in M\} \quad (3.5)$$

of the whole landscape to define a relation on M by

$$\hat{x} \sim \hat{y} := \Leftrightarrow f[\hat{x}, \hat{y}] < m. \quad (3.6)$$

If all local minima are pairwise non-adjacent, \sim is an equivalence relation on M . Its transitivity follows directly from the ultrametric inequality for the saddle height. Unless $|M| = 1$, there is at least one pair of minima that are not related. Therefore the relation \sim generates a partitioning of M into at least two equivalence classes. The argument may then be applied again to each class containing more than one element. This recursion of the partitioning into equivalence classes generates the *barrier tree*. Its leaves are the singleton classes, i.e., the minima themselves. Each inner node stands for a (sub-)partitioning at a given saddle height.

Barrier trees serve to reveal geometric differences between landscapes, e.g., by measuring tree balance [63]. Figure 3.3 shows an example for the number partitioning problem [22]. Standard “flooding” algorithms construct the barrier tree by agglomeration rather than division because the minima and saddle heights are not known a priori. By scanning the configurations of the landscape in the order of increasing fitness, local minima are detected and joined by an inner tree node when connecting walks are observed [52, 73]. Barrier trees can be defined also for *degenerate* landscapes where the assumption of non-adjacent local minima is not fulfilled [17].

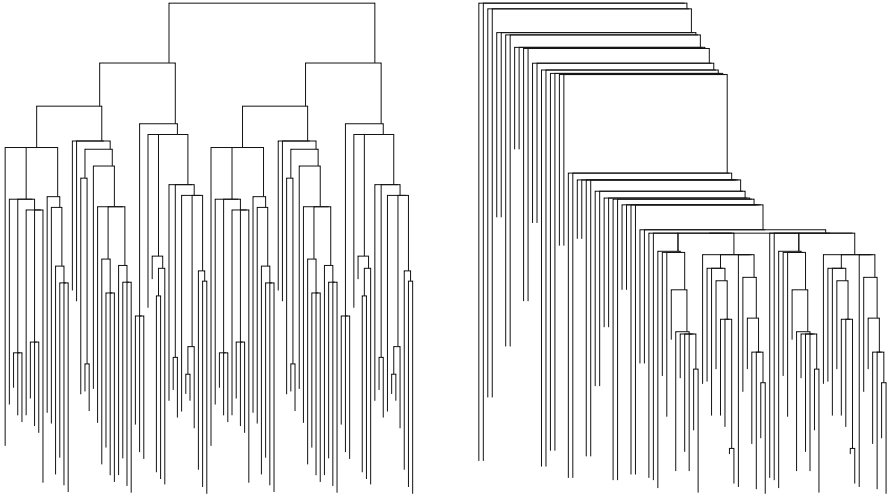


Fig. 3.3 Barrier trees of two fitness landscapes of the same size. *Left tree*: an instance of the number partitioning problem of size $N = 10$. *Right tree*: an instance of the truncated random energy model. The trees obtained for the two types of landscapes are distinguishable by measures of tree imbalance [63]

3.3.3 Basins and Inherent Structure Network

More detailed information about the geometry in terms of local minima is captured by basins and their adjacency relation. A walk (w_0, w_1, \dots, w_l) is a *gradient walk* (or *steepest descent*) if each visited configuration w_i is the one with lowest fitness in the closed neighborhood of its predecessor,

$$f(w_i) = \min\{f(x) | x \in N(w_{i-1}) \cup w_{i-1}\}, \quad 1 \leq i \leq l. \quad (3.7)$$

From each starting configuration w_0 , a sufficiently long gradient walk encounters a local minimum $w_l \in M$. If the encountered minimum $g(x)$ is unique given a starting configuration $x \in X$ of a gradient walk, this defines a mapping $g : X \rightarrow M$. In the case that neighbors with lowest fitness are not unique, ambiguity of gradient walks is resolved by an additional, e.g., lexicographic ordering on X . The *basin* or *gradient basin* of a local minimum \hat{x} is the set $B(\hat{x}) = g^{-1}(\hat{x})$ of configurations from which a gradient walk leads to \hat{x} . Each basin is non-empty because it contains the local minimum itself. Since each configuration $x \in X$ is in the basin of exactly one local minimum $g(x)$, basins are a partitioning of the set X of configurations.

The *interface* between two local minima $\hat{x}, \hat{y} \in M$ is the set

$$I(\hat{x}, \hat{y}) = \{(x, y) | x \in B(\hat{x}), y \in B(\hat{y}), x \in N(y)\} \quad (3.8)$$

containing all pairs of adjacent configurations shared between the basins. The *direct saddle height* between \hat{x} and \hat{y} is

$$h[\hat{x}, \hat{y}] = \min \{ \max \{ f(x), f(y) \} \mid (x, y) \in I(\hat{x}, \hat{y}) \} . \quad (3.9)$$

Direct saddle height is lower bounded by saddle height,

$$h[\hat{x}, \hat{y}] \geq f[\hat{x}, \hat{y}] \quad (3.10)$$

for all $\hat{x}, \hat{y} \in M$ with non-empty interface. A member of the interface $(x, y) \in I(\hat{x}, \hat{y})$ is a *direct saddle* (between \hat{x} and \hat{y}) if its cost is the direct saddle height $\max \{ f(x), f(y) \} = h(\hat{x}, \hat{y})$.

The *inherent structure network* (M, H) [13] is defined as a graph with node set M and edge set $H = \{ \{\hat{x}, \hat{y}\} \mid I(\hat{x}, \hat{y}) \neq \emptyset \}$. An edge thus connects the local minima \hat{x} and \hat{y} if and only if there is a path from \hat{x} to \hat{y} that lies in the union of basins $B(\hat{x}) \cup B(\hat{y})$. The saddle heights $f[\hat{x}, \hat{y}]$ can be recovered from the inherent structure network by minimizing the maximum values of the direct saddle height $h[\hat{p}, \hat{q}]$ encountered along a path in (M, H) that connects \hat{x} and \hat{y} . We remark, finally, that some studies use the term “direct saddle” to denote only the subset of direct saddles for which $h[\hat{x}, \hat{y}] = f[\hat{x}, \hat{y}]$, i.e., which cannot be circumvented by a longer but lower path in (M, H) [17, 61]. Exact computation of inherent structure networks requires detection of all direct saddles and is thus restricted to small instances [66]. Efficient sampling methods exist for larger landscapes, e.g. by [38].

