# Random Field Models For Fitness Landscapes

Peter F. Stadler[a,b,*] and Robert Happel[a]

[a]Theoretische Biochemie, Institut für Theoretische Chemie
Universität Wien, Vienna, Austria

[b]Santa Fe Institute, Santa Fe, NM

[*]Mailing Address:
Peter F Stadler, Inst. f. Theoretische Chemie, Univ. Wien
Währingerstr. 17, A-1090 Wien, Austria
Phone: [43] 1 40480 665 Fax: [43] 1 40480 660
E-Mail: studla@tbi.univie.ac.at

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**Abstract**

In many cases fitness landscapes are obtained as particular instances of random fields by assigning a large number of random parameters. Models of this type are often characterized reasonably well by their covariance matrices. We characterize isotropic random fields on finite graphs in terms of their Fourier series expansions and investigate the relation between the covariance matrix of the random field model and the correlation structure of the individual landscapes constructed from this random field. Our formalism suggests to approximate landscape with known autocorrelation function by a random field model that has the same correlation structure.

# 1. Introduction

Since Sewall Wright's seminal paper [1] the notion of a *fitness landscape* underlying the dynamics of evolutionary optimization has proved to be one of the most powerful concepts in evolutionary theory. However, detailed information about biological fitness landscapes is hard to gain. In general one simply lacks a theoretical model. Even in the few cases where a computational model is available, as in the case of RNA fitness landscapes [2, 3, 4, 5], the actual evaluation of the fitness function is quite costly in terms of computational resources.

Therefore, computer simulations of evolutionary optimization often make use of landscape models borrowed from statistical mechanics, e.g., spin glasses [6], or combinatorial optimization problems, e.g., the traveling salesman problem TSP [7]. The choice of these models is rather arbitrary: in most cases there is no guarantee that they will capture even the most basic properties of the biological system that they are supposed to model.

In this contribution we shall be concerned with computing properties of random field models that can be compared with the structure of a computational model of an actual biological fitness landscape. To this end we shall focus on correlation measures. There are two good reasons for this: firstly, correlation measures can be obtained fairly easily from computational models (in fact, even determining them experimentally does not seem to be an entirely hopeless task [8]). Secondly, correlation measures are known to be closely related to the "ruggedness" of the landscape and to the performance of simple optimization heuristics [9, 10, 11, 12].

In addition, characterizing landscapes by the first few statistical moments seems to be a natural approach from a purely mathematical point of view.

The role of ridges and plateaus for the velocity of adaptation is well known in the literature [13, 14, 15]. Such special structures form outstanding landmarks in a landscapes, but they are not likely to occur in an "isotropic" landscape model. Isotropy is an inherently statistical notion. We shall therefore consider isotropy in the context of a random field rather than a single landscape. In [16], on the other hand, a measure for the anisotropies within an individual landscape was considered. One of the main topics of this contribution is the characterization of the isotropic random fields. Quite a number of different models have been investigated in some detail in the last few years. Most of them are isotropic, or at least close to being isotropic; among those are a number of well known combinatorial optimization problems, such as the Traveling Salesman Problem, the Graph Bipartitioning Problem, or the Graph Matching Problem `GMP` [11, 17, 18]. The distribution of local optima and the statistical characteristics of down-hill walks have been computed for the uncorrelated landscape of the random energy model [19, 20, 21]. Furthermore, two one-parameter families of tunably rugged landscapes have been studied extensively: the Nk model and its variants [22, 23, 24, 25], and the $p$-spin models [6, 26]. In general these models are computationally easy. They involve a large number of parameters (coupling constants in the spin glass models, or distances between the cities in the TSP) that are in general assigned using some statistical model. We will refer to such models as *random fields*. In contrast, we shall call the particular instances "*landscapes*".

This contribution is organized as follows: In section 2 we give a formal definition of landscapes and random fields. Series expansions of random fields, in particular Fourier series and Karhunen-Loève series are discussed in section 3. In section 4 we discuss partitions of the set $V \times V$ of all pairs of configurations. These partitions and their algebraic properties form the mathematical foundation of this paper. In section 5 we shall give a characterization of isotropy in terms of the Fourier expansion, and we will prove conditions under which Fourier series and Karhunen-Loève series coincide. In section 6 we define a covariance measure with respect to a given partition and investigate their algebraic properties. Our results suggest a canonical procedure for approximating a given random field as a superposition of so-called elementary random fields. The individual instance of the latter are (up to an additive constant) eigenvectors of a suitable graph Laplacian; they are described in some detail in section 7. A few applications of our formalism to important random fields are described in section 8. The discussion section 9 concludes this paper.

## 2. Landscapes and Random Fields

Two features are common to all landscapes:

(1) A *cost function* or *fitness function* $f$ assigns a value to each *configuration*,

$$f : V \to \mathbb{R},$$

e.g, an energy to each spin configuration, a fitness value to each RNA sequence, a length to each tour in a traveling salesman problem.

(2) There is a rule that determines whether two configurations $x$ and $y$ are nearest neighbors. This rule describes the elementary moves in an optimization heuristic and the elementary mutations in molecular evolution.

As a consequence of property (2), the set $V$ of all configurations can be viewed as a graph with each vertex corresponding to a configuration and an edge between any two nearest neighbors; the set of edges will be denoted by $E$. Therefore, there is a natural metric distance $d(x, y)$ between any two configurations $x, y \in V$ given by the shortest path in the graph $\Gamma$ that connects $x$ with $V$.

Many of the model landscapes mentioned in the introduction contain a stochastic element: a particular instance is generated by assigning a usually large number of parameters at random. An important example is the Sherrington-Kirkpatrick Hamiltonian [27]

$$\mathcal{H}_{SK}(x) \stackrel{\text{def}}{=} \sum_{i<j} J_{ij} x_i x_j$$

where $x = (x_1, \ldots, x_n)$ denotes a configurations of spins $x_i = \pm 1$, and the "coupling constants" are i.i.d. Gaussian random variables with mean 0 and variance 1. We shall return to this particular model and its relatives later on. We shall restrict the use of the term *landscape* to mappings $f : V \to \mathbb{R}$, while a model such as the SK spin glass will be referred to a *random field.* Instead of referring explicitly to random parameters we shall use the following more general

**Definition.** The set $\{f : V \to \mathbb{R}\}$ together with a measure $\boldsymbol{\mu}\{f\}$ forms the probability space $\Xi$, which we will call a *random field* on $\Gamma$ [28].

An element (a realization, an instance) of a random field on $\Gamma$ is a landscape. Conversely, a random field can be considered as the set of all possible landscapes on a given configuration space *together with a measure.* This measure $\boldsymbol{\mu}$ can be recast in the form $P(c_1, c_2, \ldots, c_{|V|})$ which is the probability that for all configurations $x_i \in V$ holds simultaneously $f(x_i) < c_i$, where $c_i \in \mathbb{R}$, and $|V|$ denotes the total number of configurations.

The *expected value* of a random variable $X$ defined on the random field is given by $\int X\, d\boldsymbol{\mu}$, which takes the form

$$\mathcal{E}[X] \stackrel{\text{def}}{=} \int_{\mathbb{R}^{|V|}} X \, \mathrm{d}P(c_1, \ldots, c_N) \,.$$

It will be convenient to use $\mathrm{Var}[f(x)] \stackrel{\text{def}}{=} \mathcal{E}[f(x)^2] - \mathcal{E}[f(x)]^2$ for the variance of the random field evaluated at a constant position $x \in V$.

The distinction between a random field $\Xi$ and an individual landscape $f$ drawn from $\Xi$ is important as the following degenerated example shows: Consider a Gaussian random field with $\mathcal{E}[f(x)] = 0$ for all $x$ and $\mathcal{E}[f(x)f(y)] = 1$ for all $x$ and $y$. A sample function drawn from this random field is almost always constant since the correlation of any two points is 1. The constant value value of this flat landscape, however, is drawn from a Gaussian distribution with mean zero and unit variance. In fact: $\mathrm{Var}[f(x)] = 1$ for all $x \in V$.

## 3. Series Expansions

Let $\{\phi_k\}$ denote an orthonormal basis of $\{f : V \to \mathbb{R}\}$. We can represent $\Xi$ as

$$f(x) \doteq \sum_k u_k \phi_k(x),$$

where the notation $\doteq$ emphasizes that the expansion is valid only in mean square sense. In this section we shall be concerned with finding basis functions for the corresponding series expansion has particularly desirable mathematical properties.

