NEUTRALITY IN FITNESS LANDSCAPES

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Abstract. The interplay of ruggedness and neutrality in fitness landscapes plays an important role in explaining the dynamics of evolutionary adaptation. While various measures of ruggedness (correlation functions, adaptive walks, or the density of local optima) are reasonably well understood, and models for constructing landscapes with a desired degree of ruggedness are readily available, very little is known about neutrality. We introduce the notion of additive random landscapes as a framework for tuning both neutrality and ruggedness at once, and we develop a formalism that allows the explicit computation of the most salient parameters that are associated with neutrality in landscapes of this type.

1. Introduction

The notion of a *landscape*, that is, a function from a very large discrete set V that carries an additional metric or at least topological structure, into the real numbers $\mathbb{R}$, has emerged as a powerful concept in many areas of applied sciences, since it has been introduced by Sewall Wright [59] to visualize the evolutionary adaptation of a biological species to its environment. The cost functions of combinatorial optimization problems [57, 54, 2, 1], given a particular move set or search heuristic, the energy function of disordered systems such as spin glasses [35] or folding hetero-polymers [58, 11], as well as the fitness of a biomolecule as a function of its underlying genotype [59, 14, 44] are oftentimes dealt with in the common language of landscapes.

For the purpose of this contribution we shall limit ourselves to landscapes defined on the vertex set of undirected graphs, see however [28, 55, 56] for a more general setting. Thus let $Y = Y(V, E)$

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be an undirected graph and $f : V \to \mathbb{R}$ an otherwise arbitrary function. We will refer to the triple (V, E, f) as a *landscape* over Y.

Since the vertex set V is assumed to be very large, in practice oftentimes by far too large to fit into any computer's memory, aggregate (statistical) characteristics of landscapes have to be used to classify and compare these objects. Most work was focused on the notion of *ruggedness* as expressed by the number of local optima [38] or by means of pair correlation functions [10, 48, 57, 51].

We say two configurations $x, y \in V$ are *neutral* if $f(x) = f(y)$. We colloquially refer to a landscape as "neutral" if a substantial fraction of adjacent pairs of configurations are neutral. This should not be confused with the *flat* landscape, in which f is constant. Extensive computer simulations, based on RNA secondary structures [45, 21, 22], have revealed that neutrality plays an important role in understanding the dynamics of RNA evolution [27, 43, 42].

Kimura proposed a theory of biological evolution that focuses exclusively on the aspects of neutrality [31] by assuming a flat fitness landscape. Very recently, landscapes with a large degree of neutrality have also been described in computational models such as cellular automata [23], for the mapping of sequences in combinatorial random structures [41], and in the context of sequential dynamical systems [32].

At the first glance, neutrality and ruggedness appear to be two sides of the same coin. We shall see, however, that ruggedness (as measured by the correlation length of the landscapes) and neutrality (as measured by the number of neutral neighbors) can be tuned independently of each other.

The purpose of the contribution is two-fold. We describe a rather general construction for producing ensembles of landscapes with prescribed degrees of neutrality (and ruggedness), and we (partially) develop a mathematical formalism for computing their basic properties.

This paper is organized as follows: In section 2 we briefly review some properties of general random landscapes. Then we introduce the notion of additive random landscapes and discuss their basic properties using spin glasses and well known combinatorial optimization problems as examples. Up to this point, our results are independent of the graph structure imposed on the set of configurations V. In section 4 we briefly consider landscapes on graphs and the notion of ruggedness. Neutrality and the main results of this contribution are the subject of section 5. Neutral walks, a useful tool in computational explorations of neutral landscapes, are the subject of section 6.

2. Random Landscapes

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

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

$$\Omega = (\{f : V \to \mathbb{R} \mid f \text{ has property } W\}, \mathcal{A}, \mu) \ , \tag{2.1}$$

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

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

The *covariance matrix* of the random landscape Ω, $\mathbf{C}(\Omega)$, is given by

$$\mathbf{C}_{xy} := \mathrm{Cov}[\mathrm{eval}_x, \mathrm{eval}_y] = \mathbb{E}[\mathrm{eval}_x \mathrm{eval}_y] - \mathbb{E}[\mathrm{eval}_x]\mathbb{E}[\mathrm{eval}_y] \ . \tag{2.2}$$

$\mathbf{C}$ 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

$$f(x) \doteq \sum_k b_k \psi_k(x) \qquad \text{a.s.} \qquad x \in V \tag{2.3}$$

is know as *Karhunen-Loève series* or *principal component decomposition*. For later reference we note the following classical result [25]:

Proposition 1. *Let Λ_k denote the eigenvalue of $\mathbf{C}$ belonging to the eigenvector ψ_k. Then the coefficient of the Karhunen-Loève series (2.3) are uncorrelated random variables satisfying*

$$\mathrm{Cov}[b_k, b_j] = \Lambda_k \delta_{kj} \qquad 1 \le k, l \le |V|. \tag{2.4}$$

Thus $\Lambda_k = \mathbb{V}[b_k]$.

3. Additive Random Landscapes

In this paper we will study a certain class of random landscapes, defined as follows:

Definition 1. Let V and M be finite sets and $\Theta = (\vartheta_j)_{j\in M}$ a family of maps $\vartheta_j : V \to \mathbb{R}$. Further, let c_j, $j \in M$ be independent, real valued random variables (over the respective probability spaces $\Omega_j = (\mathbb{R}, \mathcal{A}_j, \mu_j)$) and

$$\Omega_V = \{f : V \longrightarrow \mathbb{R} \mid f(x) = \sum_{j=1}^{M} c_j \vartheta_j(x)\} \ . \tag{3.1}$$

An *additive random landscape* (or *arl* for short), $\mathcal{F}(V, \Theta, (c_j))$, is the probability space

$$(\Omega_V, \otimes\mathcal{A}_j, \otimes_j \mu_j) \tag{3.2}$$

An arl is *uniform* if and only if (i) the r.v's c_i, $i \in M$ are i.i.d. and (ii) there exist $a, b \in \mathbb{R}$ such that $\sum_{x\in V} \vartheta_i(x) = |V|a$ and $\sum_{x\in V} \vartheta_i^2(x) = |V|b$. An uniform random landscape is *strictly uniform* if there exist $d, e \in \mathbb{R}$ such that $\sum_j \vartheta_i(x) = d$ and $\sum_j \vartheta_i^2(x) = e$.

Remark 1. A random landscape Ω with Gaussian measure is additive. This follows immediately from Proposition 1 and the fact that Gaussian and uncorrelated already implies independent.

We proceed by giving the following four examples:

1. **Ising spin landscapes.** Consider a collection of n Ising spins x_i, $1 \le i \le n$, $x_i = \pm 1$. In the most general case we are given a list of spin interactions $\mathcal{I}$, the elements of which are the sets of spins with non-zero interactions. For instance, $\mathcal{I}$ consists of all pairs of spins for the Sherrington Kirkpatrick (SK) model [47], while $I \in \mathcal{I}$ is of the form $I = \{j, j+1\}$ for a linear spin chain. In higher order spin glasses, such as Derrida's [9] p-spin models, there are of course sets I with a cardinality larger than 2. It is customary in spin glass physics to assume the that interaction energies are of the form $c_I \prod_{i\in I} x_i$ with i.i.d. (Gaussian) interaction coefficients c_I with mean $\mathbb{E}[c_i] = 0$. Such spin glass Hamiltonians are therefore an additive landscape with

$$\vartheta_I(x) = \prod_{i\in I} x_i \ . \tag{3.3}$$

It is further clear that $\vartheta_I(x) = \pm 1$ whence $\vartheta_I^2(x) = 1$ for all x, hence $b = 1$ for all I. Finally,

$$\sum_{x\in V} \prod_{j\in I} x_k = \prod_{i\in I} \left(\sum_{x_i=\pm 1} x_i \right) \prod_{i\notin I} \left(\sum_{x_i=\pm 1} 1 \right) = 0$$

for all $I \neq \emptyset$. Thus all spin-glass models with i.i.d. coefficients are uniform random fields. Consider a spin glass with only 2 spins and the single function $\vartheta_{12}(x) = x_1 x_2$. If $x_1 = x_2$, i.e., for the spin configuration $++$ and $--$ we have $\vartheta_{12}(x) = 1$ while $\vartheta_{12}(x) = -1$ for the other two spin configuration. We have, however, $\vartheta_I^2(x) = 1$ for all x, and hence e exists and equals the number of components of the random landscape. Thus spin glass models are in general not strictly uniform since d does not exist.

2. **Kauffman's NK landscapes.** Consider a genome with n loci each of which may have the state 0 or 1, the fitness of which is the average of "site-fitnesses". Each site fitness in turn depends on its own state and the states of the K genes to which it is "epistatically" linked. These state-dependent contributions are usually taken as independent uniform random variables [29].