For the example in Fig. 3.2, the inherent structure network is the complete graph: All basins are mutually adjacent. Remarkable graph properties, however, have been revealed when studying the inherent structure networks of larger energy landscapes of chemical clusters [13], spin-glass models [7], and NK landscapes [66]. Compared to random graphs, the inherent structure networks have a large number of closed triangles (“clustering”), modular structure, and broad degree distributions, often with power law tails.

3.3.4 Funnel

Besides barrier tree and inherent structure network, another useful graph representation is the *funnel digraph* (M, A) [34]. Here, a directed arc runs from \hat{x} to \hat{y} if the basins of \hat{x} and \hat{y} have a non-empty interface and

$$h(\hat{x}, \hat{y}) = \min \{ h(\hat{x}, \hat{z}) \mid \{\hat{x}, \hat{z}\} \in E \} . \quad (3.11)$$

Thus from each local minimum \hat{x} an arc points to that neighboring local minimum \hat{y} that is reached by the smallest direct saddle height. The node \hat{x} has more than one outgoing arc if more than one neighboring basin is reached over the same minimal directed saddle height.

The definition is motivated by stochastic variants of local search such as Metropolis sampling [39] and simulated annealing [33]. Under the assumption that the search exits a basin via its lowest saddle with the largest probability, the most likely sequences of visits to basins are the directed paths of the funnel digraph. It serves to make precise the concept of a *funnel* [23, 43, 74]. A local minimum \hat{x} is in the funnel $F(\hat{z}) \subseteq M$ of a global minimum \hat{z} if there is a directed path from \hat{x} to \hat{z} on the funnel digraph. Thus the funnel contains all those local minima from which iterative exits over the lowest barrier eventually lead to the ground state [34].

In the funnel digraph for the small TSP instance in Fig. 3.2c,d, we see that the funnel consists of the basins of the global minimum itself (cost 1294) and of the highest local minimum (cost 1389) while the basins of the other three minima are outside the funnel. Numerical studies with the number partitioning problem [22] indicate that funnel size tends to zero for large random instances [34].

3.3.5 Valleys

Adaptive walks generalize gradient walks by accepting any fitness-improving steps. We say that $x \in X$ is *reachable* from $y \in X$ if there is an adaptive walk from y to x . A *valley* [61] is a maximal connected subgraph of X such that no point $y \notin W$ is reachable from any starting point $x \in W$. In contrast to basins, valleys do not form a hierarchy but rather can be regarded as a community structure of X , see, e.g., [20]. Instead, they overlap in the upper, high-energy, parts of the landscape, where adaptive walks are not yet committed to a unique local minimum. The parts of gradient basins below the saddle points linking them to other basins therefore are valleys. Conversely, entire gradient basins are always contained in valleys.

The exact mutual relationships among the barrier trees, basins, inherent structure networks, valleys, etc., are still not completely understood, in particular in the context of degenerate landscapes.

3.4 Elementary Landscapes

3.4.1 Graph Laplacian

In the previous section we have taken a geometric or topological approach to analyzing and representing a landscape. The alternative is to adopt an algebraic point of view, interpreting the landscape as a vector of fitness values. The neighborhood structure N on the set X of configurations, which index the fitness vector, also needs an algebraic interpretation. In this contribution we only deal with graphs whose edges are defined by the (symmetric) move set $N : X \rightarrow \mathfrak{P}(X)$. The most natural choice thus are the *adjacency matrix* \mathbf{A} (with entries $\mathbf{A}_{xy} = 1$ if x and y are adjacent, i.e., $y \in N(x)$, and $\mathbf{A}_{xy} = 0$ otherwise) and the *incidence matrix* \mathbf{H} . The latter has

entries $\mathbf{H}_{ex} = +1$ if x is the “head end” of the edge e , $\mathbf{H}_{ex} = -1$ if x is the “tail end” of e , and $\mathbf{H}_{ex} = 0$ otherwise. (The assignment of head and tail to each edge is arbitrary.) The basic idea of algebraic landscape theory is to explore the connections between the fitness function f and these matrix representations of the search space, and to use combinations of these algebraic objects to derive numerical descriptors of landscape structure [49].

A convenient starting point is to consider the local variation of the fitness, e.g., in the form of fitness differences $f(x) - f(y)$ between adjacent vertices $y \in N(x)$. The sum of the local changes

$$(\mathbf{L}f)(x) := \sum_{y \in N(x)} (f(x) - f(y)) \quad (3.12)$$

defines the *Laplacian* \mathbf{L} as a linear operator associated with the graph on (X, N) that can be applied to any function f on the nodes of the graph. When we imagine a spatially extended landscape, e.g., the underlying graph being a lattice, $(\mathbf{L}f)(x)$ can be interpreted as the local “curvature” of f at configuration x . In particular, the x -th entry of $\mathbf{L}f$ is negative if x is a local minimum and $(\mathbf{L}f)(x) > 0$ for a local maximum.

Since \mathbf{L} is a linear operator, it may also be seen as a matrix. In fact, \mathbf{L} is intimately related to both the adjacency and the incidence matrix: $\mathbf{L} = \mathbf{D} - \mathbf{A}$, where \mathbf{D} is the diagonal matrix of vertex degrees $\deg(x) := \sum_{y \in X} \mathbf{A}_{xy}$, and $\mathbf{L} = \mathbf{H}^+ \mathbf{H}$. The Laplacian is thus simply a representation of the topological structure of the search space.