The common algebraic representation of a graph $\Gamma(V, E)$ is its adjacency matrix $\mathbf{A}$ which has the entries

$$\mathbf{A}_{xy} \stackrel{\text{def}}{=} \begin{cases} 1 & \text{if } \{x, y\} \in E \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

The number of neighbors of vertex $x \in V$ is called the *degree* of $x$. Let $\mathbf{D}$ be the diagonal matrix of the vertex degrees. A graph is $D$-regular if all its vertices have the same number $D$ of neighbors. In this case we have $\mathbf{D} = D\mathbf{I}$, where $\mathbf{I}$ is the identity matrix. Instead of using the adjacency matrix $\mathbf{A}$, it is often convenient to characterize a graph $\Gamma$ by its *Laplacian* matrix

$$-\Delta \stackrel{\text{def}}{=} \mathbf{D} - \mathbf{A}. \tag{2}$$

For regular graphs this definition simplifies to $\Delta = \mathbf{A} - D\mathbf{I}$. The matrix $\Delta$ can be viewed as a generalization of the more familiar differential operator $\Delta$ in continuous spaces. For the details we refer to [29, 30, 31, 32]. The graph Laplacian $-\Delta$ is non-negative definite, and the smallest eigenvalue $\lambda_0 = 0$ has multiplicity 1 if and only if $\Gamma$ is a connected graph. The corresponding eigenvector is $\mathbf{1} = (1, 1, \ldots, 1)$. In what follows we will assume that $\Gamma$ is a connected $D$-regular graph.

A series expansion in terms of a complete and orthonormal system of eigenfunctions of the Laplace operator is commonly termed a Fourier expansion. Following [33], we will adopt the same terminology here. Thus, let $f$ be a landscape on $\Gamma$ and let $\{\varphi_i\}$ denote a complete orthonormal set of eigenvectors of the graph

Laplacian. Then we call the expansion $f(x) = \sum_{i=0}^{|V|-1} a_i\varphi_i(x)$ *Fourier expansion* of the landscape $f$, [34]. It seems natural to generalize this construction to random fields on $V$; thus we call an expansion of the form

$$f(x) \doteq \sum_{i=0}^{|V|-1} a_i\varphi_i(x) \tag{3}$$

*Fourier series* of the random field $\Xi$. Note that the coefficients $a_i$ are now random variables with a distribution determined by $\Xi$.

The covariance matrix $\mathbf{C}$ of the random field $\Xi$ is defined component wise by

$$\mathbf{C}_{xy} \stackrel{\text{def}}{=} \mathrm{Cov}[f(x), f(y)] = \mathcal{E}[f(x)f(y)] - \mathcal{E}[f(x)]\mathcal{E}[f(y)] \tag{4}$$

The matrix $\mathbf{C}$ is symmetric and non-negative definite. Substituting the expansion w.r.t. an arbitrary orthonormal basis $\{\phi_k\}$ of $\{f : V \to \mathbb{R}\}$ into the definition of the covariance matrix yields after a short computation

$$\mathbf{C}_{xy} = \sum_{i,j} \mathrm{Cov}[u_i, u_j]\phi_i(x)\phi_j(y)\,, \tag{5}$$

where the covariance of the coefficients is $\mathrm{Cov}[u_i, u_j] \stackrel{\text{def}}{=} \mathcal{E}[u_i u_j] - \mathcal{E}[u_i]\mathcal{E}[u_j]$. In particular, an expression of this form exists for the Fourier expansion of $\Xi$.

The second important orthonormal basis of $\{f : V \to \mathbb{R}\}$ consists of the eigenvectors $\psi_k$ of the covariance matrix $\mathbf{C}$ itself. We will call an expansion of the form

$$f(x) \doteq \sum_k b_k\psi_k(x) \tag{6}$$

*Karhunen-Loève series* of the random field $\Xi$. Let $\Lambda_k$ denote the eigenvalue of $\mathbf{C}$ belonging to the eigenvector $\psi_k$. Hotelling [35] showed that

$$\mathrm{Cov}[b_k, b_j] = \Lambda_k\delta_{kj}\,, \tag{7}$$

i.e., the coefficients of the expansion are uncorrelated random variables. Furthermore, $\mathrm{Var}[b_k] = \mathrm{Cov}[b_k, b_k] = \Lambda_k$ is the corresponding eigenvalue. Since $|V|$ is finite, the Karhunen-Loève expansion coincides with Hotelling's principal component analysis.

In the following section 5 we shall be concerned amongst other topics with finding conditions under which Fourier expansion and Karhunen-Loève expansion coincide. It is not surprising that this question is closely related to the symmetry properties of the covariance matrix $\mathbf{C}$.

## 4. Partitions of $V \times V$

The covariance matrix $\mathbf{C}$ can be regarded as a mapping $\mathbf{C}: V \times V \to \mathbb{R}$. It seems natural to consider partitions $\mathfrak{R}$ of $V \times V$ such that $\mathbf{C}$ is constant on the classes. We shall find that the most interesting mathematical results are tightly linked to the algebraic properties of such a partition.

Let $\mathcal{I} \stackrel{\text{def}}{=} \{(x,x)|x \in V\}$ and $\mathcal{A} \stackrel{\text{def}}{=} \{\,(x,y)\,|\,\{x,y\} \in E\,\}$ denote the "diagonal" and set of pairs of vertices that are adjacent in $\Gamma$, respectively. For any class $\mathcal{X} \in \mathfrak{R}$ one defines the transpose as $\mathcal{X}^+ \stackrel{\text{def}}{=} \{(y,x)|(x,y) \in \mathcal{X}\}$. To each class $\mathcal{X} \in \mathfrak{R}$ there is an associated matrix $\mathbf{X}$ with entries

$$\mathbf{X}_{xy} \stackrel{\text{def}}{=} \begin{cases} 1 & \text{if } (x,y) \in \mathcal{X} \\ 0 & \text{otherwisel,} \end{cases} \tag{8}$$

which we call the *characteristic matrix* of the class $\mathcal{X}$. Not surprisingly, a useful theory does not arise by considering arbitrary partitions $\mathfrak{R}$. It will be necessary to impose certain regularity conditions. We found that the following properties are of particular importance:

(i) $\mathcal{X} \cap \mathcal{I} \neq \emptyset \implies \mathcal{X} \subseteq \mathcal{I}$ for any $\mathcal{X} \in \mathfrak{R}$.

(ii) $\mathcal{X} \cap \mathcal{A} \neq \emptyset \implies \mathcal{X} \subseteq \mathcal{A}$ for any $\mathcal{X} \in \mathfrak{R}$.

(iii) $\mathcal{I} \in \mathfrak{R}$.

(iv) $\mathcal{X} \in \mathfrak{R} \implies \mathcal{X}^+ \in \mathfrak{R}$.

(v) $\mathcal{X} = \mathcal{X}^+$ for all $\mathcal{X} \in \mathfrak{R}$.

(vi) $\big|\{y \in V|(x,y) \in \mathcal{X}\}\big|$ depends only on $\mathcal{X} \in \mathfrak{R}$ but not on $x \in V$.

(vii) The numbers $p^{\mathcal{Z}}_{\mathcal{X}\mathcal{Y}} \stackrel{\text{def}}{=} \left|\{z \in V \,|\, (x,z) \in \mathcal{X} \text{ and } (z,y) \in \mathcal{Y}\}\right|$ are the same for all pairs $(x,y) \in \mathcal{Z}$.

(viii) The matrices $\mathbf{X}, \mathbf{Y}$ associated with any two classes $\mathcal{X}$ and $\mathcal{Y}$ commute.

There exist a large number of implications between various combinations of these properties. A variety of special types of partitions are defined in Table 1. *Coherent configurations* will play a dominant role in this contribution. We will briefly review their most important properties after presenting proofs for the few non-trivial implications that can be found in Table 1 which are not proved in Higman's paper [36].

**Table 1.** An overview of various types of partitions of $V \times V$.

| Property | $(i)$ | $(ii)$ | $(iii)$ | $(iv)$ | $(v)$ | $(vi)$ | $(vii)$ | $(viii)$ |
|---|---|---|---|---|---|---|---|---|
| *compatible with* $\Gamma$ | • | • | | | | | | |
| *homogeneous* | ○ | | • | | | | | |
| *precoherent configuration* | • | | ○ | • | | | | |
| *symmetric* | | | | | • | | | |
| *class degree regular* | | | | | | • | | |
| *coherent configuration* | • | | | • | | | • | |
| *homogeneous coherent conf.* | ○ | | • | • | | ○ | • | |
| *c.d. regular coherent conf.* | • | | ○ | • | | • | • | |
| *association scheme* | • | | ○ | • | | ○ | • | • |
| *symmetric association scheme* | • | | ○ | ○ | • | ○ | • | ○ |

• indicates properties that are used for definition. ○ marks properties that are implied by the definition. Most of these implications are proved in [36], relations involving class degree regular partitions are discussed in the text.

**Lemma 1.** A homogeneous coherent configuration is always class degree regular. If $\mathfrak{R}$ is class degree regular and has property (i) then it is homogeneous.