It becomes clear by introducing the following notation that NK models are additive random landscapes. Let V be the set of vertices $(x_1, \ldots, x_n)$ of the Boolean n-cube, $\mathfrak{Q}_2^n$. We consider a (random) mapping

$$\phi : \mathbb{N}_n \longrightarrow \{(i_0, \ldots, i_K) \mid i_j \in \mathbb{N}_n\,,\ \forall j;\ i_j < i_{j+1}\}, \quad \text{such that } i \in \phi(i) \tag{3.4}$$

and write $\phi(i)_j = i_j$. Now, we randomly and independently assign to each $K+1$-tuple $(y_{i_0}, \ldots, y_{i_K})$ a real number $c_{(i,(y_{i_0},\ldots,y_{i_K}))}$ and set $\beta_i = \beta[\phi(i)] = \big\{(y_{i_0}, \ldots, y_{i_K}) \mid y_j \in \{0,1\}\ \big\}$. With

$$\vartheta_{(i,(y_{\phi(i)_0},\ldots,y_{\phi(i)_K}))}(x) = \frac{1}{n}\prod_{j=0}^{K} \delta(y_{\phi(i)_j}, x_{\phi(i)_j})$$

we take $M = \{(i, (y_{\phi(i)_0}, \ldots, y_{\phi(i)_K})) \mid i \in \mathbb{N}_n,\ (y_{\phi(i)_0}, \ldots, y_{\phi(i)_K}) \in \beta[\phi(i)]\ \}$ and define for $x = (x_1, \ldots, x_n)$, $f_\phi(x) = \sum_{m\in M} c_m\, \vartheta_m(x)$. Clearly, f is completely determined by the (random) map ϕ and the family of real numbers c_m. Obviously,

$$\sum_{x\in\{0,1\}^n} \vartheta_{i,\beta_i}(x) = \frac{1}{n} 2^{n-(K+1)} \qquad \text{and} \qquad \vartheta^2_{i,\beta_i}(x) = \frac{1}{n}\vartheta_{i,\beta_i}(x)\,.$$

NK models are strictly uniform because

$$\sum_i \sum_{\beta_i} \vartheta_{i,\beta_i}(x) = \frac{1}{n}\sum_i 1 = 1\,.$$

3. **Graph bipartitioning (GBP)-landscapes.** Let V be the set of all (ordered) bipartitions $\xi = [A, B]$ of the set $\{1, \ldots, n\}$, $n \equiv 0 \mod 2$, with the property $|A| = |B|$. For $i \neq j$ let $d_{j,i} = d_{i,j}$

be a family of i.i.d. real valued r.v.'s and

$$\forall i \neq j; \quad \vartheta_{i,j}(\xi) = \begin{cases} 1 & \text{if} \quad \{i,j\} \not\subset A \wedge \{i,j\} \not\subset B \\ 0 & \text{otherwise.} \end{cases} \tag{3.5}$$

Then the GBP-arl is given by $f(\xi) = \sum_{i\neq j} d_{i,j}\vartheta_{i,j}(x)$. We observe $\sum_\xi \vartheta_{ij}(\xi) = \frac{1}{4}\frac{n}{n-1}\binom{n}{n/2}$ and $\vartheta_{ij}(\xi) = \vartheta_{ij}^2(\xi)$. Finally,

$$\sum_{i\neq j}\vartheta_{ij}(x) = \sum_{i\in A}\sum_{j\in B} 1 + \sum_{i\in B}\sum_{j\in A} 1 = n^2/2$$

proves that the GBP-arl is strictly uniform.

4. TSP landscapes. Consider a traveling salesman problem with randomly assigned distances between the n cities. The set V consists of all possible tours, that is, of all permutations of the n cities. The length of a tour τ is simply $\sum_i d_{\tau(i)\tau(i-1)}$ where d_{ij} is the distance from j to i and indices are taken modulo n. We may write this in the form

$$f(\tau) = \sum_{\substack{k,l\\ k\neq l}} d_{kl} \sum_{i=1}^{n} \delta_{k,\tau(i)}\delta_{l,\tau(i-1)} \tag{3.6}$$

and obtain

$$\vartheta_{kl}(\tau) = \sum_{i=1}^{n} \delta_{k,\tau(i)}\delta_{l,\tau(i-1)} \tag{3.7}$$

A similar representation can be obtained for random symmetric TSPs. Here $d_{kl} = d_{lk}$. Since the sum runs only over independent entries we require $k < l$. In a tour we have at most one of the edges (kl) and (lk), thus

$$\vartheta_{kl}(\tau) = \sum_{i=1}^{n} \left(\delta_{k,\tau(i)}\delta_{l,\tau(i-1)} + \delta_{l,\tau(i)}\delta_{k,\tau(i-1)}\right) \qquad 1 \leq k < l \leq n\,. \tag{3.8}$$

Next we have

$$\sum_{\tau\in \mathsf{S}_n}\sum_{i=1}^{n} \delta_{\tau(i),k}\delta_{\tau(i-1),l} = \sum_{\tau\in \mathsf{S}_n} \delta_{\tau(\tau^{-1}(k)-1),l} = |\mathsf{S}_n|/n = (n-1)!$$

independent of k and l. Clearly we have $\vartheta_{kl}(\tau) = \vartheta_{kl}^2(\tau)$, since ϑ_{kl} takes only the values 0 and 1.

$$\sum_{k\neq l}\vartheta_{kl}(\tau) = \sum_k\sum_{l\neq k}\sum_i \delta_{\tau(i),k}\delta_{\tau(i-1),l} = \sum_k\sum_{l\neq k}\delta_{\tau(\tau^{-1}(k)-1),l} = n-1$$

Analogously, it can be shown that the symmetric TSPs are strictly uniform.

Lemma 1. *Let $\mathcal{F}(\Omega_V, \theta, (c_j))$ be an arl, then $\mathbf{C}(\mathcal{F})$ is given by*

$$\mathbf{C}_{xy} = \sum_i \mathbb{V}[c_i]\vartheta_i(x)\vartheta_i(y) \ . \tag{3.9}$$

Suppose now that $\sum_x \vartheta_k(x)\vartheta_i(x) = \sum_x \vartheta_i(x)^2\delta_{i,k}$ holds for all $i, k \in M$. Then we have

$$\mathbf{C}\vartheta_k = \Lambda_k\vartheta_k, \quad \text{where} \quad \Lambda_k = \mathbb{V}[c_k]\sum_y \vartheta_k(y)^2 \ . \tag{3.10}$$

Proof. Elements of $\mathcal{F}$ are of the form $f(x) = \sum_j c_j\vartheta_j(x)$ and the first assertions follows by straightforward computation, using linearity of expectation and the independence of the r.v.'s c_i, $i \in M$. The second assertion follows from $\sum_y \mathbf{C}_{x,y}\vartheta_k(y) = \Lambda_k\vartheta_k(x)$. □

Remark 2. The spin glass models exhibit the orthogonality relation $\langle\vartheta_k\,\vartheta_i\rangle = e\,\delta_{i,k}$. In many cases, however, the $\{\vartheta_i\}$ are not orthogonal, e.g., for NK, TSP, and GBP-arl.

In [53] we have introduced the following notion

Definition 2. An arl $\mathcal{F}$ is *pseudo-isotropic* if there are constants a_0, v, and w such that for all $x \in V$

(i) $\mathbb{E}[\mathrm{eval}_x] = a_0$,
(ii) $\mathbb{V}[\mathrm{eval}_x] = v^2$, and
(iii) $|V|^{-1}\sum_{y\in V}\mathbf{C}_{xy} = w$.

Proposition 2. *Let $\mathcal{F}$ be a uniform random random field. Then $\mathcal{F}$ is pseudo-isotropic if and only if at least one of the following two conditions is satisfied*

1. *$\mathcal{F}$ is strictly uniform.*
2. *$\forall i :\ \sum_{x\in V}\vartheta_i(x) = a = 0$ and $\mathbb{E}[c_i] = 0$, and $\sum_i \vartheta_i^2(x) = e$ with $e \in \mathbb{R}$.*

Remark 3. It is interesting to note that the random fields of the TSPs, the GBP, and the NK models are pseudo-isotropic because they are strictly uniform, while the spin glass models have this property as a consequence of the alternative condition *2*. In particular, the additional condition $\mathbb{E}[c_i] = 0$ on the interaction coefficients cannot be relaxed.

For a uniform arl $\mathfrak{F}$ and $a = |V|^{-1} \sum_{x\in V} \vartheta_i(x)$ we set $s^2 = \mathbb{V}[c_i]$ and

$$\tilde{\vartheta}_i : V \to \mathbb{R} \qquad \tilde{\vartheta}_i(x) = \vartheta_i(x) - a \quad \text{and} \quad \tilde{\mathbf{C}}_{xy} = s^2 \sum_i \tilde{\vartheta}_i(x)\tilde{\vartheta}_i(y) \ . \tag{3.11}$$

Note that $\tilde{\mathbf{C}}$ is the covariance matrix of the arl $\tilde{f} = \sum_j c_j \tilde{\vartheta}_j$.

Lemma 2. *Let $\mathfrak{F}$ be a pseudo-isotropic uniform arl. Then the following assertions hold:*

$$(a) \quad \mathbf{C} = \tilde{\mathbf{C}} + w\mathbf{J} \ ,$$

where w is the average correlation and $\mathbf{J}$ denotes the matrix with all entries 1. Furthermore $\mathbf{C1} = w|V|\mathbf{1}$ holds.
(b) $\tilde{\vartheta}_i$ is an eigenvector of $\mathbf{C}$ if and only if it is an eigenvector of $\tilde{\mathbf{C}}$.
(c) If the $\tilde{\vartheta}_i$ are pairwise orthogonal, then

$$\forall i \in M; \quad \mathbf{C}\tilde{\vartheta}_i = \Lambda\, \tilde{\vartheta}_i, \quad \text{where} \quad \Lambda = s^2 \sum_{y\in V} \tilde{\vartheta}_k(y)^2$$

holds. Hence $\tilde{f}$ is an eigenvalue of $\mathbf{C}$ almost surely.