3.4.2 Elementary Landscapes

Since \mathbf{L} is a symmetric operator (on a finite-dimensional vector space), it can be diagonalized by finding its eigenfunctions. Let us perform the diagonalization for the simple and useful case that the graph is an n -dimensional hypercube with node set $X = \{-1, +1\}^n$ and $x \in N(y)$ if and only if x and y differ at exactly one coordinate. For each set of indices $I \subseteq \{1, \dots, n\}$, the *Walsh functions* are defined as

$$w_I(x) = \prod_{i \in I} x_i . \quad (3.13)$$

Figure 3.4 gives an illustration for the three-dimensional case. The Walsh functions form an orthogonal basis of \mathbb{R}^{2^n} . With a Walsh function of order $|I|$, each node of the hypercube has $n - |I|$ neighbors with the opposite value and $|I|$ neighbors with the same value. This amounts to

$$\mathbf{L}w_I = 2|I|w_I . \quad (3.14)$$

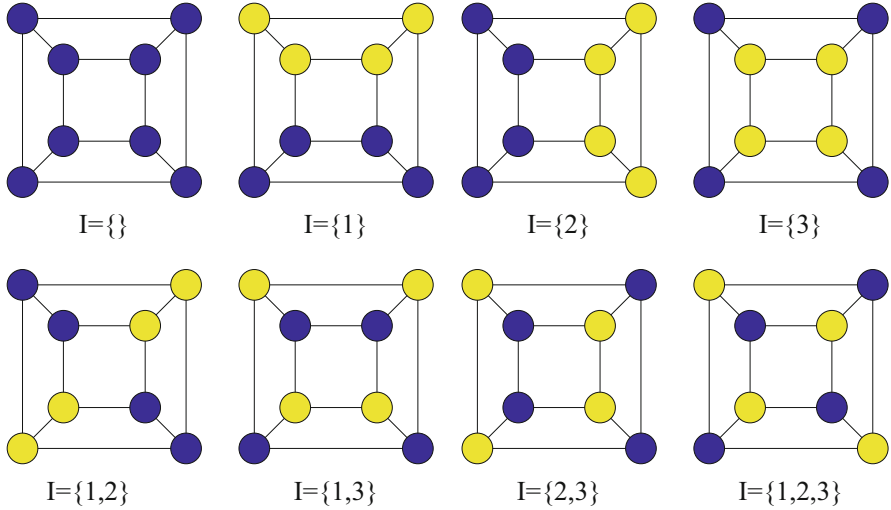


Fig. 3.4 The eight Walsh functions of the hypercube in dimension $n = 3$. *Dark* and *light* color of nodes distinguishes the values $+1$ and -1

Each Walsh function w_I is an eigenvector of \mathbb{L} for eigenvalue $2|I|$. Now consider a 2-spin glass as a landscape on the hypercube with the cost function

$$f(x) = - \sum_{i,j} J_{ij} x_i x_j \quad (3.15)$$

with arbitrary real coefficients J_{ij} . Since $x_i x_j = w_{i,j}(x)$ for all $x \in X$, we see that f is a weighted sum of Walsh functions of order 2. Therefore f is an eigenvector of the Laplacian with eigenvalue $2|I| = 4$. This observation generalizes to p -spin glasses and many other landscapes of interest.

It is convenient to consider landscapes with vanishing average fitness, i.e., instead of f , we use $\tilde{f}(x) = f(x) - \bar{f}$, where $\bar{f} = \frac{1}{|X|} \sum_{x \in X} f(x)$ is the average cost of an arbitrary configuration. A landscape is *elementary* if the zero-mean cost function \tilde{f} is an eigenfunction of the Laplacian of the underlying graph, i.e.,

$$(\mathbf{L}f)(x) = \sum_{y \in N(x)} [\tilde{f}(x) - \tilde{f}(y)] = \lambda_k \tilde{f}(x) \quad (3.16)$$

Since $\mathbf{L} = \mathbf{H}^+ \mathbf{H}$, all eigenvalues are non-negative. In the following, they will be indexed in non-decreasing order

$$0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{|X|-1}. \quad (3.17)$$

Table 3.1 Examples of elementary landscapes

| Problem | Graph | degree | λ | Order | Reference |
|--------------------------|--|---------------------|------------------------|------------------|--------------|
| p -spin glass | Q_2^n | n | $2p$ | p | Definition |
| NAES | Q_2^n | n | 4 | 2 | [24] |
| Weight partitioning | Q_2^n | n | 4 | 2 | [24, 55] |
| GBP (constrained) | Q_2^n | n | 4 | 2 | [1] |
| Max cut | Q_2^n | n | 4 | 2 | [1] |
| Graph α -coloring | Q_α^n | $(\alpha - 1)n$ | 2α | 2 | [55] |
| XY-spin glass | Q_α^n | $(\alpha - 1)n$ | 2α | 2 | [21] |
| for $\alpha > 2$: | \mathcal{C}_α^n | 2 | $8 \sin^2(\pi/\alpha)$ | 2 | [21] |
| Linear assignment | $\Gamma(\mathcal{S}_n, \mathcal{T})$ | n | | 1 | [51] |
| TSP symmetric | $\Gamma(\mathcal{S}_n, \mathcal{T})$ | $n(n - 1)/2$ | $2(n - 1)$ | 2 | [9, 24] |
| | $\Gamma(\mathcal{S}_n, \mathcal{J})$ | $n(n - 1)/2$ | n | 2 | [9, 24] |
| | $\Gamma(\mathcal{A}_n, \mathcal{C}_3)$ | $n(n - 1)(n - 2)/6$ | $(n - 1)(n - 2)$ | ? | [9] |
| Antisymmetric | $\Gamma(\mathcal{S}_n, \mathcal{T})$ | $n(n - 1)/2$ | $2n$ | 3 | [2, 55] |
| | $\Gamma(\mathcal{S}_n, \mathcal{J})$ | $n(n - 1)/2$ | $n(n + 1)/2$ | $\mathcal{O}(n)$ | [2, 55] |
| Graph matching | $\Gamma(\mathcal{S}_n, \mathcal{T})$ | $n(n - 1)/2$ | $2(n - 1)$ | 2 | [55] |
| Graph bipartitioning | $J(n, n/2)$ | $n^2/4$ | $2(n - 1)$ | 2 | [24, 55, 57] |

Q_α^n is the n -fold Cartesian product of the complete graph K_α , also known as a Hamming graph. $\Gamma(\mathcal{A}, \Omega)$ is the Cayley graph of the group \mathcal{A} with generating set Ω , where \mathcal{S}_n and \mathcal{A}_n denote the symmetric and alternating groups, resp., \mathcal{T} , \mathcal{J} , and \mathcal{C}_3 are the transpositions, reversals, and permutations defined by a cycle of length 3, resp. $J(p, q)$ is a Johnson graph.