**Proof.** Let $\mathfrak{R}$ be a homogeneous coherent configuration. Then

$$\left|\{y \in V | (x,y) \in \mathcal{X}\}\right| = \left|\{y \in V | (x,y) \in \mathcal{X} \,\wedge\, (y,x) \in \mathcal{X}^+\}\right| = p^{\mathcal{I}}_{\mathcal{X}\mathcal{X}^+}\,,$$

which is of course independent of $x \in V$.
Consider a class $\cap J \subseteq \mathcal{I}$ and a vertex $x_0$ such that $(x_0, x_0) \in \mathcal{J}$. Then $|\{y \in V|(x_0, x) \in \mathcal{J}\}| = 1$. This is independent of $x$ only if $(x, x) \in \mathcal{J}$ for all $x \in V$, i.e., if $\mathcal{J} = \mathcal{I}$. ∎

The most important feature of a coherent configuration $\mathfrak{R}$ is that the characteristic matrices of its classes form an algebra $\langle\mathfrak{R}\rangle$ which is closed under (conjugate) transposition, ordinary matrix multiplication, and component-wise (Hadamard) multiplication. Matrix algebras of this type have been termed *coherent algebras* and have been studied in great detail by D.G. Higman [37, 36, 38, 39]. The *intersection numbers* $p^{\mathcal{Z}}_{\mathcal{X}\mathcal{Y}}$ defined together with property (vii) above give rise to a matrix algebra $\langle\hat{\mathfrak{R}}\rangle$ on $\mathfrak{R} \times \mathfrak{R}$ by means of the definition

$$\hat{\mathbf{Y}}_{\mathcal{X}\mathcal{Z}} \stackrel{\text{def}}{=} p^{\mathcal{Z}}_{\mathcal{X}\mathcal{Y}}.$$

It can be shown that $\langle\mathfrak{R}\rangle$ and $\langle\hat{\mathfrak{R}}\rangle$ are isomorphic. For the basis matrices $\mathbf{X}$ the isomorphism has the explicit representation

$$\imath : \langle\mathfrak{R}\rangle \to \langle\hat{\mathfrak{R}}\rangle, \quad \mathbf{X} \mapsto \hat{\mathbf{X}} \qquad \text{for all } \mathcal{X} \in \mathfrak{R}\,.$$

If $\mathfrak{R}$ is an association scheme then the commutative algebra $\langle\mathfrak{R}\rangle$ is commonly called *Bose-Mesner algebra* [40, 41].

If $\mathfrak{R}$ is compatible with the graph $\Gamma$, then $\mathbf{A} \in \langle\mathfrak{R}\rangle$ [34]. The *collapsed adjacency matrix* $\hat{\mathbf{A}}$ is then the image of $\mathbf{A}$ under the isomorphism $\imath : \langle\mathfrak{R}\rangle \to \langle\hat{\mathfrak{R}}\rangle$, or more explicitly:

$$\hat{\mathbf{A}}_{\mathcal{X}\mathcal{Y}} = \sum_{\substack{\mathcal{Z}\in\mathfrak{R} \\ \mathcal{Z}\cap\mathcal{A}\neq\emptyset}} p^{\mathcal{Y}}_{\mathcal{X}\mathcal{Z}} = \sum_{\substack{\mathcal{Z}\in\mathfrak{R} \\ \mathcal{Z}\cap\mathcal{A}\neq\emptyset}} p^{\mathcal{Z}}_{\mathcal{X}\mathcal{Y}}\,, \tag{9}$$

see [34] for a proof. An alternative way of constructing the collapsed adjacency matrix based on so-called equitable partitions is discussed for instance in [42, 43, 34].

A particularly important class of coherent configurations are symmetric association schemes [41], which play a prominent role in coding theory. Suppose $\mathfrak{R}$ is a symmetric association scheme that is compatible with $\Gamma$. Then the algebra $\langle \mathfrak{R} \rangle$ coincides with the so-called *adjacency algebra* $\langle \mathfrak{A} \rangle$ of $\Gamma$ [29], that is, any $\mathbf{X} \in \mathfrak{R}$ can be written as a polynomial in terms of the adjacency matrix $\mathbf{A}$, [37]. As a consequence $\varphi_k$ diagonalizes simultaneously all elements of $\mathfrak{R}$ and the functions

$$\omega_p(\mathcal{X}) \stackrel{\text{def}}{=\!=} \frac{|V|}{|\mathcal{X}|} \frac{\langle \varphi_i, \mathbf{X}\varphi_i \rangle}{\langle \varphi_i, \varphi_i \rangle} \qquad \text{for all } i \in I_p \tag{10}$$

are well defined, where $I_p$ is the set of all indices for which $\Delta\varphi_i = \lambda_p \varphi_i$. These functions will play a special role later on. In particular, it can be shown [34] that $\omega_p$ is a left eigenvector of the collapsed adjacency matrix $\hat{\mathbf{A}}$ with eigenvalue $\mu_p = D - \lambda_p$. The functions $\omega_k$ are orthogonal with respect to the scalar product

$$\langle \theta_i; \theta_j \rangle \stackrel{\text{def}}{=\!=} \frac{1}{|V|^2} \sum_{\mathcal{X} \in \mathfrak{R}} \theta_i(\mathcal{X}) \theta_j(\mathcal{X}) |\mathcal{X}| \,. \tag{11}$$

One finds explicitly [29]:

$$\langle \omega_p; \omega_q \rangle = \frac{1}{m(\lambda_p)}\, \delta_{pq} \tag{12}$$

where $m(\lambda_p)$ is the multiplicity of $\lambda_p$ as an eigenvalue of the graph Laplacian $-\Delta$.

So far, we have used the partition $\mathfrak{R}$ as the basis of our discussion. Intuitively, however, one would like to link the formalism much stronger to the graph $\Gamma$ on which the random field is defined. Hence we shall insist that the choice of $\mathfrak{R}$ is compatible with $\Gamma$. It is important, therefore, to know what types of graphs admit coherent configurations or even association schemes on their vertex sets. As an immediate consequence of the definition of the edge set $E$ we obtain a partitioning of $V \times V$ with respect to the canonical distance $d : V \times V \to \mathbb{N}_0^+$ on $V$. The properties of this metric on $V$ are discussed in detail in the book [44]. If $\Gamma$ is finite and connected, as it is always assumed in this contribution, then there is a maximum distance, called the *diameter* $d^*$ of $\Gamma$. The metric $d(\,.\,,\,.\,)$ induces in a natural way the *distance partition* $\mathfrak{D}$ of $V \times V$, which has the classes

$$\mathcal{D}_d \stackrel{\text{def}}{=\!=} \left\{ (x,y) \in V \,\middle|\, d(x,y) = d \right\} .$$

Note that $\mathcal{D}_0 = \mathcal{I}$ and $\mathcal{D}_1 = \mathcal{A}$. A coherent configuration $\mathfrak{R}$ is compatible with $\Gamma$ if and only if each class $\mathcal{X} \in \mathfrak{R}$ is a subset of a distance class $\mathcal{D}_k \in \mathfrak{D}$ for some $k = 0, \ldots, d^*$ [34]. Furthermore, the distance partition $\mathfrak{D}$ is symmetric by construction, i.e., it is a coherent configuration if and only if it is a symmetric association scheme.

The class of *distance regular* graphs is characterized by the fact that $\mathfrak{D}$ is a symmetric association scheme. These graphs have received considerable attention, see the monograph [45]. The following well-studied graphs are distance regular: the sequences spaces $\mathcal{Q}_\alpha^n$ with arbitrary alphabets, the Johnson graphs, the odd graphs, the Grassmann graphs, and all distance transitive graphs.

A graph $\Gamma$ is vertex transitive if its automorphism group $\mathbf{Aut}[\Gamma]$ acts transitively on the vertex set $V$. It can be shown [37, 36] that the orbits of the automorphism group of $\Gamma$ acting on $V \times V$ form a homogeneous coherent configuration. An important sub-class of the class of vertex transitive graphs is derived from groups: Let $H$ be a finite group and let $\Phi$ be a set of generators[1] of $H$ such that (i) the group identity $e \notin \Phi$, and (ii) $x \in \Phi$ implies $x^{-1}$ in $\Phi$. Then the graph $\Gamma(H, \Phi)$ with vertex set $V = H$ and edge set $E = \big\{ \{x, y\} | xy^{-1} \in \Phi \big\}$ is called the Cayley *graph* of the group $H$ with respect to the set of generators $\Phi$. Not all vertex transitive graphs are Cayley graphs, however. A famous counter-example is the Petersen graph. If $H$ is a commutative group then the coherent configuration implied by the automorphism group of $\Gamma(H, \Phi)$ is also commutative. This follows immediately from [33, 46, 34].

[1] $\Phi$ is a set of generators of the group $H$ if each element $x \in G$ can be represented as a product of members of $H$.

## 5. Isotropy

The most obvious way of defining isotropy would require the probability distribution of $\Xi$ to be invariant under all symmetries of the configuration space $\Gamma$. In practice, however, such a definition would be too restrictive for the following two reasons: (i) We would like to develop a second order theory of random fields revolving around correlation measures. Consequently we want to use the covariance matrix $\mathbf{C}$ instead of the probability distribution itself. (ii) Graphs oftentimes exhibit a high degree of regularity without having a large group of automorphisms. For instance, most distance regular graphs do not have a transitive group of automorphisms. We shall therefore use the more general "combinatorial" regularities rather than the symmetries of $\Gamma$. The discussion in section 4 has shown that these combinatorial properties can be conveniently dealt with in terms of partitions of $V \times V$. Hence we begin our exhibition with a definition of isotropy based on a partition $\mathfrak{R}$.