Proof. (a) Substituting equ.(3.11) into the definition of the covariance matrix (2.2) we find

$$\mathbf{C}_{xy} = s^2 \sum_i \tilde{\vartheta}_i(x)\tilde{\vartheta}_i(y) + s^2\ a\ \left(a + \sum_i \tilde{\vartheta}_i(x) + \sum_i \tilde{\vartheta}_i(y)\right) \ .$$

If $\mathfrak{F}$ is strictly uniform, then sums in the parenthesis are independent of x and y. Thus $\mathbf{C} = \tilde{\mathbf{C}} + q\mathbf{J}$ for some $q \in \mathbb{R}$. Clearly we have for pseudo-isotropic arl $\mathbf{C1} = w|V|\mathbf{1}$. Finally, to prove $q = w$ we compute $\mathbf{C1} = \tilde{\mathbf{C}}\mathbf{1} + w\mathbf{J1}$. Now, $\mathbf{C1} = w|V|\mathbf{1}$, $\tilde{\mathbf{C}}\mathbf{1} = 0$ and $\mathbf{J1} = |V|\mathbf{1}$, whence the assertion.
(b) The assertion follows from $w\mathbf{J}\tilde{\vartheta}_k = 0$.
(c) Since $\mathfrak{F}$ is an uniform arl $\sum_y \tilde{\vartheta}_k^2(y)$, $k \in M$, is independent of k. Hence,

$$\sum_{y\in V} \tilde{\mathbf{C}}_{xy}\tilde{\vartheta}_k(y) = s^2 \sum_i \tilde{\vartheta}_i(x) \sum_{y\in V} \tilde{\vartheta}_i(y)\tilde{\vartheta}_k(y) = s^2\tilde{\vartheta}_k(x) \sum_{y\in V} \tilde{\vartheta}_k(y)^2$$

and the assertion follows. □

4. Random Landscapes over Graphs: Ruggedness and Neutrality

We have introduced a *random landscape* in section 2 making use of the following data: a base space of maps Ω_V, (Ω_V-elements are mappings $V \to \mathbb{R}$ where V is a finite set), a σ-field, $\mathcal{A}$, and a probability measure, μ,. No additional structure on the set V has been required. In practice, however, we are most interested in those properties of a landscape that depend explicitly on a notion of "closeness" among the elements of V, namely ruggedness and neutrality. To this end we assume that there is an adjacency relation between V-elements, that is, one considers V as the vertex set of a finite, simple, loop-free graph Y. Furthermore, we shall assume throughout this contribution that Y is regular.

Remark 4. The concept of ruggedness can be dealt with in settings far more general. R. Seitz [46], generalizing E. Weinberger's approach [57], recently suggested to use a Markov process on V to describe the mutual location of V-elements. The set of configurations V is interpreted as (the vertex set of) a hypergraph in the "theory of recombination spaces" [19, 55, 56]. Fontana [12, 13] focuses on the notion of "accessibility", thereby relaxing the symmetry of the adjacency relation and the regarding V as a (finite) topological space.

In many cases the model at hand suggests a "natural" adjacency structure on V and we obtain a graph that captures the regularities of constructing the configurations in V. For instance, when the configurations are n-tuples (such as strings of length n taken from a fixed alphabet of size a as in the case of the NK models, or a list of up/down spins in a spin glass model) point mutation (or the flipping of individual spins) is the obvious choice. The resulting graphs are the Hamming graph $\mathcal{Q}^n_\alpha$. Bipartitions of a set are naturally modified by exchanging an element between the two classes. This gives rise to the Johnson graph $\mathcal{J}(n, n/2)$. The tours of the TSP are naturally encoded as permutations of the list of cities. Hence we can interpret the set of TSP tours as a symmetric group S_n. Sets of generators of the S_n thus are natural move sets, leaving us with a variety of Cayley graphs of S_n, see Figure 4.

As usual, let $\mathbf{A}$ denote the adjacency matrix of Y and let $\mathbf{D}$ be the diagonal matrix of vertex degrees, i.e., $\mathbf{D}_{xx} = \sum_{y\in V} \mathbf{A}_{xy}$ and $\mathbf{D}_{xy} = 0$ for $x \neq y$. Furthermore, we introduce $\mathbf{T} = \mathbf{A}\mathbf{D}^{-1}$, the (bistochastic) transition matrix of a *simple random walk* on Y. (In previous studies we have mostly used the graph Laplacian $\mathbf{\Delta} = \mathbf{A} - \mathbf{D}$ instead of $\mathbf{T}$ [51].) It will be convenient to use the decomposition $f(x) = \tilde{f}(x) + \bar{f} \times \mathbf{1}(x)$, where $\sum_{x\in V} \tilde{f}(x) = 0$, $\bar{f} = |V|^{-1} \sum_x f(x)$ and $\mathbf{1}(x) = 1$

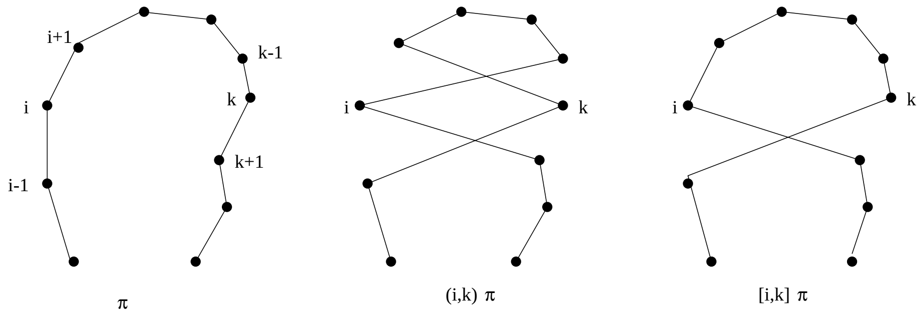

FIGURE 1. The two most widely used move-sets for TSPs are transpositions (i,k) and so-called reversals [34], denoted by $[i,k]$. In a transposition, two cities i and k are exchanged. As a consequence, four connections are deleted from the tour π and four new connections are introduced, provided i and k are adjacent in π. If i and k are adjacent the corresponding transposition is called canonical; it causes the deletion of only two old and the insertion of only two new connections. A reversal move inverts the orientation of the tour between two cities i and k. This causes two old connections to be replaced by two new ones. Note that inverting the orientation between i and k has no effect in a symmetric TSP but replaces $|k-i|$ connections by new ones in the non-symmetric case.

for all $x \in V$. It seems natural to define ruggedness and neutrality as random variables given that the mathematical object underlying our study is the probability space $\Omega = (\Omega_V, \mathcal{A}, \mu)$:

Definition 3. Let Y be a finite simple loop-free graph, $y \in \mathrm{v}[Y]$ and $\mathcal{F}(\mathrm{v}[Y], \Theta, (c_j))$ an arl. The *ruggedness* of $\mathcal{F}$ is the family of random variables

$$\forall\, s \le \mathrm{diam}(Y), \quad r_s : \mathcal{F} \longrightarrow \mathbb{R}, \quad r_s(f) = \frac{\langle \tilde f, \mathbf{T}^s \tilde f\rangle}{\langle \tilde f, \tilde f\rangle}\ , \tag{4.1}$$

where $\langle\, .\,,\, .\,\rangle$ denotes the standard scalar product.

Remark 5. The r.v. $r_s(f)$ can be interpreted as the autocorrelation function of the "time series" that is obtained by sampling the values $eval_x(f)$ along a random walk on V with transition matrix T [57, 50].

In general, we can write the correlation function of a landscape in the following form: Let $\{\varphi_i\}$ denote an orthonormal basis of eigenfunctions of $\mathbf{T}$, and let I_p be the set of indices of the eigenfunctions belonging to the same eigenvalue λ_p of $\mathbf{T}$, i.e., $\mathbf{T}\varphi_i = \lambda_p \varphi_i$ if and only if $i \in I_p$. Let $\lambda_0 = 1$

and φ_0 be the normalized Peron-Frobenius eigenvector. We can write f in the form $f = \sum_i a_i\varphi_i$ with $a_i = \langle f, \varphi_i^* \rangle$. As a consequence we have [51]

$$r_s = \sum_{p\neq 0} B_p \lambda_p^s \qquad \text{with} \qquad B_p = \frac{\sum_{i\in I_p} |a_i|^2}{\sum_{i\neq 0} |a_i|^2} \ . \tag{4.2}$$

By linearity of expectation we obtain $\mathbb{E}[r_s] = \sum_{p\neq 0} \mathbb{E}[B_p]\lambda_p^s$. Instead of r_s we can therefore use the *amplitude spectrum* B_p, $p \leq 1$, as a measure for the ruggedness of a landscape that in many cases is easier to interpret, see e.g. [51, 16, 24].

Lov Grover and others [7, 20, 51] observed that $\tilde{f}$ is in many cases an eigenfunction of the graph Laplacian, and hence also of $\mathbf{T}$, in many cases. We call a random landscape f elementary w.r.t. $\mathbf{T}$ iff $\mathbf{T}\tilde{f} = \lambda_p \tilde{f}$ with an eigenvalue $\lambda_p < 1$ almost surely. Equivalently, f is elementary if $r_s = \lambda_p^s$ for some $p \neq 0$, i.e., $\mathbb{E}[B_p] > 0$ for exactly one "mode" p. This value of p therefore determines the ruggedness of an elementary landscape.

These conditions are satisfied for many of the best-studied models, in particular for the p-spin models, for the TSP with both transpositions and reversals, and for the graph bipartitioning problem which exchange moves. It is interesting to note furthermore, that most of the well-studied combinatorial optimization problems, the symmetric TSPs and the Graph Bipartitioning problem among them, are elementary with eigenvalue λ_2 (assuming that the eigenvalues labeled such that $1 = \lambda_0 > \lambda_1 > \dots$). Recall that the Perron-Frobenius eigenvalue $\lambda_0 = 1$ corresponds to the flat landscape. For landscapes on Hamming graphs it is well known that the elementary landscapes belonging to λ_1 are additive functions of the form $f(x) = \sum_{i=1}^n f_i(x_i)$. The TSP and the GBP thus belong to the class of the "smoothest rugged landscapes". NK models, on the other hand, are **not** elementary for $K \neq 1$ [53]. In cases like this, it is often useful to condense the information contained in r_s into a single random variable, the *correlation length*

$$\ell = \sum_{s=0}^{\infty} r_s = \sum_{p>0} B_p/(1-\lambda_p) \tag{4.3}$$

Let λ_1 and λ_- denote the second largest eigenvalue and the smallest eigenvalue of $\mathbf{T}$, respectively. With this notation, the feasible values of the correlation length ℓ therefore form the compact interval $[(1-\lambda_-)^{-1}, (1-\lambda_1)^{-1}]$.