First examples of elementary landscapes were identified by Grover and others [9, 24, 55]. Table 3.1 lists some of them. Additional examples are discussed, e.g., by [36, 53, 54, 70]. In most cases, k is small: \hat{f} lies in the eigenspace of one of the first few eigenvalues of the Laplacian.

Lov Grover [24] showed that, if f is an elementary landscape, then

$$f(\hat{x}_{\min}) \leq \bar{f} \leq f(\hat{x}_{\max}) \quad (3.18)$$

for every local minimum \hat{x}_{\min} and every local maximum \hat{x}_{\max} . This *maximum principle* shows that elementary landscapes are in a sense well-behaved: There are no local optima with worse than average fitness \bar{f} . A bound on the global maxima in terms of the maximal local fitness differences can be obtained using a similar argument [12]:

$$\lambda |f(\hat{x}) - \bar{f}| \leq \deg(\hat{x}) \varepsilon^*, \quad (3.19)$$

where $\varepsilon^* = \max_{\{x, y\} \in E} |f(x) - f(y)|$ is the ‘‘information stability’’ introduced by [67].

The eigenvalues, λ_i , convey information about the underlying graph [42]. For instance, G is connected if and only if $\lambda_1 > 0$. The value of λ_1 is often called the algebraic connectivity of the graph G [16]. The corresponding eigenfunctions have a particularly simple form: The vertices with non-negative (non-positive) values of f are connected. More generally, a *nodal domain* of a function g on G is a

maximal connected vertex set on which g does not change sign. A strong nodal domain is a maximal connected vertex set on which g has the same strict sign, $+$ or $-$. The discrete version of *Courant's nodal domain theorem* [6, 10, 15, 46] asserts that an eigenfunction f to eigenvalue λ_k (counting multiplicities) has no more than $k + 1$ weak and $k + m_k$ strong nodal domains, where m_k is the multiplicity of λ_k . The theorem restricts ruggedness in terms of the eigenvalue. Intuitively, the nodal domain theorem ascertains that the number of big mountain ranges (and deep sea valleys) is small for the small eigenvalues of \mathbf{L} .

There is, furthermore, a simple quantitative relationship between λ and the autocorrelation function of f of (X, \mathcal{X}) [55]. For a D -regular graph G , we have

$$r(s) = (1 - \lambda/D)^s \quad (3.20)$$

$r(s)$ is the autocorrelation function of f along a uniform random walk on G [19, 68]. Similar equations can be derived for correlation measures defined in terms of distances on G [55] and for non-regular graphs [3, 11, 62].

Whitley et al. [71] interpret the eigenvalue equation (3.16) as a statement on the average fitness of the neighbors of a point,

$$\langle f \rangle_x = \frac{1}{\deg(x)} \sum_{y \in N(x)} f(y) \quad (3.21)$$

and discuss some implications for local search processes. Local conditions for the existence of improving moves are considered by [70].

3.4.3 Fourier Decomposition

Of course, in most cases, a natural move set \mathcal{T} does not make f an elementary landscape. In case of the TSP landscape, for example, transpositions and reversals lead to elementary landscapes. One easily checks, on the other hand,

$$\begin{aligned} (\mathbf{L}f)(\pi) &= \sum_{i,j} \left\{ d_{\pi(i)\pi(i+1)} + d_{\pi(i+1)\pi(i+2)} + d_{\pi(j)\pi(j+1)} \right. \\ &\quad \left. - d_{\pi(i)\pi(i+2)} - d_{\pi(j)\pi(i+1)} - d_{\pi(i+1)\pi(j+1)} \right\} \\ &= 2n(f(\pi) - \bar{f}) + nf(\pi) - \sum_{i=1}^n d_{\pi(i)\pi(i+2)} \end{aligned} \quad (3.22)$$

which is clearly not of the form $a_1 f(\pi) + a_0$ due to the explicit dependence of the last term on the next-nearest neighbors w.r.t. π . Exchange moves therefore do not make the TSP an elementary landscape.

A Fourier-decomposition-like formalism can be employed to decompose arbitrary landscapes into their elementary components [28, 51, 69]:

$$f = a_0 + \sum_{k>0}^{n-1} a_k f_k \quad (3.23)$$

where the f_k form an orthonormal system of eigenfunctions of the graph Laplacian ($\mathbf{L}f_k = \lambda_k f_k$, and $a_0 = \bar{f}$ is the average value of the function f). Let us denote the distinct eigenvalues of \mathbf{L} by $\bar{\lambda}_p$, sorted in increasing order starting with $\bar{\lambda}_0 = \lambda_0 = 0$. We call p the *order* of the eigenvalue $\bar{\lambda}_p$. The *amplitude spectrum* of $f: X \rightarrow \mathbb{R}$ is defined by

$$B_p = \sum_{k:\lambda_k=\bar{\lambda}_p} |a_k|^2 / \sum_{k>0} |a_k|^2. \quad (3.24)$$

By definition, $B_p \geq 0$ and $\sum_p B_p = 1$. The amplitude measures the relative contribution of the eigenspace of the eigenvalue with order p to the function f . Of course, a landscape is elementary if and only if $B_p = 1$ for a single order and 0 for all others. For Ising spin-glass models, for example, the order equals the number of interacting spins, Table 3.1.

In some cases, landscapes are not elementary but at least exhibit a highly localized spectrum. The landscape of the “Low-Autocorrelated Binary String Problem”, for instance, satisfies $B_p = 0$ for $p > 4$ [44]. Quadratic assignment problems are also superpositions of eigenfunctions of quasi-abelian Cayley graphs of the symmetric group with the few lowest eigenvalues [51]. A similar result holds for K -SAT problems. An instance of K -SAT consists of n Boolean variables x_i , and a set of m clauses each involving exactly K variables in disjunction. The cost function $f(x)$ measures the number of clauses that are satisfied. [64] showed that $B_p = 0$ for $p > K$. Similar results are available for frequency assignment problems [72], the subset sum problem [8], or genetic programming parity problems [35]. Numerical studies of the amplitude spectra of several complex real-world landscapes are reported in [4, 25, 51, 65]. A practical procedure for algebraically computing the decomposition of a landscape into its elementary constituents is discussed in [8]. This approach assumes that $f(x)$ is available as an algebraic equation and that an orthonormal basis $\{f_k\}$ is computable.