**Definition.** A random field $\Xi$ is *isotropic*[2] w.r.t. a partition $\mathfrak{R}$ of $V \times V$ if

(i) $\mathcal{E}[f(x)] = a_0$ for all $x \in V$,

(ii) $\mathrm{Var}[f(x)] = s^2$ for all $x \in V$, and

(iii) the covariance matrix $\mathbf{C}$ is constant on the classes of $\mathfrak{R}$, i.e., there is a function $c : \mathfrak{R} \to \mathbb{R}$ such that $\mathbf{C}_{xy} = c(\mathcal{X})$ for all $(x, y) \in \mathcal{X}$.

We are not aware of any interesting implications of this definition by itself. However, if we insist that the partition $\mathfrak{R}$ is sufficiently regular we obtain a very interesting characterization of isotropy.

**Theorem 1.** The random field $\Xi$ is isotropic with respect to the homogeneous coherent configuration $\mathfrak{R}$ if and only if $\mathcal{E}[f(x)] = a_0$ for all $x \in V$ and $\mathbf{C} \in \langle \mathfrak{R} \rangle$.

[2] The notion of isotropy for random fields is analogous to the definition of stationarity for stochastic processes. Following the conventions of Karlin and Taylor [47] our notion of isotropy would be called "covariance isotropic", "weakly isotropic", or "wide sense isotropic". For a Gaussian random field the notions of (weak) isotropy and strict isotropy coincide.

**Proof.** We observe that $\mathbf{C}_{xy} = c(\mathcal{X})$ for all $(x, y) \in \mathcal{X}$ and all $\mathcal{X} \in \mathfrak{R}$ is equivalent to $\mathbf{C} = \sum_{\mathcal{X} \in \mathfrak{R}} c(\mathcal{X})\mathbf{X}$. Thus property (iii) of the definition of isotropy is satisfied if and only if $\mathbf{C} \in \langle \mathfrak{R} \rangle$. Since $\mathfrak{R}$ is homogeneous we have $\mathcal{I} \in \mathfrak{R}$ and thus $\mathrm{Var}[f(x)] = c(\mathcal{I})$, independent of $x \in V$, i.e., condition (ii) is satisfied as well. ∎

**Corollary.** Let $\Gamma$ be vertex transitive and let $\mathfrak{R}$ be the partition formed by the orbits of the automorphism group $\mathbf{Aut}[\Gamma]$ acting on $V \times V$. Then the random field is isotropic (w.r.t. $\mathfrak{R}$) if and only if $\mathcal{E}[f(x)] = a_0$ for all $x \in V$ and $\mathbf{C} \in \langle \mathfrak{R} \rangle$.

**Proof.** The orbits on $V \times V$ of a permutation group that acts transitively on $V$ form a homogeneous coherent configuration [37]. ∎

**Corollary.** Let $\mathfrak{R}$ be an association scheme (i.e., a commutative coherent configuration) on $V \times V$ that is compatible with $\Gamma$ and let $\Xi$ be isotropic w.r.t. $\mathfrak{R}$. Then the Fourier series and the Karhunen-Loève series of $\Xi$ coincide.

**Proof.** As a consequence of the theorem above we have $\mathbf{C} \in \langle \mathfrak{R} \rangle$ and compatibility implies $\mathbf{A} \in \langle \mathfrak{R} \rangle$. Since $\langle \mathfrak{R} \rangle$ is commutative by assumption we have $\mathbf{CA} = \mathbf{AC}$, and hence both matrices have a common basis of orthonormal eigenfunctions. ∎

**Definition.** A random field $\Xi$ on $\Gamma$ is **-isotropic* if $\mathcal{E}[f(x)] = a_0$ for all $x \in V$ and its covariance matrix $\mathbf{C}$ is a polynomial in terms of the adjacency matrix $\mathbf{A}$ of $\Gamma$.

**Theorem 2.** Let $\Xi$ be a random field on $\Gamma$, and let $\mathfrak{R}$ be a homogeneous coherent configuration compatible with $\Gamma$. If $\Xi$ is *-isotropic then it is isotropic w.r.t. $\mathfrak{R}$.

**Proof.** The adjacency algebra $\langle \mathfrak{A} \rangle$ of $\Gamma$, which consists of all polynomials in $\mathbf{A}$, is always contained in the algebra $\langle \mathfrak{R} \rangle$ associated with the homogeneous coherent configuration $\mathfrak{R}$, provided $\mathfrak{R}$ is compatible with $\Gamma$ [34]. *-Isotropy means $\mathbf{C} \in \langle \mathfrak{A} \rangle \subseteq \langle \mathfrak{R} \rangle$, i.e., $\Xi$ is isotropic w.r.t. $\mathfrak{R}$. ∎

Since the adjacency algebra $\langle \mathfrak{A} \rangle$ and the Bose-Mesner algebra $\langle \mathfrak{R} \rangle$ coincide for symmetric association schemes that are compatible with $\Gamma$ the following two statements are true as well:

**Corollary.** The random field $\Xi$ is isotropic w.r.t. a symmetric association scheme $\mathfrak{R}$ that is compatible with $\Gamma$ if and only if $\mathcal{E}[f(x)] = a_0$ for all $x \in V$ and $\mathbf{C}$ is a polynomial in terms of the adjacency matrix $\mathbf{A}$ of $\Gamma$.

**Corollary.** Let $\mathfrak{R}$ be a symmetric association scheme compatible with $\Gamma$. Then $\Xi$ is isotropic w.r.t. $\mathfrak{R}$ if and only if it is *-isotropic.

*-Isotropic random fields have a convenient characterization in terms of their Fourier coefficients:

**Theorem 3.** A random field $\Xi$ is *-isotropic if and only if its Fourier coefficients satisfy

(i) $\mathcal{E}[a_k] = 0$ for all $k \neq 0$; the coefficient $a_0$ belonging to the flat mode is arbitrary.

(ii) $\mathrm{Cov}[a_k, a_j] = \mathrm{Var}[a_k]\delta_{kj}$.

(iii) $\mathrm{Var}[a_k] = \mathrm{Var}[a_j]$ for all $k, j \in I_p$, i.e., the expected value of the amplitude depends only on the corresponding eigenvalue of the graph Laplacian.

**Proof.** $\mathcal{E}[a_k] = 0$ for all $k \neq 0$ is equivalent to $\mathcal{E}[f(x)] = a_0$ for all $x \in V$. Thus we need to proof that $\mathbf{C} \in \langle \mathfrak{A} \rangle$ is equivalent to properties (ii) and (iii).
($\Longrightarrow$) We have seen already that Fourier series and Karhunen-Loève series coincide for $*$-isotropic landscapes. The properties (i), (ii), and (iii) are valid for all Karhunen-Loève series, see section 3.3.
($\Longleftarrow$) There is a set of idempotent matrices $\{\mathbf{E}_l\}$ associated with the eigenspaces of $\mathbf{A}$ such that (i) $\mathbf{A} = \sum_l \mu_l \mathbf{E}_l$, where the $\mu_l$ are the distinct eigenvalue of A, and (ii) $\mathbf{E}_i\mathbf{E}_j = \delta_{ij}\mathbf{E}_i$. The idempotents $\mathbf{E}_l$ depend only on the eigenspaces of $\mathbf{A}$, not on the eigenvalues $\mu_l$. Thus they can be constructed uniquely, given the Fourier basis $\{\varphi_k\}$ and the knowledge which of the basis vectors belong to different eigenvectors $\mu_k$ of $\mathbf{A}$ (or equivalently, to the different eigenvectors $\lambda_p$ of $-\Delta$). The idempotents $\mathbf{E}_l$ form a basis of the adjacency algebra $\langle \mathfrak{A} \rangle$ and thus they can be expressed as polynomials in $\mathbf{A}$. Properties (ii) and (iii) of the Fourier series implies that the Fourier series is a Karhunen-Loève series, i.e., the $\varphi_k$ are eigenvectors of $\mathbf{C}$. Furthermore, as a consequence of property (iii), any two basis functions $\varphi_k$

and $\varphi_l$ which belong to the same eigenspace of $\mathbf{A}$ have the same eigenvalue $\mathrm{Var}[a_k]$ with respect to $\mathbf{C}$, i.e., each eigenspace of $\mathbf{A}$ is also an eigenspaces of $\mathbf{C}$. Thus $\mathbf{C}$ can be written in the form $\mathbf{C} = \sum_l q_l \mathbf{E}_l$, and hence $\mathbf{C} \in \langle \mathfrak{A} \rangle$. In other words, $\mathbf{C}$ is a polynomial in terms of the adjacency matrix $\mathbf{A}$, and thus $\Xi$ is *-isotropic. ∎

Note that the theorem also characterizes isotropy w.r.t. any symmetric association scheme that is compatible with $\Gamma$. Some interesting results can be obtained using only a very weak notion of isotropy:

**Definition.** A random field $\Xi$ is *pseudo-isotropic* if there are constants $a_0$, $s$, and $w$ such that the following statements are true for all $x \in V$:

(i) $\mathcal{E}[f(x)] = a_0$,

(ii) $\mathrm{Var}[f(x)] = s^2$, and

(iii) $\displaystyle\frac{1}{|V|}\sum_{y\in V} \mathbf{C}_{xy} = w$.