We can therefore construct additive random landscapes with a desired (feasible) correlation length $\hat{\ell}$ by the following procedure: Given a graph Γ, we consider an arl of the form

$$f(x) = \sum_j c_j \varphi_j(x) \tag{4.4}$$

where $\{\varphi_j(x)\}$ is an ONB of the $\mathbf{T}$. For simplicity we may even assume that the coefficients belonging to the same eigenvalues of $\mathbf{T}$ are i.i.d. It is clear from equ.(4.2) and equ.(4.3) that by choosing the variances of these distributions appropriately, we can reproduce the desired value of $\hat{\ell}$. More explicitly, set $\mathbb{E}[c_i] = 0$ for all i, determine p such that $1\ (1-\lambda_p) \le \hat{\ell} < 1\ (1-\lambda_p)$, set $\mathbb{V}[c_i] = 0$ unless c_i belongs to the modes p or $p-1$ and finally adjust variances of c_i's belonging to these two modes such that $\mathbb{E}[\ell] = \hat{\ell}$.

A variety of landscapes, in particular those associated with biopolymers, are the composite of two maps: First a space of "genotypes" is mapped into a space of "phenotypes", which in the second step are assigned a fitness, see Figure 4. Computer simulations using both RNA [45] and polypeptides [3] indicate that a substantial degree of redundancy is inherent to the genotype-phenotype map. Fitness landscapes of this type inherit their overall structure essentially from the underlying genotype-phenotype map and therefore exhibit neutrality.

This decomposability of the landscapes and the resulting neutrality are not confined to biomolecular folding maps. The problem of finding CA rules that perform a prescribed task, such as global synchronization of an arbitrary initial pattern [8], also gives rise to a landscape admitting a large number of neutral mutations [23].

A quite different type of models, termed *sequential dynamical systems* (SDS), arise in the formal description of computer simulations [6]. The basic idea is to model a simulation using an undirected graph Γ (with vertex set $\{1,\ldots,n\}$), a collection of Boolean function (F_i) that update the state of vertex i as a function of its neighbors while leaving all other vertices unchanged, and 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 $(\mathfrak{F},\pi) = \prod_{i=1}^{n} F_{\pi(i)} : \mathbb{F}_2^n \longrightarrow \mathbb{F}_2^n$. The question then becomes to analyze the set of all schedules π' that lead to the same SDS. It is shown in [40] that there is one-to-one correspondence between SDS and the acyclic orientations of Γ. The acyclic orientations of Γ therefore serve as the "phenotypes" of the following mapping:

$$\psi_\Gamma : \mathsf{S}_n \longrightarrow \mathrm{Acyc}(\Gamma) \tag{4.5}$$

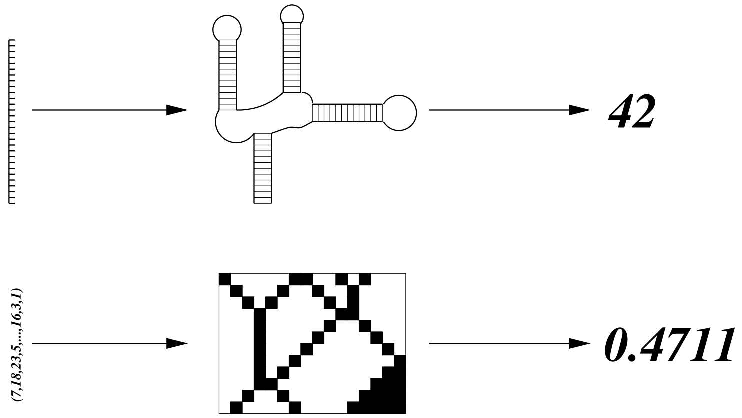

FIGURE 2. Landscapes derived from biopolymer folding and those associated with discrete dynamical systems share crucial features. In both cases first "genotypes" are mapped onto "phenotypes". This mapping is in general many-to-one. This redundancy of the genotype-phenotype map translates into neutrality in the fitness landscape that is obtained by evaluating the phenotypes.

Fitness can be introduced into this model by evaluating how close the behavior of an SDS is to a desired target. Obviously, permutations with the same image under ψ_Γ are neutral in the sense of having the same fitness.

Definition 4. Let Y be a finite simple loop-free graph, $y \in \mathrm{v}[Y]$ and $\mathcal{F}(\mathrm{v}[Y], \Theta, (c_j))$ an arl. Let $S_1(x)$ denotes the set of vertices that are adjacent to x in Y. The *neutrality of* $\mathcal{F}$ *in* x is the random variable

$$\nu_x : \mathcal{F} \longrightarrow \mathbb{Z}, \quad \nu_x(f) = \sum_{x' \in S_1(x)} \delta\big(f(x), f(x')\big) \ . \tag{4.6}$$

Definition 5. Let f be a landscape on a graph Y, and let Q be a maximal subset of the vertex set of Y such that f is constant on Q. The we call Q a neutral set of f and the induced subgraph $\Gamma[Q]$ is referred to as a *neutral networks.*

In other words, a neutral set is a set $\emptyset \neq Q \subseteq V$ satisfying $Q \in f^{-1}(t)$ for some $t \in \mathbb{R}$.

Three approaches have been explored to study the geometric properties of neutral sets: a mathematical model of genotype-phenotype mapping based on random graph theory [43], extensive sample statistics [45] and exhaustive folding of all sequences with given chain length n [22].

In the random graph model of neutral networks vertices are selected with the independent probability $\tilde{\nu}$. In case of generalized n-cubes the random graph evolution exhibits various threshold values as $\tilde{\nu}$ increases from 0 to 1. In particular for $\tilde{\nu} = \mathcal{O}(\log(n)/n)$ a giant component is a.s. present [39], while connectivity emerges a.s. for $\tilde{\nu} = 1 - \sqrt[\alpha-1]{\alpha^{-1}}$ [43]. Since $\tilde{\nu} = \mathbb{E}[\nu_x]/\deg(x)$ holds, the number of neutral neighbors turns out to be the key parameter of the random graph model.

Computational data from RNA folding show that $\tilde{\nu}$ is typically larger than the above connectivity threshold. The implications of the existence of extensive "percolating" neutral networks is discussed for instance in [27, 26, 17, 18, 42].

Neutral walks [45], a useful tool in computational explorations of neutral landscapes, will be discussed in some detail in section 6. We shall see there that some global (long range) properties of the seemingly benign additive random landscapes strongly deviate from the predictions of the random graph model.

5. Neutrality in Additive Random Landscapes

We begin our investigations of neutrality with the following technical

Lemma 3. *Let M be a finite index set and c_j, $j \in M$, be independent real valued random variables such that*

$$\mu\{c_j = \xi\} = \begin{cases} \mu_0 > 0 & \text{if } \xi = 0 \\ 0 & \text{otherwise} \end{cases} \tag{5.1}$$

Then we have for any set $\Phi \subseteq M$ of non-zero constants $0 \neq \eta_j \in \mathbb{R}$

$$\mu\{\sum_{j\in\Phi} c_j\eta_j = 0\} > 0 \quad \Rightarrow \quad \forall\, j \in \Phi,\ c_j = 0\ . \tag{5.2}$$

Proof. Suppose that we seek for given $\eta_j \neq 0$, $j \in M$ a solution of $\sum_{j\in M} c_j\eta_j = 0$. Then we can select $|M|-1$ values c_j to be arbitrary, while the last coefficient, $c_{|M|}$, is determined by the linear equation. By construction, $\mu\{c_j = \xi\} = 0$ for $\xi \neq 0$, and hence (5.2) follows. □

Remark 6. In fact we will analyze neutrality assuming that the random variables c_i, $i \in M$ fulfill (5.1).

We next introduce the random variables:

$$\forall\{x,y\} \in E : \quad X_{\{y,x\}}(f) = \begin{cases} 1 & \text{if } f(x) = f(y) \\ 0 & \text{otherwise.} \end{cases} \tag{5.3}$$

Clearly, we have $X_{\{x,y\}} = X_{\{y,x\}}$ and we can write $\nu_x(f)$ (see equ.(4.6) as

$$\nu_x(f) = \sum_{y\in S_1(x)} X_{\{y,x\}}(f) \tag{5.4}$$

For the following, it will be convenient to define the following parameters

$$c_x(y) \quad = \quad \left|\{j \in \Phi \mid \vartheta_j(x) \neq \vartheta_j(y)\}\right| \qquad y \in S_1(x) \tag{5.5}$$

$$w_x(y',y'') \quad = \quad \left|\{j \in \Phi \mid \vartheta_j(x) \neq \vartheta_j(y') \ \wedge \vartheta_j(x) \neq \vartheta_j(y'')\}\right| \qquad y',y'' \in S_1(x) \tag{5.6}$$

$$\Xi \quad = \quad \mathbb{E}\left[\frac{1}{|V|}\sum_x \left(\nu_x - \frac{1}{|V|}\sum_{x'} \nu_{x'}\right)^2\right] \ , \tag{5.7}$$