A *block-model* [70, 71] is a landscape of the form

$$f(x) = \sum_{q \in \mathcal{Q}(x)} w_q \quad (3.25)$$

where \mathcal{Q} is a set of “building blocks” with weights w_q . The subset $\mathcal{Q}(x) \subseteq \mathcal{Q}$ consists of the blocks that contribute to a particular state x . For instance, the TSP is of this type: \mathcal{Q} is the collection of intercity connections, and w_q is their length.

Necessary conditions for block models to be elementary are discussed, e.g., by [70]. Equation (3.25) can be rewritten in the form

$$f(x) = \sum_{q \in \Omega} w_q \vartheta_q(x) \quad (3.26)$$

where $\vartheta_q(x) = 1$ if $q \in \Omega(x)$, and $\vartheta_q(x) = 0$ otherwise. They form a special case of the additive landscapes considered in the next section.

3.5 Additive Random Landscapes

Many models of landscapes contain a random component. In spin-glass Hamiltonians of the general form

$$f(\sigma) = \sum_{i_1 < i_2 < \dots < i_p} a_{i_1, i_2, \dots, i_p} \sigma_1 \sigma_2 \dots \sigma_{i_p} \quad (3.27)$$

with n Ising spin variables $\sigma_i = \pm 1$, the coefficients a_{i_1, i_2, \dots, i_p} are usually considered as random variables drawn from some probability distribution. Similarly, the “thermodynamics” of TSPs can be studied with the distances w_q in Eq. (3.25) interpreted as random variables. [48, 58] studied this type of model in a more general setting motivated by Eq. (3.26).

Let $\vartheta_q : X \rightarrow \mathbb{R}$, $q \in I$, be a family of fitness functions on X , where I is some index set, and let c_q , $q \in I$, be independent, real-valued, random variables. We consider additive random fitness functions of the form

$$f(x) = \sum_{q \in I} c_q \vartheta_q(x) \quad (3.28)$$

on $G = (X, \mathcal{J})$. The associated probability space is referred to *additive random landscape* (a.r.l.) [48]. An a.r.l. is *uniform* if (1) the c_q , $q \in I$, are independently and identically distributed (i.i.d.) and (2) there are constants b_0 and b_1 such that $\sum_{x \in V} \vartheta_q(x) = |V|b_0$ and $\sum_{x \in V} \vartheta_q(x)^2 = |V|b_1$ independent of q . An a.r.l. is *strictly uniform* if, in addition, $\sum_q \vartheta_q(x) = b_2$ and $\sum_q \vartheta_q(x)^2 = b_3$ independently of $x \in X$.

For block models, $\vartheta_q(x) = \vartheta_q(x)^2$. Hence a block model is uniform if each block is contained in the same number configurations and is strictly uniform if in addition, $|\mathcal{Q}(x)|$ is independent of x . Furthermore, every a.r.l. with Gaussian measure is additive. This follows immediately by the Karhunen-Loève theorem [30], using the fact that uncorrelated jointly normal distributed variables are already independent. Random versions of elementary landscapes, i.e., those with i.i.d. Fourier coefficients, are of course also a.r.l.s.

Maybe the most famous a.r.l.s are Kauffman’s NK landscape models. Consider a binary “genome” x of length n . Each site is associated with a site fitness that is determined from a set of K sequence positions to which position i is epistatically linked. These state-dependent contributions are usually taken as independent uniform random variables [31]. In order to see that an NK model is an a.r.l., we introduce the functions

$$\vartheta_{i,y(i)}(x) = \prod_{k=0}^{|y(i)|} \delta_{y(i)_k, x_k} \quad (3.29)$$

where $y(i)_k$ denotes a particular (binary) state of position k in the epistatic neighborhood $y(i)$ of i . In other words, $\vartheta_{i,y(i)}(x) = 1$ if the argument x coincides on the K epistatic neighbors of i with a particular binary pattern $y(i)$. It is not hard to check that NK models are strictly uniform [48].

An important observation in this context is that short-range spin-glass models can be understood as a.r.l.s for which the p -spin eigenfunctions (of the Laplacian of the Boolean hypercube)

$$\vartheta_{i_1 i_2 \dots i_p}(\sigma) = \prod_{k=1}^p \sigma_{i_k} \quad (3.30)$$

take on the role of the characteristic functions $\{\vartheta_j\}$. The coefficients are then taken from a mixed distribution of the form $\rho(c) = (1 - \mu)\text{Gauss}_{(0,s)}(c) + \mu\delta(c)$. Thus there is a finite probability p that a coefficient c_j vanishes. In this setting one can easily evaluate the *degree of neutrality*, i.e., the expected fraction of neutral neighbors

$$\nu(x) = \frac{1}{|N(x)|} \mathbb{E} [|\{y \in N(x) : f(x) = f(y)\}|] \quad (3.31)$$

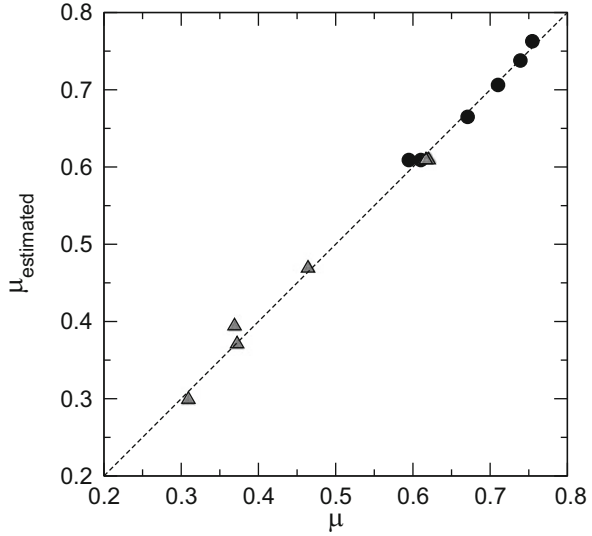
One finds

$$\nu(x) = \frac{1}{D} \sum_{y \in N(x)} \mu^{c_y(x)} \quad c_y(x) := |\{q \in I | \vartheta_q(x) \neq \vartheta_q(y)\}| \quad (3.32)$$

which, for the case of the p -spin models can be evaluated explicitly as $\nu(x) = \mu^{\binom{n-1}{p-1}}$ [48]. The value of ν can thus be tuned by μ , the fraction of vanishing coefficients. On the other hand, the Laplacian eigenvalue and hence the algebraic measures of ruggedness depend only on the interaction order p . Hence, ruggedness and neutrality are *independent* properties of landscapes.