We will call $w$ the *average correlation* of the random field $\Xi$. Condition (iii) is equivalent to insisting that $\mathbf{1}$ is an eigenvector of $\mathbf{C}$.

**Theorem 4.** Let $\Xi$ be isotropic w.r.t. a homogeneous class degree regular partition $\mathfrak{R}$ of $V \times V$. Then $\Xi$ is pseudo-isotropic.

**Proof.** $\displaystyle w = \frac{1}{|V|}\sum_{y\in V}\mathbf{C}_{xy} = \frac{1}{|V|}\sum_{\mathcal{X}\in\mathfrak{R}}\sum_{x,y\in\mathcal{X}}\mathbf{C}_{xy}$

$\displaystyle = \frac{1}{|V|}\sum_{\mathcal{X}\in\mathfrak{R}} \overline{c}(\mathcal{X})\big|\{y\in V|(x,y)\in\mathcal{X}\}\big| = \frac{1}{|V|}\sum_{\mathcal{X}\in\mathfrak{R}} \overline{c}(\mathcal{X}) p^{\mathcal{I}}_{\mathcal{X}\mathcal{X}^+}$ for all $x \in V$. ∎

**Lemma 2.** If $\Xi$ is both pseudo-isotropic and isotropic w.r.t. a partition of $\mathfrak{R}$ of $V \times V$ then the average correlation is given by $\displaystyle w = \frac{1}{|V|^2}\sum_{\mathcal{X}\in\mathfrak{R}} |\mathcal{X}|\, c(\mathcal{X})$.

**Proof.** $\displaystyle w = \frac{1}{|V|}\sum_{x\in V}\mathbf{C}_{xy} = \frac{1}{|V|^2}\sum_{x,y\in V}\mathbf{C}_{xy} = \frac{1}{|V|^2}\sum_{\mathcal{X}\in\mathfrak{R}}\sum_{(x,y)\in\mathcal{X}}\mathbf{C}_{xy} = \frac{1}{|V|^2}\sum_{\mathcal{X}\in\mathfrak{R}} c(\mathcal{X})|\mathcal{X}|$. ∎

## 6. Covariance Functions

It is often convenient to fix a particular partition $\mathfrak{R}$ of $V \times V$ and to consider the "average" correlation

$$\overline{c}(\mathcal{X}) \stackrel{\text{def}}{=} \frac{1}{|\mathcal{X}|} \sum_{(x,y)\in\mathcal{X}} \mathrm{Cov}[f(x), f(y)] \tag{13}$$

within the classes of $\mathfrak{R}$. Of course we have $\overline{c}(\mathcal{X}) = c(\mathcal{X})$ whenever the random field is isotropic w.r.t. $\mathfrak{R}$. The virtue of this approach is its close connection with the individual realizations of $\Xi$, i.e., with the properties of the *landscapes* drawn from the random field.

For each realization $f$ of the random field $\Xi$ we define the random variables

$$\overline{f} \stackrel{\text{def}}{=} \frac{1}{|V|} \sum_{x\in V} f(x) \qquad \text{and} \qquad \sigma_f^2 \stackrel{\text{def}}{=} \overline{f^2} - \overline{f}^2 . \tag{14}$$

Furthermore, we introduce

$$\chi(\mathcal{X}) \stackrel{\text{def}}{=} \frac{1}{|\mathcal{X}|} \sum_{(x,y)\in\mathcal{X}} (f(x) - \overline{f})(f(y) - \overline{f}) \tag{15}$$

for each class $\mathcal{X}$ of a partition $\mathfrak{R}$. The function $\chi$ measures the covariance within the landscape $f$. In fact, it is used to define "empirical" correlation measures for landscapes that are not viewed as instances of random field, see [34]. Examples of this type are the landscapes of free energies and reaction rate constants derived from RNA secondary structures, see e.g., [25, 48]. In the context of this paper, of course, $\chi(\mathcal{X})$ is a random variable. In the following we shall evaluate the expected values of $\overline{f}$, $\sigma_f^2$ and $\chi(\mathcal{X})$ for a broad class of random fields.

**Theorem 5.** Let $\Xi$ be a random field for which $\mathcal{E}[f(x)] = a_0$ independent of $x \in V$ and let $\mathfrak{R}$ be a homogeneous class degree regular partition of $V \times V$. Then:

$$\mathcal{E}[\overline{f}] = a_0, \qquad \mathcal{E}[\sigma_f^2] = \overline{c}(\mathcal{I}) - w, \qquad \text{and} \qquad \mathcal{E}[\chi(\mathcal{X})] = \overline{c}(\mathcal{X}) - w . \tag{16}$$

**Proof.** We first observe $\mathcal{E}[\overline{f}] = \frac{1}{|V|}\sum_x \mathcal{E}[f(x)] = a_0$. The definition of $\sigma_f^2$ coincides with $\chi(\mathcal{I})$, thus it suffices to prove the third expression. To this end we need to evaluate

$$\sum_{(x,y)\in\mathcal{X}} \mathcal{E}[f(x)\overline{f}] = \sum_{x\in V}\big|\{y\in V|(x,y)\in\mathcal{X}\}\big|\mathcal{E}[f(x)\overline{f}] = \frac{1}{|V|}\sum_{z\in V}\sum_{x\in V}\frac{|\mathcal{X}|}{|V|}\mathcal{E}[f(x)f(y)].$$

Here we have used explicitly that $\mathfrak{R}$ is a class degree regular partition. One obtains the same result for $\sum\limits_{(x,y)\in\mathcal{X}} \mathcal{E}[f(x)\overline{f}]$ . As a consequence we arrive at

$$\mathcal{E}[\chi(\mathcal{X})] = \frac{1}{|\mathcal{X}|}\sum_{(x,y)\in\mathcal{X}}\mathcal{E}[f(x)f(y)] - \frac{1}{|V|^2}\sum_{x,y\in V}\mathcal{E}[f(x)f(y)]$$

Recalling that $\mathcal{E}[f(x)]\mathcal{E}[f(y)] = a_0^2$ we find that this can be written as

$$\begin{aligned}\mathcal{E}[\chi(\mathcal{X})] =& \frac{1}{|\mathcal{X}|}\sum_{(x,y)\in\mathcal{X}}\{\mathcal{E}[f(x)f(y)] - \mathcal{E}[f(x)]\mathcal{E}[f(y)]\}\\ &- \frac{1}{|V|^2}\sum_{x,y\in V}\{\mathcal{E}[f(x)f(y)] - \mathcal{E}[f(x)]\mathcal{E}[f(y)]\}\ .\end{aligned}$$

Using the definitions of $\overline{c}(\mathcal{X})$ and $w$, respectively completes the proof. ∎

We note that $\sum_{\mathcal{X}\in\mathfrak{R}}|\mathcal{X}|\mathcal{E}[\chi(\mathcal{X})] = 0$ for any random field, as can be seen by direct evaluation of this expression. Thus $\sum_{\mathcal{X}\in\mathfrak{R}}|\mathcal{X}|\overline{c}(\mathcal{X}) = |V|^2\,w$.

A number of very useful results can be obtained by substituting the Fourier expansion into the definition of $\chi$. It is easy verify that

$$\sum_k a_k\varphi_k(x) - \overline{f} = \sum_{k\neq 0} a_k\varphi_k(x)\,.$$

A simple short computation then yields the representation

$$\mathcal{E}[\chi(\mathcal{X})] = \sum_{k,l\neq 0}\mathcal{E}[a_k a_l]\cdot\frac{1}{|\mathcal{X}|}\langle\varphi_k,\mathbf{X}\varphi_l\rangle\,. \tag{17}$$

Recall that $I_p$ is defined as the set of all indices $i$ for which $-\Delta\varphi_i = \lambda_p\varphi_i$.