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 1. *For any arl whose coefficients c_i fulfill (5.1) the following assertions hold*

$$\mathbb{E}[\nu_x] \quad = \quad \sum_{y\in S_1(x)} \mu_0^{c_x(y)} \tag{5.8}$$

$$\mathbb{V}[\nu_x] \quad = \quad \sum_{y',y''} \mu_0^{c_x(y')+c_x(y'')} \left[\mu_0^{-w_x(y',y'')} - 1\right] \tag{5.9}$$

$$\begin{aligned} \Xi \quad &= \quad \frac{1}{|V|}\left[\sum_y \mathbb{V}(\nu_y) - \frac{1}{|V|}\sum_{y,y'} \mathrm{Cov}(\nu_y,\nu_{y'})\right] \\ &\quad + \frac{1}{|V|}\sum_y \mathbb{E}[\nu_y]^2 - \left(\frac{1}{|V|}\sum_y \mathbb{E}[\nu_y]\right)^2 \end{aligned} \tag{5.10}$$

where $\frac{1}{|V|}\sum_{y,y'}\mathrm{Cov}(\nu_y,\nu_{y'})\geq 0$. *In particular, if* $\mathbb{E}[\nu_y]$ *is independent of* y *we have*

$$\Xi=\frac{1}{|V|}\left[\sum_y \mathbb{V}(\nu_y)-\frac{1}{|V|}\sum_{y,y'}\mathrm{Cov}(\nu_y,\nu_{y'})\right]\ . \tag{5.11}$$

Proof. By linearity of expectation we have $\mathbb{E}[\nu_y]=\sum_{y'\in S_1(y)}^n \mathbb{E}[X_{\{y',y\}}]$ and in view of the independence of the r.v.'s c_j and equ.(5.2) we observe

$$\mathbb{E}[X_{\{y,x\}}]=\mu\{X_{\{y,x\}}=1\}=\mu_0^{|\{j\,|\,\vartheta_j(x)\neq\vartheta_j(y)\}|}\ .$$

To prove the second assertion we compute

$$\mathbb{E}[X_{\{y',x\}}X_{\{y'',x\}}]=\mu_0^{|\{j\,|\,\vartheta_j(x)\neq\vartheta_j(y')\ \vee\ \vartheta_j(x)\neq\vartheta_j(y'')\}|}=\mu_0^{c_x(y')+c_x(y'')-w(y',y'')}\ .$$

whence $\mathrm{Cov}[X_{\{y',x\}}X_{\{y'',x\}}]=\mu_0^{c_x(y')+c_x(y'')}\left[\mu_0^{-w(y',y'')}-1\right]$. It remains to write

$$\mathbb{V}[\sum_{y\in S_1(x)}X_{\{y,x\}}]=\sum_{y',y''\in S_1(x)}\mathrm{Cov}[X_{\{y',x\}},X_{\{y'',x\}}]$$

and the second assertion follows.
To prove the third assertion we compute

$$\begin{aligned}
\mathbb{E}[\frac{1}{|V|}\left(\sum_{x\in V}\nu_x-\frac{1}{|V|}\sum_{x\in V}\nu_x\right)^2] &= \frac{1}{|V|}\sum_{x\in V}\mathbb{E}(\nu_x^2)-\mathbb{E}[\left(\frac{1}{|V|}\sum_{x\in V}\nu_x\right)^2]\\
&= \frac{1}{|V|}\left[\sum_{x\in V}\mathbb{V}[\nu_x]+\sum_{x\in V}\mathbb{E}[\nu_x]^2\right]-\frac{1}{|V|^2}\,\mathbb{E}[\sum_{x,y}\nu_x\nu_y]\\
&= \frac{1}{|V|}\sum_{x\in V}\mathbb{V}[\nu_x]-\frac{1}{|V|^2}\sum_{x,y}\mathrm{Cov}[\nu_x,\nu_y]\\
&\quad +\frac{1}{|V|}\sum_{x\in V}\mathbb{E}[\nu_x]^2-\left(\frac{1}{|V|}\sum_x\mathbb{E}[\nu_x]\right)^2\ .
\end{aligned}$$

Obviously, if $\mathbb{E}[\nu_x]$ is independent of x we have $\frac{1}{|V|}\sum_x\mathbb{E}[\nu_x]^2-\left(\frac{1}{|V|}\sum_x\mathbb{E}[\nu_x]\right)^2=0$. □

Remark 7. The study of neutrality in the general case, however, requires to determine the distribution of

$$\delta(x,x'):=\sum_{i:\,\vartheta_i(x)\neq\vartheta_i(x')}c_i\,[\vartheta_i(x)-\vartheta_i(x')] \tag{5.12}$$

Since in an additive landscape the c_i are independent by definition, we have to compute the convolution

$$g_{x,x'}(\delta) = \mathop{\star}_{i:\vartheta_i(x)\neq\vartheta_i(x')} \rho_i\big(c_i/[\vartheta_i(x)-\vartheta_i(x')]\big) \tag{5.13}$$

where $\star_j$ denotes convolution of all functions indexed by j, $g_{x,x'}(\delta)$ is the density of the values of $\delta(x,x')$, and $\rho_i(.)$ is the density functions of c_i, which in this case has to be evaluated for $c_i/[\vartheta_i(x) \neq \vartheta_i(x')$. Then we have

$$\mathrm{Prob}[X_{x'}(x)=1] = \lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} g_{x,x'}(\delta)d\delta\ .$$

If $\{i|\,\vartheta_i(x)\neq\vartheta_i(x')\}=\varnothing$, x and x' are neutral for any distribution of the c_i. This is observed for instance in the *graph matching problem* [49].

In practice, evaluation of the convolution (5.13) oftentimes boils down to a combinatorial exercise, as for instance in the case of the integer-valued NK model proposed by Newman and Engelhardt [36]. Finally we remark that $g(\,.\,)$ would also be the appropriate starting point for a theory of *nearly neutral landscapes* [37], in which the condition $|f(x)-f(x')|<\varepsilon$ for some finite $\varepsilon>0$ replaces the condition $f(x)=f(x')$.

In the following we consider a few prominent examples in some detail.

1. p-spin landscapes. Recall that the p-spin landscape is an arl generated by the maps $\vartheta_k(x)$ as defined in (3.3). Let now $x_i^{(k)}=x_i$ for $i\neq k$ and $x_k^{(k)}=-x_k$, then

$$X_k(x) = \begin{cases} 1 & \text{if } f(x)=f(x^{(k)}) \\ 0 & \text{otherwise.}\end{cases} \tag{5.14}$$

A short computation verifies that $X_k(x)=0$ if and only if

$$2x_k \sum_{\substack{i_2<i_3<\cdots<i_p\\ i_l\neq k}} c_{k,i_2,i_3,\ldots,i_p} x_{i_2}x_{i_3}\ldots x_{i_p} = 0\,,$$

i.e., if each of the coefficients $c_{k,i_2,i_3,\ldots,i_p}$, with $i_2<i_3<\cdots<i_p$ and $i_l\neq k$, $l=2,\ldots,p$ vanished. Thus $X_k(x)$ is independent of $x\in V$ and we can write ν instead of ν_x.

Proposition 3. *For a p-spin model, where the coefficients c_i fulfill (5.1) the following assertions hold:*

$$\mathbb{E}[\nu] = n\,\mu_0^{\binom{n-1}{p-1}} \tag{5.15}$$

$$\mathbb{V}[\nu] = n(n-1)\mu_0^{2\binom{n-1}{p-1}}\left[\mu_0^{-\binom{n-2}{p-2}}-1\right] + n\,\mu_0^{\binom{n-1}{p-1}}\left[1-\mu_0^{\binom{n-1}{p-1}}\right] \tag{5.16}$$

$$\Xi = 0\,. \tag{5.17}$$

Proof. By linearity of expectation we obtain $\mathbb{E}[\nu] = \sum_{k=1}^{n}\mathbb{E}[X_k]$. Now, exactly $\binom{n-1}{p-1}$ p-sets do not contain a given element k and we immediately obtain in view of (5.2) $\mathbb{E}[X_k] = \mu_0^{\binom{n-1}{p-1}}$. To prove the second assertion we compute $\mathbb{V}[X_k] = \mu_0^{\binom{n-1}{p-1}}\left[1-\mu_0^{\binom{n-1}{p-1}}\right]$ and for $i \neq j$ $\mathbb{E}[X_iX_j] = \mu_0^{2\binom{n-1}{p-1}-\binom{n-2}{p-2}}$. The assertion follows from $\mathbb{V}\left[\sum_k X_k\right] = \sum_{i,j}\mathrm{Cov}[X_i, X_j]$ □

Remark 8. In the previous section we have seen that the p-spin models are elementary w.r.t. spin-flip moves. On the other hand, we may use μ_0 above 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 p-spin landscape and arl.

Remark 9. 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

$$\mu_0 = 1 - \frac{z}{n^{p-1}} \tag{5.18}$$

where $z > 0$ is a parameter determined by the connectivity of the lattice.

As an immediate consequence we have

Proposition 4. *A short range p-spin glass, $p \geq 2$, whose coefficients c_i fulfill (5.1) has a finite fraction of neutral mutations, i.e.,*

$$\lim_{n\to\infty}\mathbb{E}[\nu/n] = \mathrm{e}^{-z} \quad \text{and} \quad \lim_{n\to\infty}\mathbb{V}[\nu/n] = 0\,. \tag{5.19}$$

2. **NK-landscapes.** In Kauffman's original construction [30], we have a fixed, specific, mapping $\phi : \mathbb{N}_n \to \{(i_0, \dots, i_K)\}$ as defined in equ. (3.4). In case of *random* NK landscapes, the mapping ϕ is constructed as follows[1]: for given i one selects i itself and randomly K indices different from i and writes them as the ordered $K+1$-tuple $\phi(i) = (i_0, \dots, i_K)$.

Barnett considers in [6] the following version of the random NK model. Let $c_{(i,(y_{\phi(i)_0},\dots,y_{\phi(i)_K}))}$ be a random number such that for $\xi \neq 0$: $\mu\{c_{(i,(y_{\phi(i)_0},\dots,y_{\phi(i)_K}))} = \xi\} = 0$ and $\mu\{c_{(i,(y_{\phi(i)_0},\dots,y_{\phi(i)_K}))} = 0\} = p > 0$. (We use p instead of μ_0 here in order to keep the notation consistent with ref. [6].)