Elementary landscapes have restrictions on “plateaus”, that is, on connected subgraphs on which the landscape is flat. In particular, Sutton et al. [64] show for 3-SAT that plateaus cannot contain large balls in G unless their fitness is close to average. A more general understanding of neutrality in elementary landscapes is still missing, however.

Fig. 3.5 Empirically, the number \mathcal{N} of local optima in many landscape scales exponentially with system size n . The values of $\mu := \lim_{n \rightarrow \infty} \frac{1}{n} \log \mathcal{N}(n)$ can be estimated surprisingly accurately by the correlation length conjecture for *-isotropic landscapes (●) and nearly *-isotropic landscapes (▲) (Data are taken from [58])



There is a close connection between the Fourier decomposition of a (random) landscape and a “symmetry” property of random fields: Stadler and Happel [58] call a random field **-isotropic* if its covariance matrix \mathbf{C} is a polynomial of the adjacency matrix \mathbf{A} of the underlying graph. The interest in this symmetry property arises from the observation that **-isotropy* is equivalent to three regularity conditions on the distributions of the Fourier coefficients:

1. $\mathbb{E}[a_k] = 0$ for $k \neq 0$.
2. $\text{Cov}[a_k, a_j] := \mathbb{E}[a_k a_j] - \mathbb{E}[a_k]\mathbb{E}[a_j] = \text{Var}[a_k]\delta_{kj}$.
3. $\text{Var}[a_k] = \text{Var}[a_j]$ if $\varphi_k(x)$ and $\varphi_j(x)$ are eigenfunctions to the same eigenvalue of the graph Laplacian.

In Gaussian case, **-isotropy* also has an interpretation as a maximum entropy condition: Gaussian random fields satisfying these three conditions maximize entropy subject to the constraint of a given amplitude spectrum [56].

An interesting empirical observation in this context is the *correlation length conjecture* [59]. It states that we should expect about one local optimum within a ball B in G whose radius r is given by the distance covered by random walk of length ℓ on G , where

$$\ell = \sum_{s=0}^{\infty} r(s) \quad (3.33)$$

is the *correlation length* of the landscape. This simple rule yields surprisingly accurate estimates of the number of local optima in isotropic and nearly isotropic landscapes, see Fig. 3.5. The accuracy of the estimate seems to decline with increasing deviations from **-isotropy* [21, 44, 58].

3.6 Outlook

Most of the theoretical results for fitness landscapes have been obtained for very simple search processes, i.e., for landscapes on simple graphs. In the field of genetic algorithms, on the other hand, the search operators themselves are typically much more complex, involving recombination of pairs of individuals drawn from a population. A few attempts have been made to elucidate the mathematical structure of landscapes on more general topologies [18, 60, 61], considering generalized versions of barrier trees and basins. A generalization of the Fourier decomposition and a notion of elementary landscapes under recombination was explored in [62], introducing a Markov chain on X that in a certain sense mimics the action of crossover. In this formalism, a close connection between elementary landscapes and Holland's schemata [27] becomes apparent. It remains a topic for future research, however, if and how spectral properties of landscapes can be formulated in general for population-based search operators in which offsprings are created from more than one parent.

Despite the tentative computational results that suggest a tight connection between spectral properties of a landscape, statistical features of the Fourier coefficients, and geometric properties such as the distribution of local minima, there is at present no coherent theory that captures these connections. We suspect that a deeper understanding of relations between these different aspects of landscapes will be a prerequisite for any predictive theory of the performance of optimization algorithms on particular landscape problems.

References

1. E. Angel, V. Zissimopoulos, On the classification of NP-complete problems in terms of their correlation coefficient. *Discr. Appl. Math.* **99**, 261–277 (2000)
2. J. Barnes, S. Dokov, R. Acevedoa, A. Solomon, A note on distance matrices yielding elementary landscapes for the TSP. *J. Math. Chem.* **31**, 233–235 (2002)
3. J.W. Barnes, B. Dimova, S.P. Dokov, A. Solomon, The theory of elementary landscapes. *Appl. Math. Lett.* **16**, 337–343 (2003)
4. O. Bastert, D. Rockmore, P.F. Stadler, G. Tinhofer, Landscapes on spaces of trees. *Appl. Math. Comput.* **131**, 439–459 (2002)
5. K. Binder, A.P. Young, Spin glasses: experimental facts, theoretical concepts, and open questions. *Rev. Mod. Phys.* **58**, 801–976 (1986)
6. T. Bıyıkođlu, J. Leydold, P.F. Stadler, in *Laplacian Eigenvectors of Graphs: Perron-Frobenius and Faber-Krahn Type Theorems*. Lecture Notes in Mathematics, vol. 1915 (Springer, Heidelberg, 2007)
7. Z. Burda, A. Krzywicki, O.C. Martin, Network of inherent structures in spin glasses: scaling and scale-free distributions. *Phys. Rev. E* **76**, 051107 (2007)
8. F. Chicano, L.D. Whitley, E. Alba, A methodology to find the elementary landscape decomposition of combinatorial optimization problems. *Evol. Comp.* (2011). doi:10.1162/EVCO_a_00039
9. B. Codenotti, L. Margara, Local properties of some NP-complete problems. Technical Report TR 92-021, International Computer Science Institute, Berkeley, 1992