**Theorem 6.** Let $\mathfrak{R}$ be a symmetric association scheme. Then $\mathcal{E}[\chi(\mathcal{X})]$ is of the form

$$\mathcal{E}[\chi(\mathcal{X})] = \sum_{p\neq 0} \left\{ |V| \sum_{k\in I_p} \mathcal{E}[|a_k|^2] \right\} \omega_p(\mathcal{X}) \stackrel{\text{def}}{=\!=} \sum_{p\neq 0} A_p \omega_p(\mathcal{X}) .$$

**Proof.** Each vector $\varphi_k$ is an eigenvector of any $\mathbf{X} \in \mathfrak{R}$, with eigenvalue $\mathbf{p}_k(\mathcal{X})$. Thus

$$\begin{aligned}\mathcal{E}[\chi(\mathcal{X})] &= \sum_{k,l\neq 0} \mathcal{E}[a_k a_l] \cdot \frac{1}{|\mathcal{X}|} \mathbf{p}_k(\mathcal{X}) \langle \varphi_k, \varphi_l \rangle = \sum_{k,l\neq 0} \mathcal{E}[a_k a_l] \cdot \frac{1}{|\mathcal{X}|} \mathbf{p}_k(\mathcal{X}) \delta_{kl} \\ &= \sum_{k\neq 0} \mathcal{E}[|a_k|^2] \frac{\mathbf{p}_k(\mathcal{X})}{|\mathcal{X}|} .\end{aligned}$$

The definition of $\omega_k$ completes the proof. ∎

**Corollary.** Let $\mathfrak{R}$ be a symmetric association scheme and define $A_0 \stackrel{\text{def}}{=\!=} w$. Then

$$\overline{c}(\mathcal{X}) = \sum_{p} A_p \omega_p(\mathcal{X}) \qquad \text{with} \qquad A_p = |V| \sum_{k\in I_p} \mathcal{E}\left[|a_k|^2\right] . \tag{18}$$

Correlation functions have been used successfully as a measure for the *ruggedness* of landscapes and random fields. The measure that has been used most often for random field models is

$$R(\mathcal{X}) \stackrel{\text{def}}{=\!=} \frac{\overline{c}(\mathcal{X})}{\overline{c}(\mathcal{I})} . \tag{19}$$

The results above imply immediately

$$R(\mathcal{X}) = \frac{\mathcal{E}[\chi(\mathcal{X})] + w}{\mathcal{E}[\sigma_f^2] + w} = \sum_{p} \left[ \frac{A_p}{\sum_q A_q} \right] \omega_p(\mathcal{X}) \stackrel{\text{def}}{=\!=} \sum_p \tilde{B}_p \omega_p(\mathcal{X}) . \tag{20}$$

Instead of the correlation function $R$ is is often convenient to characterize a random field by means of the *normalized amplitudes* $\tilde{B}_p$.

On the other hand, on empirical landscapes $f$ it is convenient to use the "direct correlation function" w.r.t. a partition $\mathfrak{R}$ [34], which is defined by

$$\rho(\mathcal{X}) \stackrel{\text{def}}{=\!=} \frac{1}{|\mathcal{X}|} \sum_{(x,y)\in\mathcal{X}} \frac{(f(x)-\overline{f})(f(y)-\overline{f})}{\overline{f^2} - \overline{f}^2} = \frac{\chi(\mathcal{X})}{\chi(\mathcal{I})} . \tag{21}$$

If $\mathfrak{R}$ is a symmetric association scheme that one can expand $\rho$ in terms of the functions $\omega_p$ as $\rho(\mathcal{X}) = \sum_{p\neq 0} B'_p\omega_p$, and consequently we can write $\mathcal{E}[\rho(\mathcal{X})] = \sum_p B_p\omega_p$. Here we have used $B_p \stackrel{\text{def}}{=} \mathcal{E}[B'_p]$. It is convenient to set $B_0 \stackrel{\text{def}}{=} 0$. It is instructive to compare the explicit definition of $B_k$ and $\tilde{B}_k$ in terms of the Fourier coefficients:

$$B_p = \mathcal{E}\left[\frac{\sum\limits_{k\in I_p} |a_k|^2}{\sum\limits_{j\neq 0} |a_j|^2}\right] \qquad \tilde{B}_p = \left[\frac{\sum\limits_{k\in I_p} \mathcal{E}[|a_k|^2]}{w + \sum\limits_{j\neq 0} \mathcal{E}[|a_j|^2]}\right] \tag{22}$$

for all $p \neq 0$. For $p = 0$ we have $B_0 = 0$ and $\tilde{B}_0 = w/(w + \sum_{j\neq 0} \mathcal{E}[|a_j|^2])$.

## 7. Elementary Landscapes and Elementary Random Fields

**Definition.** A landscapes $f : V \to \mathbb{R}$ is *elementary* if there are constants $f^*$ and $\lambda > 0$ such that

$$(\Delta f)(x) + \lambda\,[f(x) - f^*] = 0 \qquad \text{for all } x \in V\,. \tag{23}$$

The main result of [34] is that elementary landscapes are characterized by their correlation functions.

Random walk autocorrelation function have been proposed in [9] as a measure of landscapes. A simple random walk [49] has transition matrix $\mathbf{T} = \mathbf{D}^{-1}\mathbf{A}$. It is shown in [34] that the autocorrelation function of a "time series" sampled along a simple random walk on a $D$-regular graph $\Gamma$ can be written as

$$r(s) = \frac{\frac{1}{D|V|}\langle f, \mathbf{A}f\rangle - \overline{f}^2}{\overline{f^2} - \overline{f}^2}$$

We will not consider $r(s)$ in any details in this contribution. We refer to the following references instead [50, 25, 51, 11, 17, 18, 52, 24, 33].

**Proposition.** [34] Let $\Gamma$ be connected $D$-regular graph, and let $\mathfrak{R}$ be a homogeneous coherent configuration which is compatible with $\Gamma$. Furthermore let $f$ be a non-flat landscape on $\Gamma$ with "random walk" correlation function $r$ and "direct" correlation function $\rho$ w.r.t. $\mathfrak{R}$. Then the following statements are equivalent:

(i) $f$ is elementary.

(ii) $f - \overline{f}\mathbf{1}$ is an eigenvector the Laplacian $-\Delta$ of $\Gamma$ with a positive eigenvalue.

(iii) $r$ is of the form $r(s) = a^{-s}$ (with $-1 \leq a < 1$).

(iv) $\rho$ is a left eigenvector of the collapsed adjacency matrix $\hat{\mathbf{A}}$ of $\Gamma$ (with an eigenvalue smaller than $D$).

The notion of an elementary landscape can be carried over immediately to random fields:

**Definition.** A random field $\Xi$ is *elementary* if its sample functions are elementary with the same eigenvalue $\lambda$.

**Theorem 7.** Let $\mathfrak{R}$ be a symmetric association scheme compatible with $\Gamma$ and let $\Xi$ be an elementary random field on $\Gamma$. Then the "direct" correlation function $\rho$ coincides with one of the functions $\omega_p$ for some $p \neq 0$ for almost all instances of $\Xi$, i.e., $\mathcal{E}[\rho(\mathcal{X})] = \omega_p(\mathcal{X})$.

**Proof.** Since almost all instance of $f$ are elementary with the same eigenvalue $\lambda + p$ by construction we have almost always $\rho(\mathcal{X}) = \omega_p(\mathcal{X})$. The theorem then follows. ∎

The following combinatorial optimization problems, all of which can be regarded as random fields, are elementary: the symmetric traveling salesman problem, the graph matching problem, the graph bipartitioning problem, the graph coloring problem with a fixed set of colors, and the spin glass models discussed in section 8.2 [53, 34].

# 8. Model Random Fields

## 8.1. The Random Energy Model

In the *Random Energy Model* (REM) the values $f(x)$ are i.i.d. random variables (see, e.g., [54]. This model has been introduced by Derrida [55, 56, 57], and it has been applied to a variety of problems, amongst others also to the maturation of the immune system [23, 19]. The REM has covariance $c(\mathcal{X}) = 0$ for all $\mathcal{X} \neq \mathcal{I}$, and $\mathcal{E}[f(x)^2]$ is independent of $x \in V$ since the values of $f(x)$ are i.i.d. Thus $\mathbf{C} = s^2\mathbf{I}$ with some constant $s^2 \geq 0$, i.e., REM is isotropic w.r.t. to any partition of $V \times V$ for which $\mathcal{X} \cap \mathcal{I} \neq \emptyset$ implies $\mathcal{X} \subseteq \mathcal{I}$.

**Theorem 8.** Let $\Gamma$ a $D$-regular graph, and let $\mathfrak{R}$ be a homogeneous coherent configuration that is compatible with $\Gamma$. Furthermore let $\{\omega_k\}$ be a basis of left eigenvectors of the collapsed adjacency matrix $\hat{\mathbf{A}}$ of $\Gamma$ which are orthogonal w.r.t. the scalar product $\langle\, .\, ;\, .\, \rangle$ defined in section 4. Then the normalized amplitudes of a REM on $\Gamma$ are given by

$$\tilde{B}_p = \frac{1}{|V|} \cdot \frac{1}{\langle \omega_p ; \omega_p \rangle}. \tag{24}$$

**Proof.** $\tilde{B}_p = \dfrac{\langle \omega_p ; \rho \rangle}{\langle \omega_p ; \omega_p \rangle} = \dfrac{1}{\langle \omega_p ; \omega_p \rangle} \dfrac{1}{|V|^2} \sum\limits_{\mathcal{X} \in \mathfrak{R}} \delta_{\mathcal{I}\mathcal{X}} \omega_p(\mathcal{X}) |\mathcal{X}| = \dfrac{\omega_p(\mathcal{I})|\mathcal{I}|}{|V|^2 \langle \omega_p ; \omega_p \rangle}$. Using $\omega_p(\mathcal{I}) = 1$ and $|\mathcal{I}| = |V|$ completes the proof. ∎

On a boolean hypercube $\mathcal{Q}_2^n$ one finds explicitly $B_p = \dfrac{1}{2^n}\dbinom{n}{p}$ for the random energy model.