Proposition 5. *Let ϕ be a fixed (3.4) and*

$$f_\phi(x) = \sum_{(r,,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))} c_{(r,,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))}\ \vartheta_{(r,,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))}(x)$$

an NK-landscape whose coefficients c_i fulfill (5.1). Then the following assertions hold

$$\begin{aligned}
\mathbb{E}[\nu_x] &= \sum_{i=1}^n \left[p^2\right]^{|\{r|r\in\phi(i)\}|} \\
\mathbb{V}[\nu_x] &= \sum_{i=1}^n \left[p^2\right]^{|\{r|r\in\phi(i)\}|} \left(1-\left[p^2\right]^{|\{r|r\in\phi(i)\}|}\right) \\
&\quad + \sum_{i\neq j} \left[p^2\right]^{|\{r|r\in\phi(i)\setminus\phi(j)\cup\phi(j)\setminus\phi(i)\}|} + \left[p^3\right]^{|\{r|r\in\phi(i)\cap\phi(j)\}|}
\end{aligned}$$

If ϕ is a random map and f_ϕ is an element of an NKp-landscape we have

$$\begin{aligned}
\mathbb{E}[\nu_y] &= n\, p^2\rho^{n-1} \\
\mathbb{V}[\nu_y] &= np^2\rho^{n-1}(1-p^2\rho^{n-1}) + n(n-1)\left[\left\{p^2\left(1-\eta(1-p)\right)\right\}^2\ \tau^{n-2} - (p^2\rho^{n-1})^2\right]
\end{aligned}$$

where $\eta = \frac{K}{n-1}$, $\rho = \left[1-\eta\,(1-p^2)\right]$ and $\tau = \left[(1-\eta)^2 + 2\eta(1-\eta)p^2 + \eta^2p^3\right]$.

Proof. Let X_i be the random variable that is defined in (5.14). By Lemma 3, $X_i = X_j = 1$ for arbitrary i, j implies that for all $(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))$ and $t \in \{i,j\}$

$$c_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))}\left\{\vartheta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))}(x) - \vartheta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))}(x^{(t)})\right\} = 0\ . \tag{5.20}$$

Since $\vartheta_{(i,(y_{\phi(i)_0},\dots,y_{\phi(i)_K}))}(x) = \frac{1}{n}\prod_{j=0}^K \delta(y_{\phi(i)_j}, x_{\phi(i)_j})$,

$$\left\{\vartheta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))}(x) - \vartheta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))}(x^{(t)})\right\} = 0,\ t\in\{i,j\} \quad\Longleftrightarrow\quad t\notin\phi(r)$$

[1] Note that there are *two* randomizations to distinguish, the first one is the random construction of ϕ and the second one is induced by the coefficients c_j of the arl.

holds. Let ϕ, as defined in equ. (3.4), be fixed. We set the LHS of (5.20) to be $\Delta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))}$ and immediately observe for $i \neq j$

$$\begin{array}{rcl} \forall\, r \notin \phi(i) \,\cup\, \phi(j); \quad \mu\{\Delta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))} = 0 \quad \forall\,(y_{\phi(r)_0},\dots,y_{\phi(r)_K})\} & = & 1 \\ \forall\, r \in \phi(i)\setminus\phi(j) \,\cup\, \phi(j)\setminus\phi(i);; \quad \mu\{\Delta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))} = 0 \quad \forall\,(y_{\phi(r)_0},\dots,y_{\phi(r)_K})\} & = & p^2 \\ \forall\, r \in \phi(j)\cap\phi(i); \quad \mu\{\Delta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))} = 0 \quad \forall\,(y_{\phi(r)_0},\dots,y_{\phi(r)_K})\} & = & p^3\ . \end{array}$$

Thus we have for fixed ϕ:

$$\begin{array}{rcl} \mathbb{E}[X_i] & = & \left[p^2\right]^{|\{r|r\in\phi(i)\}|} \\ \mathbb{V}[X_i] & = & \left[p^2\right]^{|\{r|r\in\phi(i)\}|}\ (1-\left[p^2\right]^{|\{r|r\in\phi(i)\}|}) \\ \forall\, i\neq j \quad \mathrm{Cov}[X_i,X_j] & = & \left[p^2\right]^{|\{r|r\in\phi(i)\setminus\phi(j)\cup\phi(j)\setminus\phi(i)\}|} + \left[p^3\right]^{|\{r|r\in\phi(i)\cap\phi(j)\}|} \end{array}$$

In particular, the above equations allow for the computation of $\mathbb{E}[\nu_y]$ and $\mathbb{V}[\nu_y]$ for the original Kaufmann-NK-landscape. Next we consider random NKp-landscapes. First, $\mathbb{E}[X_i]$ has already been computed in [5]. To compute $\mathbb{V}[\nu_y]$ we consider $\mathbb{E}[X_iX_j]$.
Claim.

$$\forall i\neq j; \quad \mathbb{E}[X_iX_j] = \left\{p^2\,(1-\eta(1-p)\ )\right\}^2\ \left\{(1-\eta)^2+2\eta(1-\eta)p^2+\eta^2p^3\right\}^{n-2}\ . \tag{5.21}$$

To prove the claim we first observe that $\mathbb{E}[X_iX_j] = \mu(\{X_i = 1\ \wedge\ X_j = 1\})$. Obviously, $\mu\{r \in \phi(i)\setminus\phi(j)\} = \mu\{r\in\phi(j)\setminus\phi(i)\} = \eta(1-\eta)$, $\mu\{r\in\phi(i)\cap\phi(j)\} = \eta^2$ and we derive

$$\forall\, r\neq i,j; \quad \mu\{\Delta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))} = 0 \quad \forall\,(y_{\phi(r)_0},\dots,y_{\phi(r)_K})\} = (1-\eta)^2+2\eta(1-\eta)p^2+\eta^2p^3\ .$$

Thus it remains to consider the case $r\in\{i,j\}$ in which we immediately obtain

$$\mu\{\Delta_{(r,(y_{\phi(r)_0},\dots,y_{\phi(r)_K}))} = 0 \quad \forall\,(y_{\phi(r)_0},\dots,y_{\phi(r)_K})\} = p^2\,((1-\eta)+\eta\ p\ )\ .$$

Now, $\mathbb{V}[\nu_y] = \mathbb{V}[\sum_i X_i] = \sum_i \mathbb{V}[X_i] + \sum_{i\neq j}\mathrm{Cov}[X_i,X_j]$ and we have

$$\begin{array}{rcl} \mathbb{V}[X_i] & = & \left\{p^2\left[1-\eta(1-p^2)\right]^{n-1}\right\}\left(1-\left\{p^2\left[1-\eta(1-p^2)\right]^{n-1}\right\}\right) \\ \mathrm{Cov}[X_i,X_j] & = & \left\{p^2\,(1-\eta(1-p)\ )\right\}^2\ \left\{(1-\eta)^2+2\eta(1-\eta)p^2+\eta^2p^3\right\}^{n-2} - (p^2\rho^{n-1})^2\ . \end{array}$$

□

3. Graph bipartitioning landscapes. The natural graph structure underlying the GBP-arl is the Johnson graph $\mathcal{J}(n,n/2)$, see e.g. [52]. Two vertices $\xi = [A,B]$ and $\xi' = [A',B']$ are adjacent

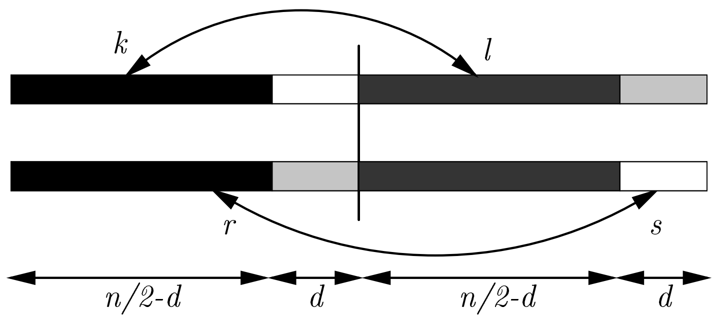

FIGURE 3. The vertices of a graph can be sorted in such a way that on each side of the bipartition, we have first the vertices are in common to two different configurations, and then the vertices in which they differ. Two different mutations, $[kl]$ and $[rs]$ are indicated by arrows.

if they differ by the exchange of a pair (k,l), $k \in A$, $l \in B$. The metric induced by this adjacency relation is given by

$$d(\xi,\xi') = \frac{n}{2} - |A \cap A'| = \frac{n}{2} - |B \cap B'| \,. \tag{5.22}$$

The parameter μ_0 described the connectivity of the graph Γ that is partitioned. It plays an important role in the statistical mechanics of this combinatorial optimization problem, see e.g., [4, 15, 33].

Proposition 6. *Let $\mathcal{F}$ be an GBP-arl whose coefficients c_i fulfill (5.1) then*

$$\begin{aligned}
\mathbb{E}[\nu_\xi] &= \frac{n^2}{4}\mu_0^{2n-4} \\
\mathbb{V}[\nu_\xi] &= \frac{n^2}{4}\mathbb{E}[\nu_y]\left[1-\mu_0^{2n-4}+(n-2)\mu_0^{n-2}(1-\mu_0^{n-2})+\frac{n^2-4(n-1)}{4}\mu_0^{2n}(1-\mu_0^4)\right] \\
\mathrm{Cov}[\nu_\xi,\nu_{\xi'}] &= \mu_0^{4n-8}\left[a_n(d)(\mu_0^{-4}-1)+b_n(d)(\mu_0^{-(n-2)}-1)+c_n(d)(\mu_0^{-(2n-4)}-1)\right]
\end{aligned}$$

where

$$c_n(d) = n^2/4 - nd + 2d^2\,, \qquad b_n(d) = n^2(n-2)/4 + 4(n/2-d)d\,, \qquad a_n(d) = n^4/16 - b_n(d) - c_n(d)\,.$$

Proof. In order to prove the first assertion let $\xi,\xi' \in V$ be adjacent w.r.t. the exchange (k,l). We observe $c_\xi(\xi') = 2n-4$. The assertion follows now from Theorem 1.