10. E.B. Davies, G.M.L. Gladwell, J. Leydold, P.F. Stadler, Discrete nodal domain theorems. *Lin. Algebra Appl.* **336**, 51–60 (2001)
11. B. Dimova, J.W. Barnes, E. Popova, Arbitrary elementary landscapes & AR(1) processes. *Appl. Math. Lett.* **18**, 287–292 (2005)
12. B. Dimova, J.W. Barnes, E. Popova, E. Colletti, Some additional properties of elementary landscapes. *Appl. Math. Lett.* **22**, 232–235 (2009)
13. J.P.K. Doye, Network topology of a potential energy landscape: a static scale-free network. *Phys. Rev. Lett.* **88**, 238701 (2002)
14. G. Dueck, New optimization heuristics: the great deluge algorithm and the record-to-record travel. *J. Comp. Phys.* **104**, 86–92 (1993)
15. A.M. Duval, V. Reiner, Perron-Frobenius type results and discrete versions of nodal domain theorems. *Lin. Algebra Appl.* **294**, 259–268 (1999)
16. M. Fiedler, Algebraic connectivity of graphs. *Czechoslovak Math. J.* **23**, 298–305 (1973)
17. C. Flamm, I.L. Hofacker, P.F. Stadler, M.T. Wolfinger, Barrier trees of degenerate landscapes. *Z. Phys. Chem.* **216**, 155–173 (2002)
18. C. Flamm, B.M.R. Stadler, P.F. Stadler, Saddles and barrier in landscapes of generalized search operators, in *Foundations of Genetic Algorithms IX*, ed. by C.R. Stephens, M. Toussaint, D. Whitley, P.F. Stadler. *Lecture Notes Computer Science*, vol. 4436 (Springer, Berlin/Heidelberg, 2007), pp. 194–212. 9th International Workshop, FOGA 2007, Mexico City, 8–11 Jan 2007
19. W. Fontana, P.F. Stadler, E.G. Bornberg-Bauer, T. Griesmacher, I.L. Hofacker, M. Tacker, P. Tarazona, E.D. Weinberger, P. Schuster, RNA folding landscapes and combinatorial landscapes. *Phys. Rev. E* **47**, 2083–2099 (1993)
20. S. Fortunato, Community detection in graphs. *Phys. Rep.* **486**, 75–174 (2010)
21. R. García-Pelayo, P.F. Stadler, Correlation length, isotropy, and meta-stable states. *Physica D* **107**, 240–254 (1997)
22. M.R. Garey, D.S. Johnson, *Computers and Intractability: A Guide to the Theory of NP-Completeness* (W.H. Freeman, San Francisco, 1979)
23. P. Garstecki, T.X. Hoang, M. Cieplak, Energy landscapes, supergraphs, and “folding funnels” in spin systems. *Phys. Rev. E* **60**, 3219–3226 (1999)
24. L.K. Grover, Local search and the local structure of NP-complete problems. *Oper. Res. Lett.* **12**, 235–243 (1992)
25. R. Happel, P.F. Stadler, Canonical approximation of fitness landscapes. *Complexity* **2**, 53–58 (1996)
26. D. Heidrich, W. Kliesch, W. Quapp, in *Properties of Chemically Interesting Potential Energy Surfaces*. *Lecture Notes in Chemistry*, vol. 56 (Springer, Berlin, 1991)
27. J. Holland, *Adaptation in Natural and Artificial Systems* (MIT, Cambridge, 1975)
28. W. Hordijk, P.F. Stadler, Amplitude spectra of fitness landscapes. *Adv. Complex Syst.* **1**, 39–66 (1998)
29. L. Kallel, B. Naudts, C.R. Reeves, Properties of fitness functions and search landscapes, in *Theoretical Aspects of Evolutionary Computing*, ed. by L. Kallel, B. Naudts, A. Rogers (Springer, Berlin Heidelberg, 2001), pp. 175–206
30. K. Karhunen, Zur Spektraltheorie Stochastischer Prozesse. *Ann. Acad. Sci. Fennicae, Ser. A I* **34**, 7 (1947)
31. S.A. Kauffman, *The Origin of Order* (Oxford University Press, New York/Oxford, 1993)
32. S.A. Kauffman, S. Levin, Towards a general theory of adaptive walks on rugged landscapes. *J. Theor. Biol.* **128**, 11–45 (1987)
33. S. Kirkpatrick, C.D. Gelatt Jr., M.P. Vecchi, Optimization by simulated annealing. *Science* **220**, 671–680 (1983)
34. K. Klemm, C. Flamm, P.F. Stadler, Funnels in energy landscapes. *Europ. Phys. J. B* **63**, 387–391 (2008)
35. W.B. Langdon, 2-bit flip mutation elementary fitness landscapes, in *11th International Workshop on Foundations of Genetic Algorithms, FOGA 2011*, Schwarzenberg, ed. by H.G. Beyer, W.B. Langdon (ACM, 2011), pp. 25–42