### 8.2. Boolean Hypercubes and p-Spin Models

The vertices of a Boolean hypercube are the sequences of length $n$ taken from an alphabet of size $\alpha = 2$. Without loosing generality we may use the alphabet $\{+1, -1\}$. A configurations is then a string $x$ of "spins" $x_k \in \{+1, -1\}$. The following result is well known in the literature, see e.g., [33, 34] for more details.

Any landscape $f$ on the Boolean Hypercube can be written as

$$f(x) = J_0 + \sum_{p=1}^{n} \sum_{i_1<i_2<\ldots<i_p} J_{i_1 i_2 \ldots i_p} x_{i_1} x_{i_2} \ldots x_{i_p}\,, \tag{25}$$

where the $J_{i_1 i_2 \ldots i_p}$ are constants. In particular, this is exactly a Fourier-series representation of $f$ up to the normalization of the basis functions

$$\varepsilon_{i_1,i_2,\ldots,i_p}(x) \stackrel{\text{def}}{=} \frac{1}{\sqrt{|V|}} x_{i_1} x_{i_2} \ldots x_{i_p} \tag{26}$$

which belong to the eigenvalue $\lambda_p = 2p$ of $-\Delta$. Thus $a_{i_1 i_2 \ldots i_p} = \sqrt{|V|} J_{i_1 i_2 \ldots i_p}$ are the Fourier coefficients of these landscapes. The boolean hypercube is distance transitive and thus also distance regular. Consequently, its distance partition $\mathfrak{D}$ forms a symmetric association scheme. We shall therefore consider the correlation functions w.r.t. $\mathfrak{D}$ in this subsection. For simplicity we write $\rho(d)$ instead of $\rho(\mathcal{D}_d)$.

The $p$-spin Hamiltonian $\mathcal{H}_p(x) = \sum_{i_1<i_2<\ldots<i_p} J_{i_1 i_2 \ldots i_p} x_{i_1} x_{i_2} \ldots x_{i_p}$ was introduced in order to bridge the gap between the Sherrington-Kirkpatrick (SK) model [27], which is the special case $p = 2$, and the random energy model discussed above. The coefficients $J_{i_1 i_2 \ldots i_p}$ are i.i.d. Gaussian random variables with mean 0 and unit variance.[3]

**Theorem 9.** Let $\Xi$ be a $p$-spin type model with an arbitrary distribution of the non-zero coefficients $J_{i_1 i_2 \ldots i_p}$, $i_1 < i_2 < \ldots < i_p$. Then

$$\mathcal{E}[\rho(d)] = R(d) = \omega_p(d) = \frac{1}{\binom{n}{p}(\alpha-1)^p} \sum_{j=0}^{p} (-1)^j (\alpha-1)^{p-j} \binom{d}{j} \binom{n-d}{p-j} \tag{27}$$

[3] In Derrida's original formulation the variance was chosen to be $S_p^2 = p!/n^p$, such that the variance of the Hamiltonian itself is independent of $n$.

is a suitably normalized Krawtchouk polynomial of degree $p$.

**Proof.** Each realization of a $p$-spin model is an elementary landscape on the boolean hypercube. This is still true if the non-zero (Fourier) coefficients are correlated as long as they belong to the same eigenvalue $\lambda_p$. Thus the correlation function $\rho(d)$ is given by the left eigenvector $\omega_p$ of the collapsed adjacency matrix $\hat{\mathbf{A}}$ belonging to the eigenvalue $\mu_p = D - \lambda_p$. For Hamming graphs (sequence spaces) these vectors are known to be suitably normalized Krawtchouk polynomials of degree $p$, see e.g., [58, 34]; these polynomials play an important role in coding theory [59, 60]. Since the $p$-spin models are elementary we conclude immediately $\mathcal{E}[\rho(d)] = \omega_p(d)$. In [26] the identity $R(d) = \omega_p(d)$ has been shown by direct computation of the autocorrelation function $R$. ∎

**Corollary.** The average correlation $w$ vanishes under the assumptions of theorem 9.

**Proof.** We have $\tilde{B}_p = B_p$ for all $p \geq 0$ as an immediate consequence of theorem 9. In particular, $\tilde{B}_0 = w/s^2 = B_0 = 0$, and therefore $w = 0$. ∎

**Theorem 10.** Derrida's $p$-spin models are isotropic w.r.t. the distance partition $\mathfrak{D}$ on the boolean hypercube for all $p > 0$.

**Proof.** By definition of the $p$-spin Hamiltonian we have $\mathcal{E}[J^2_{i_1 i_2 \ldots i_p}] = 1$ and thus $\mathcal{E}[a^2_{i_1 i_2 \ldots i_p}] = |V|$. Furthermore the coefficients have mean zero and are uncorrelated. Thus theorem 3 guarantees that the $p$-spin Hamiltonian is *-isotropic. Since $\mathfrak{D}$ is a symmetric association scheme $\mathcal{H}_p$ is isotropic w.r.t. the distance partition $\mathfrak{D}$ on the boolean hypercube. ∎

### 8.3. Superpositions of Random Fields

For the next result we have to state precisely what we mean by a "sum" of random fields.

**Definition**. Let $\Xi_i = (\{f : V \to \mathbb{R}\}, \boldsymbol{\mu}_i)$ be random fields on $\Gamma$. The *superposition* of two random fields on $\Gamma$ with fixed coefficients $a, b \in \mathbb{R}$ is the probability space

$$a\Xi_1 + b\Xi_2 \stackrel{\text{def}}{=\!=} (\{f : V \to \mathbb{R}\}, \boldsymbol{\mu}^*) \quad \text{with} \quad \boldsymbol{\mu}^*(f) = \int_g \boldsymbol{\mu}_1(\frac{1}{a}g)\boldsymbol{\mu}(\frac{1}{b}(f-g)).$$

The effect of this definition is that elements of the probability spaces $\Xi_i$ are added as independent random variables: $f(x) = af_1(x) + bf_2(x)$ for all $x \in V$.

**Theorem 11.** A Gaussian isotropic random field on the Boolean hypercube is a superposition of $p$-spin models with independent coefficients.

**Proof.** On a boolean hypercube *-isotropy and isotropy w.r.t. the distance partition $\mathfrak{D}$ is the same. Consider the Fourier expansion of $\Xi$. Since the random field is isotropic, theorem 3 guarantees that the Fourier coefficients are uncorrelated random variables and that their variance depends only on $p$. Furthermore, for Gaussian distribution functions uncorrelatedness implies independence. Therefore, the coefficients are i.i.d. Gaussian random variables for each value of $p$, and $S_p^2 \stackrel{\text{def}}{=\!=} \mathcal{E}[J^2_{i_1 i_2 \dots i_p}]$ is well-defined. Hence any Gaussian isotropic random field is of the form $\Xi = \sum_p S_p \mathcal{H}_p(\sigma)$. ∎

As a consequence, a Gaussian REM on a Boolean hypercube – that is, Derrida's original model – is a superposition of $p$-spin models. Derrida argued that the REM is the limit $p \to \infty$ of the $p$-spin models. We are now in the position to make the sense in which this is true more precise. We have seen that $B_p = 2^{-n}\binom{n}{p}$, hence the REM is a superposition of a "continuum" of $p$-spin models with $p \approx n/2$. The width of this peak in the $\tilde{B}_p$-spectrum is on the order $\mathcal{O}(\sqrt{n})$.