Let $\xi \in V$ and $\xi', \xi'' \in S_1(\xi)$ where ξ' and ξ'' differ from ξ by the exchange of (k,r) and (l,s), respectively. A tedious but straightforward calculation verifies that

$$w_\xi(\xi', \xi'') = \big|\{j \mid \vartheta_j(\xi) = \vartheta_j(\xi') = \vartheta_j(\xi'') = 1\}\big|$$

depends exclusively on $|\{k,l\} \cap \{r,s\}|$. Explicitly,

$$w_\xi(\xi', \xi'') = \begin{cases} 4 & \text{if} \quad |\{k,l\} \cap \{r,s\}| = 0 \\ n-2 & \text{if} \quad |\{k,l\} \cap \{r,s\}| = 1 \\ 2n-4 & \text{if} \quad |\{k,l\} \cap \{r,s\}| = 2 \ . \end{cases} \tag{5.23}$$

Now the second assertion follows directly from

$$\mathrm{Cov}[X_{\{\xi,\xi'\}} X_{\{\xi,\xi''\}}] = \mu_0^{2(2n-4)} \left(\mu_0^{-w_\xi(\xi',\xi'')} - 1\right) \ .$$

Finally, we have to compute

$$\mathrm{Cov}[\nu_\xi, \nu_{\xi'}] = \sum_{(k,l)} \sum_{(r,s)} \mathrm{Cov}[X_{\{\xi,\xi_{(kl)}\}}, X_{\{\xi',\xi'_{(rs)}\}}]$$

where $\xi_{(kl)}$ is the neighbor of ξ that is obtained by applying the exchange (k,l). The sums above run over all neighbors of ξ and ξ', resp. We find

$$\mathrm{Cov}[X_{\{\xi,\xi_{(kl)}\}}, X_{\{\xi',\xi'_{(rs)}\}}] = \mu_0^{2(2n-4)} \left(\mu_0^{-w_{\xi,\xi'}(\xi_{(kl)},\xi'_{(rs)})} - 1\right)$$

where $w_{\xi,\xi'}(\xi_{(kl)}$ depends only on $|\{k,l\} \cap \{r,s\}|$ but not on the distance between ξ and ξ', whence $w_{\xi,\xi'}(\xi_{(kl)}$ is given by equ.(5.23). Evaluating the sums therefore reduces to a straightforward (but tedious) combinatorial exercise: As explained in Figure 5 we write $\xi = [A \cup B | A' \cup B']$ and $\xi' = [A \cup B' | A' \cup B]$, where $d(\xi, \xi') = |B| = |B'|$. We have to distinguish four cases for the exchange (k,l), namely (i) $k \in A \wedge\ l \in A'$; (ii) $k \in A \wedge\ l \in B'$; (iii) $k \in B \wedge\ l \in A'$; (iv) $k \in B \wedge\ l \in B'$. Analogously, there are four cases to be considered for the (r,s). For each of the resulting 16 sub-cases, we determine the number of combinations of indices with $|\{k,l\} \cap \{r,s\}| = 0$, 1, or 2, respectively. For example, case (i.i), $k \in A \wedge\ l \in A'$ and $r \in A \wedge\ s \in A'$ consists of a total of $(n/2-d)^4$ index combinations. Of these $(n/2-d)^2$ are of the form $|\{k,l\} \cap \{r,s\}| = 2$, $2(n/2-d)^2(n/2-d-1)$ have one common index, and $(n/2-d)^2(n/2-d-1)^2$ index pairs have only distinct indices. The other 15 cases are treated analogously. □

Remark 10. Suppose $\mu = 1 - \rho/n$, then we have

$$\lim_{n\to\infty} \frac{4}{n^2} \mathbb{E}[\nu_x] = e^{-2\rho} \ . \tag{5.24}$$

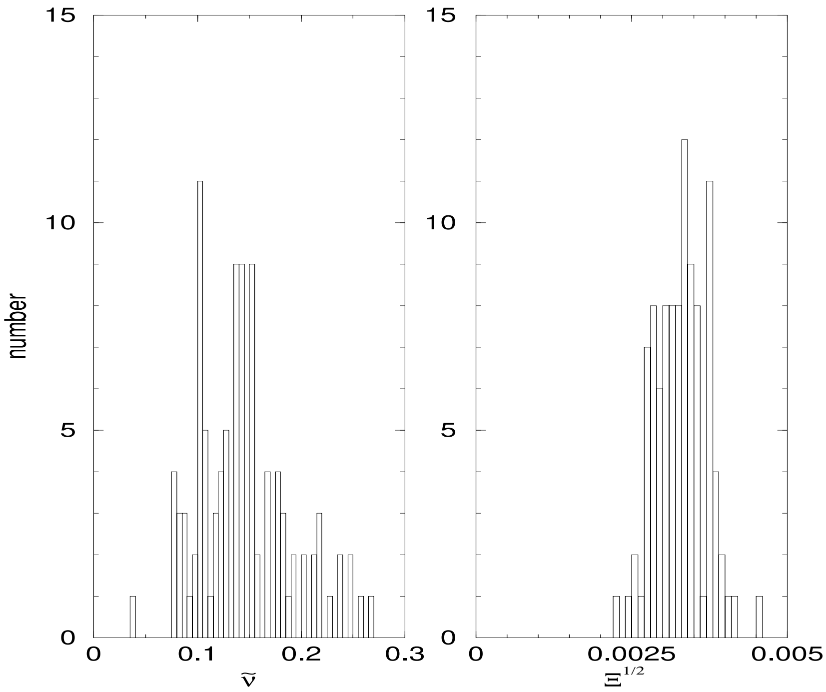

FIGURE 4. Distribution of the fraction of neutral neighbors, $\tilde{\nu}_\xi = \nu_\xi/(n^2/4)$, for GBP landscapes with $n = 100$ and $\mu_0 = 0.99$, LHS. Note the rather large variance (standard deviation $\sigma \approx 0.047$) across independently generated instances. For comparison, the variation of ν_ξ a cross a single landscape is very small, $\sqrt{\Xi} \approx 0.003$, RHS.

In particular for $\mu = 1 - z \log n/n$, $z > 0$ we find $\lim_{n\to\infty} \mathbb{E}[\nu_x] = \frac{n^2}{4}\ e^{-2\,z}$, while for $\mu = 1 - z \log n/n$ $\lim_{n\to\infty} \mathbb{E}[\nu_x] = \frac{1}{4} n^{2\,(1-z)}$ holds.

4. **TSP with reversals.** In order to introduce neutrality into a symmetric TSP, eqns.(3.6) and (3.8), we assume that there is special value of the road length, say $d_{ij} = 1$, such that $\boldsymbol{\mu}(d_{ij} = 1) = \mu_0$, while $\boldsymbol{\mu}(d_{ij} = \xi) = 0$ for all $\xi \neq 1$.

TABLE 1. Values of $w(\rho, \rho')$ for the TSP with reversals

l=	k= i-1	i	i+1	other
j-1	2	2	2	1
j	2	(4)	1	1
j+1	2	1	0	0
other	1	1	0	0

The difference of the lengths of two tours is given by the length of the roads that are not common between two tours. For *reversals* (2opt moves) we immediately compute

$$(5.25)\quad X_{[ij]}(\pi) = \begin{cases} 1 & \text{iff} \quad d_{\pi(i-1),\pi(j)} = 1 \wedge d_{\pi(i-1),\pi(i)} = 1 \wedge d_{\pi(i),\pi(j+1)} = 1 \wedge d_{\pi(j),\pi(j+1)} = 1 \\ 0 & \qquad\qquad\qquad\qquad \text{otherwise.} \end{cases}$$

Proposition 7. *For the TSP-arl whose coefficients c_i fulfill (5.1) the following assertions hold:*

$$\begin{aligned} \mathbb{E}[\nu_\pi] &= \binom{n}{2}\mu_0^4 \\ \mathbb{V}[X_{[ij]}(\pi)X_{[kl]}(\pi)] &= \mu_0^8(\mu_0^{-w([ij],[kl])} - 1) \end{aligned}$$

where $w([ij],[kl])$ are listed in Table 1. Further we have

$$(5.26)\qquad \frac{4}{n^2(n-1)^2}\mathbb{V}[\nu_\pi] = \mathcal{O}(n^{-1})\mu_0^8(\mu_0^{-1} - 1) + \mathcal{O}(n^{-2})\mu_0^8(\mu_0^{-2} - 1) + \mathcal{O}(n^{-2})\mu_0^8(\mu_0^{-2} - 1)\ .$$

Proof. The first assertion follows immediately from linearity of expectation and equ.(5.25). In order to compute $\mathbb{V}[\nu_\pi]$ we write

$$(5.27)\qquad \frac{4}{n^2(n-1)^2}\mathbb{V}[\nu_\pi] = \sum_{[ij],[kl]} \mathbb{V}[X_{[ij]}(\pi)X_{[kl]}(\pi)]\ .$$

A close inspection of the co-variations listed in table 1 shows that there are $\mathcal{O}(n^3)$ pairs $([ij],[kl])$ with $w = 1$, $\mathcal{O}(n^2)$ pairs $([ij],[kl])$ with $w = 2$, and, of course, the $\binom{n}{2}$ diagonal terms with $w = 4$. Thus equ.(5.26) follows. □

Remark 11. The situation is more complicated for the seemingly simpler Cayley graph that arises from using the transpositions as move set. In general we have

$$\begin{aligned} \delta_{(ij)}(\pi) &= d_{\pi(j),\pi(i-1)} + d_{\pi(i+1),\pi(j)} + d_{\pi(i),\pi(j-1)} + d_{\pi(j+1),\pi(i)} \\ &- d_{\pi(i),\pi(i-1)} - d_{\pi(i+1),\pi(i)} - d_{\pi(j),\pi(j-1)} - d_{\pi(j+1),\pi(j)}\ . \end{aligned}$$