36. G. Lu, R. Bahsoon, X. Yao, Applying elementary landscape analysis to search-based software engineering, in *2nd International Symposium on Search Based Software Engineering*, Benvento (IEEE Computer Society, Los Alamitos, 2010), pp. 3–8
37. C.A. Macken, P.S. Hagan, A.S. Perelson, Evolutionary walks on rugged landscapes. *SIAM J. Appl. Math.* **51**, 799–827 (1991)
38. M. Mann, K. Klemm, Efficient exploration of discrete energy landscapes. *Phys. Rev. E* **83**(1), 011113 (2011)
39. N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, Equation of state calculations by fast computing machines. *J. Chem. Phys.* **21**, 1087–1092 (1953)
40. M. Mézard, G. Parisi, M. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987)
41. P.G. Mezey, *Potential Energy Hypersurfaces* (Elsevier, Amsterdam, 1987)
42. B. Mohar, Graph laplacians, in *Topics in Algebraic Graph Theory, Encyclopedia of Mathematics and Its Applications*, vol. 102, ed. by L.W. Beineke, R.J. Wilson (Cambridge University Press, Cambridge, 2004), pp. 113–136
43. K.i. Okazaki, N. Koga, S. Takada, J.N. Onuchic, P.G. Wolynes, Multiple-basin energy landscapes for large-amplitude conformational motions of proteins: structure-based molecular dynamics simulations. *Proc. Natl. Acad. Sci. U.S.A.* **103**, 11844–11849 (2006)
44. V.M. de Oliveira, J.F. Fontanari, P.F. Stadler, Metastable states in high order short-range spin glasses. *J. Phys. A: Math. Gen.* **32**, 8793–8802 (1999)
45. R. Palmer, Optimization on rugged landscapes, in *Molecular Evolution on Rugged Landscapes: Proteins, RNA, and the Immune System*, ed. by A.S. Perelson, S.A. Kauffman (Addison-Wesley, Redwood City, 1991), pp. 3–25
46. D.L. Powers, Graph partitioning by eigenvectors. *Lin. Algebra Appl.* **101**, 121–133 (1988)
47. R. Rammal, G. Toulouse, M.A. Virasoro, Ultrametricity for physicists. *Rev. Mod. Phys.* **58**, 765–788 (1986)
48. C.M. Reidys, P.F. Stadler, Neutrality in fitness landscapes. *Appl. Math. Comput.* **117**, 321–350 (2001)
49. C.M. Reidys, P.F. Stadler, Combinatorial landscapes. *SIAM Rev.* **44**, 3–54 (2002)
50. H. Rieger, The number of solutions of the Thouless-Anderson-Palmer equations for p -spin interaction spin glasses. *Phys. Rev. B* **46**, 14655–14661 (1992)
51. D. Rockmore, P. Kostelec, W. Hordijk, P.F. Stadler, Fast Fourier transform for fitness landscapes. *Appl. Comput. Harmonic Anal.* **12**, 57–76 (2002)
52. P. Sibani, R. van der Pas, J.C. Schön, The lid method for exhaustive exploration of metastable states of complex systems. *Comput. Phys. Commun.* **116**, 17–27 (1999)
53. A. Solomon, J.W. Barnes, S.P. Dokov, R. Acevedo, Weakly symmetric graphs, elementary landscapes, and the TSP. *Appl. Math. Lett.* **16**, 401–407 (2003)
54. A. Solomon, B.W. Colletti, Quasiabelian landscapes of the traveling salesman problem are elementary. *Discret. Optim.* **6**, 288–291 (2009)
55. P.F. Stadler, Landscapes and their correlation functions. *J. Math. Chem.* **20**, 1–45 (1996)
56. P.F. Stadler, Spectral landscape theory, in *Evolutionary Dynamics—Exploring the Interplay of Selection, Neutrality, Accident, and Function*, ed. by J.P. Crutchfield, P. Schuster (Oxford University Press, New York, 2002), pp. 231–272
57. P.F. Stadler, R. Happel, Correlation structure of the landscape of the graph-bipartitioning-problem. *J. Phys. A: Math. Gen.* **25**, 3103–3110 (1992)
58. P.F. Stadler, R. Happel, Random field models for fitness landscapes. *J. Math. Biol.* **38**, 435–478 (1999)
59. P.F. Stadler, W. Schnabl, The landscape of the travelling salesman problem. *Phys. Lett. A* **161**, 337–344 (1992)
60. B.M.R. Stadler, P.F. Stadler, Generalized topological spaces in evolutionary theory and combinatorial chemistry. *J. Chem. Inf. Comput. Sci.* **42**, 577–585 (2002)
61. B.M.R. Stadler, P.F. Stadler, Combinatorial vector fields and the valley structure of fitness landscapes. *J. Math. Biol.* **61**, 877–898 (2010)

62. P.F. Stadler, R. Seitz, G.P. Wagner, Evolvability of complex characters: population dependent Fourier decomposition of fitness landscapes over recombination spaces. *Bull. Math. Biol.* **62**, 399–428 (2000). Santa Fe Institute Preprint 99-01-001
63. P.F. Stadler, W. Hordijk, J.F. Fontanari, Phase transition and landscape statistics of the number partitioning problem. *Phys. Rev. E* **67**, 0567011–6 (2003)
64. A.M. Sutton, A.E. Howe, L.D. Whitley, A theoretical analysis of the k -satisfiability search space, in *Proceedings of SLS 2009*, Brussels. Lecture Notes in Computer Science, vol. 5752 (2009), pp. 46–60
65. A.M. Sutton, L.D. Whitley, A.E. Howe, A polynomial time computation of the exact correlation structure of k -satisfiability landscapes, in *Genetic and Evolutionary Computation Conference, GECCO 2009*, Montréal, 2009, ed. by F. Rothlauf, pp. 365–372
66. M. Tomassini, S. Vérel, G. Ochoa, Complex-network analysis of combinatorial spaces: the NK landscape case. *Phys. Rev. E* **78**, 066114 (2008)
67. V.K. Vassilev, T.C. Fogarty, J.F. Miller, Information characteristics and the structure of landscape. *Evol. Comput.* **8**, 31–60 (2000)
68. E.D. Weinberger, Correlated and uncorrelated fitness landscapes and how to tell the difference. *Biol. Cybern.* **63**, 325–336 (1990)
69. E.D. Weinberger, Local properties of Kauffman’s N-K model: a tunably rugged energy landscape. *Phys. Rev. A* **44**, 6399–6413 (1991)
70. L.D. Whitley, A.M. Sutton, Partial neighborhoods of elementary landscapes, in *Genetic and Evolutionary Computation Conference, GECCO 2009*, Montréal, 2009, ed. by F. Rothlauf, pp. 381–388
71. L.D. Whitley, A.M. Sutton, A.E. Howe, Understanding elementary landscapes, in *Genetic and Evolutionary Computation Conference, GECCO 2008*, Atlanta, ed. by C. Ryan, M. Keijzer (ACM, 2008), pp. 585–592
72. L.D. Whitley, F. Chicano, E. Alba, F. Luna, Elementary landscapes of frequency assignment problems, in *Proceedings of the 12th Annual Conference of Genetic and Evolutionary Computation GECCO*, Portland, ed. by M. Pelikan, J. Branke (ACM, 2010), pp. 1409–1416
73. M.T. Wolfinger, W.A. Svrcek-Seiler, C. Flamm, I.L. Hofacker, P.F. Stadler, Exact folding dynamics of RNA secondary structures. *J. Phys. A: Math. Gen.* **37**, 4731–4741 (2004)
74. P. Wolynes, J. Onuchic, D. Thirumalai, Navigating the folding routes. *Science* **267**, 1619–1620 (1995)
75. S. Wright, The roles of mutation, inbreeding, crossbreeding and selection in evolution, in *Proceedings of the Sixth International Congress on Genetics*, New York, vol. 1, ed. by D.F. Jones (Brooklyn Botanic Gardens, New York, 1932), pp. 356–366
76. S. Wright, “Surfaces” of selective value. *Proc. Natl. Acad. Sci. U.S.A.* **58**, 165–172 (1967)