However, if the transposition is canonical, i.e., if $i = j \pm 1$, four of the terms in the above equation cancel and we are left with

$$\delta_{(i,i+1)}(\pi) = d_{\pi(i+1),\pi(i-1)} + d_{\pi(i+2),\pi(i)} - d_{\pi(i),\pi(i-1)} - d_{\pi(i+2),\pi(i+1)} \ .$$

Hence we have $\mathbb{E}[\nu(\pi)] = \sum_\tau \mathbb{E}[X_\tau(\pi)]$ and $\mathbb{E}[X_\tau(\pi)] = \mu_0^4$ if τ is one of the n canonical transpositions and $\mathbb{E}[X_\tau(\pi)] = \mu_0^8$ if τ is one of the $\binom{n}{2} - n$ other transpositions. A short computation now verifies

$$\mathbb{E}[\nu(\pi)] = \binom{n}{2}\left[\mu_0^8 + \frac{2}{n-2}(\mu_0^4 - \mu_0^8)\right] \ . \tag{5.28}$$

This example shows that a detailed analysis of the TSP landscape with transpositions will be a rather tedious enterprise; indeed, $\mathbb{E}[X_{(pq)}(\pi)X_{(rs)}(\pi)]$ depends explicitly on whether (pq), (rs), or both are canonical, and on the differences between all the indices. It is not hard to verify, however, that $\mathbb{E}[X_{(pq)}(\pi)X_{(rs)}(\pi)] = \mathbb{E}[X_{(pq)}]\mathbb{E}[X_{(rs)}]$ if differences between any two of the indices p, q, r, s are sufficiently large. Thus only $\mathcal{O}(n^3)$ out of $\mathcal{O}(n^4)$ pairs of transpositions will have exchanged edges in common. In other words, only a minority of size $\mathcal{O}(1/n)$ of the pairs of transpositions will be correlated.

6. Neutral Walks

Neutral walks 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 [45, 21, 22]. Formally, neutral walks are defined in algorithm 1. In a nutshell, in each step we attempt to find a neutral neighbor such that the distance from the starting point increases. Therefore neutral walks terminate at latest after $\mathrm{diam}(Y)$ steps.

Consider a pair of vertices $x, y \in V$ with $d(x, y) = d$. For each neighbor of y we have of course $d(x, y) - 1 \leq d(x, z) \leq d(x, y) + 1$.

Let us now restrict ourselves to distance transitive graphs (such as hypercubes or the Johnson graphs). In this case, the number $\alpha(d)$ of "forward steps" is independent of the choice of x, y with prescribed distance $d(x, y) = d$.

algorithm 1 Neutral Walk

Input: landscape

$x_0 \leftarrow$ random configuration;
$\mathsf{walk} \leftarrow x_0$; $\quad d \leftarrow 0$; $\quad \xi \leftarrow \mathsf{neutral\_neigbors}(x_0)$;
while $\xi \neq \emptyset$ **do**
  randomize the order of the list ξ;
  search for a $y \in \xi$ such that $d(x_0, y) > d$;
  if found y **then**
    append y to walk; $\quad \xi \leftarrow \mathsf{neutral\_neigbors}(y)$; $\quad d \leftarrow d(x_0, y)$;
  else
    $\xi \leftarrow \emptyset$;
return walk;

Let $\tilde{\nu}$ denote the probability that two adjacent vertices are neutral. Assuming furthermore, that the probabilities that any two edges connect neutral neighbors are independent (this is the assumption of the random graph model described in [43]) we obtain $(1-\tilde{\nu})^{\alpha(d)}$ for the probability that a neutral walk with d steps cannot be elongated any further. Hence $1-(1-\tilde{\nu})^{\alpha(d)}$ is the probability that we can make a further step. The probability that a neutral walk on a distance transitive graph terminates after exactly d steps is:

$$\mathrm{Prob}[\mathcal{L} = d] = (1-\tilde{\nu})^{\alpha(d)} \times \prod_{d'=1}^{d} \left[1-(1-\tilde{\nu})^{\alpha(d'-1)}\right] \ . \tag{6.1}$$

This can be recast as a recursion which can be used to numerically compute the length of a neutral walk.

Note that the above independence assumption is not strictly valid for any of the models discussed in this paper. While the correlations between two edges are small in general, $\mathcal{O}(1/n)$, or only a small number of edge pairs is strongly correlated, these weak correlations add up along a neutral walk and cause the large deviations between the values of $\mathcal{L}$ as obtained from simulations with the algorithm 1, and from the analytical estimate (6.1).

These deviations can be understood easily in the case of spin glasses. In this case the random variables $X_k(x)$ are independent of x, i.e., flipping a particular spin is neutral independent of the actual values of all other bits. As an immediate consequence, the neutral network containing $x \in V$ is the entire sub-hypercube spanned by the spins for which $X_k(x) = 1$. Consequently, the length

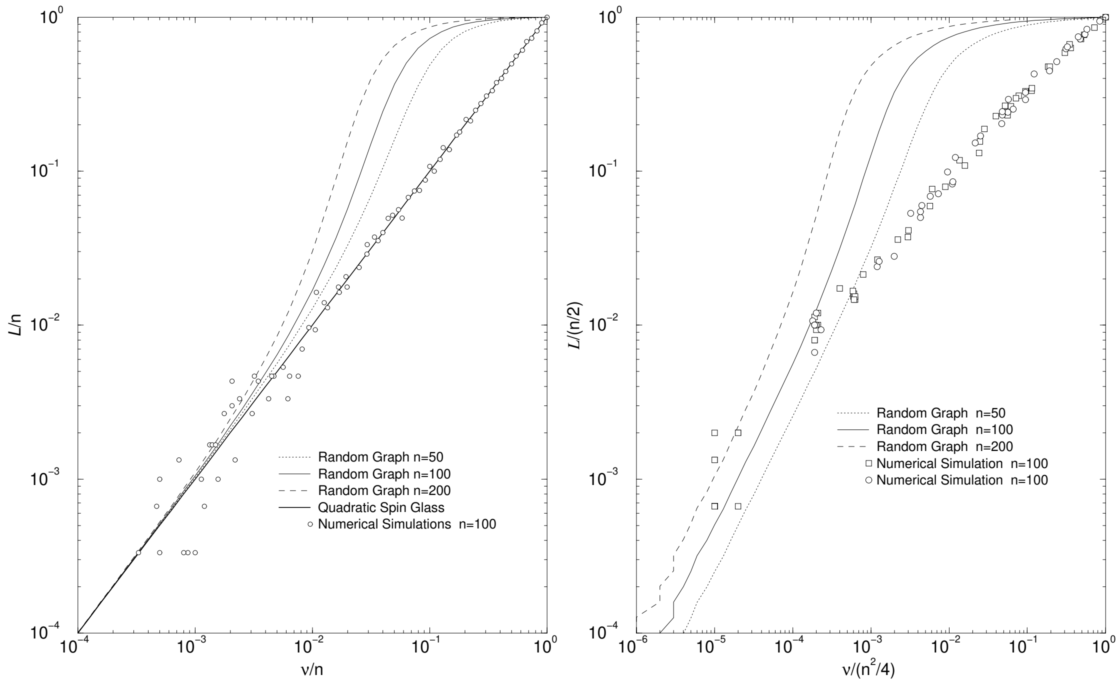

FIGURE 5. The accumulation of correlations causes large deviation of the average length $\mathcal{L}$ of neutral walks compared to what would be expected from an uncorrelated random graph model. L.h.s.: quadratic spin glass model ($p = 2$). R.h.s.: graph bipartitioning.

of a neutral walk is

$$\mathcal{L} = \left|\{k|X_k(x) = 1\}\right| \tag{6.2}$$

for the spin glass models described in Section 5.2, i.e., $\mathbb{E}[\mathcal{L}] = \mathbb{E}[\nu_x]$. The prediction of the uncorrelated model (6.1) and data from numerical simulations for the quadratic spin glass model and graph bipartitioning are shown in Figure 6.

We have seen that additive random landscapes provide a useful framework for constructing models of landscapes in which both ruggedness and neutrality are tunable. Not surprisingly, the best known examples of landscapes in spin glass physics and combinatorial optimization are of this type. While a desired degree of ruggedness can be obtained by choosing the "generating functions" ϑ_j, neutrality can introduced into the model by selecting the distribution(s) of the random coefficients c_i. We find that neutrality is linked to the discrete part of these distrbutions: As long as the random variables c_i have "smooth" densities, we cannot expect neutral neighbors unless symmetries of the "generating functions" ϑ_j cause their existence independent of the coefficients c_i.

We have restricted ourselves to the simplest cases here: The discrete part of the distribution of the c_i's consists of a single special value occurring with finite probability μ_0. Structural properties of the corresponding neutral networks (subgraphs with constant values of f) differ significantly from random subgraphs obtained by independent vertex selections with probability $\mathbb{E}[\nu_x]/\delta_x$ (δ_x being the vertex degree) [39]: neutral networks of additive random landscapes are more "localized" whence neutral walks are shorter than those in random graphs.

We finally remark that it is of some importance to obtain a detailed analysis of the neutral networks that arise from additive random landscapes. As in the case of folding landscapes of RNA secondary structures, where important features like connectivity and density could be studied by random induced subgraphs of generalized n-cubes, the structure of neutral networks of arl landscapes has yet to be explored. Further one might ask whether there exists a simple construction for a p-spin type landscape that satisfies the independence requirements of the random graph model. Since neutrality is a property that is derived from the distribution of the coefficients c_i, is seems natural to search for a classification of (uniform) additive random fields in terms of these distributions.

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