### 8.4. Kauffman's Nk Models

The Nk model assigns a real valued "fitness" to the bit string $\mathbf{b}$ by first assigning a real valued "fitness contribution", $f_i$ , to the $i^{\text{th}}$ bit, $b_i$, in $\mathbf{b}$. Each such assignment depends, not just on $i$ and the value of $b_i$, but also on $0 \le k < n$ other bits, which we call its "neighbors". The fitness contribution of each site is a random function, $f_i(\mathbf{b}_i)$, of the substring, $\mathbf{b}_i$, formed by the $i^{\text{th}}$ bit and its $k$ neighbors. $f_i(\mathbf{b}_i)$ is assigned by selecting an independent random variable from some distribution, such as the uniform or Gaussian distributions, for each of the $2^{k+1}$ possible values of $\mathbf{b}_i$, thus generating a "fitness table" for the $i^{\text{th}}$ site. There is a different, independently generated table for each of the $n$ sites. Then, given any string of $n$ bits, the total fitness of the string, $f$, is defined as the average of the fitness contributions of each site; that is,

$$f(\mathbf{b}) = \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{b}_i). \tag{28}$$

The Nk model comes a different "flavors" depending on the choice of neighbors influencing a particular site fitness. The simplest — but not the only — way of choosing neighbors, at least for even $k$, is to use the $k$ sites adjacent to site $i$; that is, the bits at sites $i - k/2$ through $i + k/2$. Let us use the convention that site $i$ is influenced by the $k/2$ sites to its right and to its left if $k$ is even and by $(k-1)/2$ sites to is left and $(k+1)/2$ sites to its right for odd $k$. As in the original formulation of the model, we introduce periodic boundary conditions to assign neighbors to sites $i$ with $i \le k/2$ and $i \ge n - k/2$. In other words, we assume that the sites are arranged in a circle, such that site $n$ is next to site 1. This choice of neighbors gives rise to a class of short range spin glasses. We will call this arrangement the "*adjacent neighborhood*" model, AN. Alternatively, we could assign the neighbors by randomly selecting, for each site $i$, $k$ other sites. This assignment of neighbors makes the model similar to a long range, dilute spin glass. It will be referred to as "*random neighborhood*" model, RN. In a third variation we drop the requirement

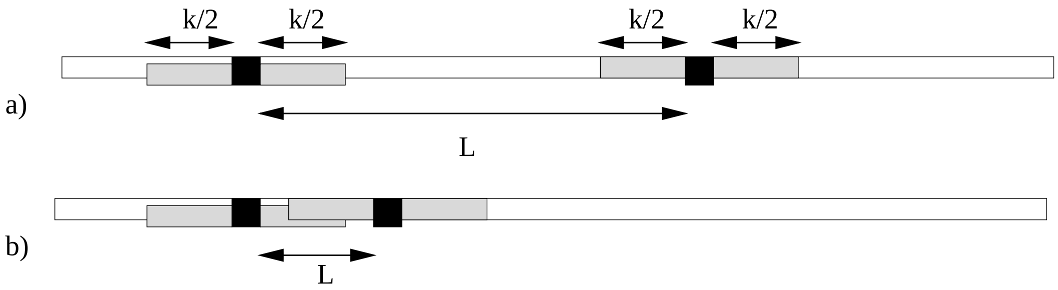


**Figure 1:** Sites influenced by point mutations in an AN-Nk model.
The black squares indicate the positions of two point mutations. The grey bars mark all sites whose site fitness values differ between the wild-type and the mutant. The number of such sites depends on the separation $\ell$ between the mutated positions.
a) $\ell \geq k$, b) $\ell < k$.

that $f_i$ depends on bit $i$. This version will be called "*purely random*" model, PR. The Nk model reduces to the REM for $k+1=n$, see e.g., [51].

**Theorem 12.** The RN and the PR version of the Nk model are isotropic w.r.t. $\mathfrak{D}$. The AN version of the Nk model is not isotropic w.r.t. $\mathfrak{D}$.

**Proof.** Let us first consider isotropy of Nk models. Let $c_0$ and $c_1^2$ be the mean and variance of the entries of the fitness tables, respectively. It is trivial to check then, that

$$\mathcal{E}[f(x)] = c_0 \qquad \text{and} \qquad \mathrm{Var}[f(x)] = \frac{1}{n}c_1^2 \,.$$

Thus the conditions (i) and (ii) for isotropy are always satisfied.
Explicit constructing the covariance matrix yields

$$\begin{aligned}
\mathbf{C}_{xy} =& \frac{1}{n^2}\sum_{i,j}\{\mathcal{E}[f_i(x)f_j(y)] - \mathcal{E}[f_i(x)]\mathcal{E}[f_j(y)]\} \\
=& \frac{1}{n^2}\sum_{i}\{\mathcal{E}[f_i(x)f_i(y)] - \mathcal{E}[f_i(x)]\mathcal{E}[f_j(y)]\} \\
=& \frac{1}{n^2}c_1^2\mathcal{E}\left[|\{i \in \mathbb{N} \,|\, f_i(x) = f_i(y)\}|\right] \stackrel{\text{def}}{=\!=} \frac{c_1^2}{n^2}[n - U(x,y)]\,.
\end{aligned}$$

The crucial quantity here is the number

$$U(x,y) = \mathcal{E}\left[\,\left|\,\{i \in \mathbb{N} \,|\, f_i(x) \neq f_i(y)\,\}\,\right|\,\right]$$

of entries in the site fitness tables that are different for the strings $x$ and $y$. Thus an Nk model is isotropic w.r.t. to a partition $\mathfrak{R}$ if and only if $U$ is constant on the classes of $\mathfrak{R}$.

Both the RN and the PR version of the Nk model do not imply any particular arrangement between the sites (i.e., the fact that we write them as a linear sequence with a particular order is irrelevant). In both models the sites contributing to the site-fitnesses $f_i$ are assigned independently and uniformly with the table entries themselves. As an immediate consequence, $U(x,y)$ depends only on the number of positions that are differ between $x$ and $y$, and thus $\mathcal{N}_{PR}$ and $\mathcal{N}_{RN}$ are isotropic w.r.t. the distance partition $\mathfrak{D}$ on the boolean hypercube for all $k$.

The situation is different in the AN version of the Nk model with $k \geq 1$. Consider a sequence $x$ and its two-error mutants $x^{r,s}$ which differ in the positions $r$ and $s$ with $r < s$. The the number of positions between $r$ and $s$ is $\ell \stackrel{\text{def}}{=} \min\{s-r, n+r-s\}-1$. Figure 1 shows that there the table entries for $2(k+1)$ sites are affected if the two point mutations are $\ell \geq k$ sites apart from each other. On the other hand, only $2+k+\ell < 2(k+1)$ sites are affected if $\ell < k$. $U(x, x^{r,s})$ depends explicitly on $\ell$ for all $k > 0$ and consequently the adjacent neighbor Nk model $\mathcal{N}_{AN}$ cannot be isotropic w.r.t. the distance partition $\mathfrak{D}$ on the boolean hypercube. ∎

**Lemma 3.** All three versions of the Nk model discussed above are pseudo-isotropic random fields.

**Proof.** The PR and the RN version are isotropic (and therefore also pseudo-isotropic) as a consequence of theorem 4. In the AN-version pseudo-isotropy is guaranteed by the cyclic boundary conditions. In this case $\mathbf{C}_{xy}$ depends on the relative location of the difference between $x$ and $y$ but neither on their absolute position in the sequences nor on the sequence of $x$ itself. Thus the sum of $\mathbf{C}_{xy}$ over all possible $y$ is independent of $x$. ∎

The autocorrelation functions $R$ w.r.t. the distance partition $\mathfrak{D}$ of the boolean hypercube are known explicitly for all the three versions of the Nk model discussed above. For a derivation see, e.g., the appendix of [25].

**Proposition.** The "direct" autocorrelation functions of the the Nk model with random, purely random, and adjacent neighborhood, respectively, are given by

$$\begin{aligned} R_{RN}(d) &= (1-\frac{d}{n})(1-\frac{k}{n-1})^d \\ R_{PR}(d) &= (1-\frac{k+1}{n})^d \\ R_{AN}(d) &= 1-\frac{k+1}{n}d+\frac{1}{\binom{n}{d}}\sum_{j=1}^{\min(k,n+1-d)}(k-j+1)\binom{n-j-1}{d-2}. \end{aligned} \tag{29}$$

**Theorem 13.** The autocorrelation function of the adjacent neighbor Nk model, $R_{AN}$, is a polynomial of degree $k+1$. It is therefore of the form

$$R_{AN}(d) = \sum_{p=0}^{k+1} \tilde{B}_p \omega_p(d). \tag{30}$$

**Proof.** We start by rewriting $R_{AN}$ without using binomial coefficients:

$$\begin{aligned} R_{AN}(d) &= 1-\frac{k+1}{n}d+\sum_{j=1}^{\min(k,n+1-d)}(k+1-j)\frac{(n-j-1)!\,d!\,(n-d)!}{(n-j-d+1)!\,(d-2)!\,n!} \\ &= 1-\frac{k+1}{n}d+\frac{d(d-1)}{n(n-1)}\sum_{j=1}^{k}(k+1-j)\prod_{\ell=0}^{j-2}\frac{n-d-\ell}{n-2-\ell} \end{aligned}$$

where an empty product is 1 by definition. This is obviously a polynomial in $d$. We have for $k \geq 1$

$$\text{Degree}[R_{AN}] = \max\left\{0;\ 1;\ 2+\max_{1\leq j\leq k}[j-1]\right\} = k+1,$$

since $d^{k-1}$ appears with non-zero coefficient in the product. For $k=0$ we have explicitly $R_{AN}(d) = 1-d/n$, i.e., the degree is 1. The Krawtchouk polynomial $\omega_j$ has degree $j$, and thus we can write $R_{AN}$ as a superposition of the eigenfunctions $\omega_j$ for $j \leq k+1$. ∎

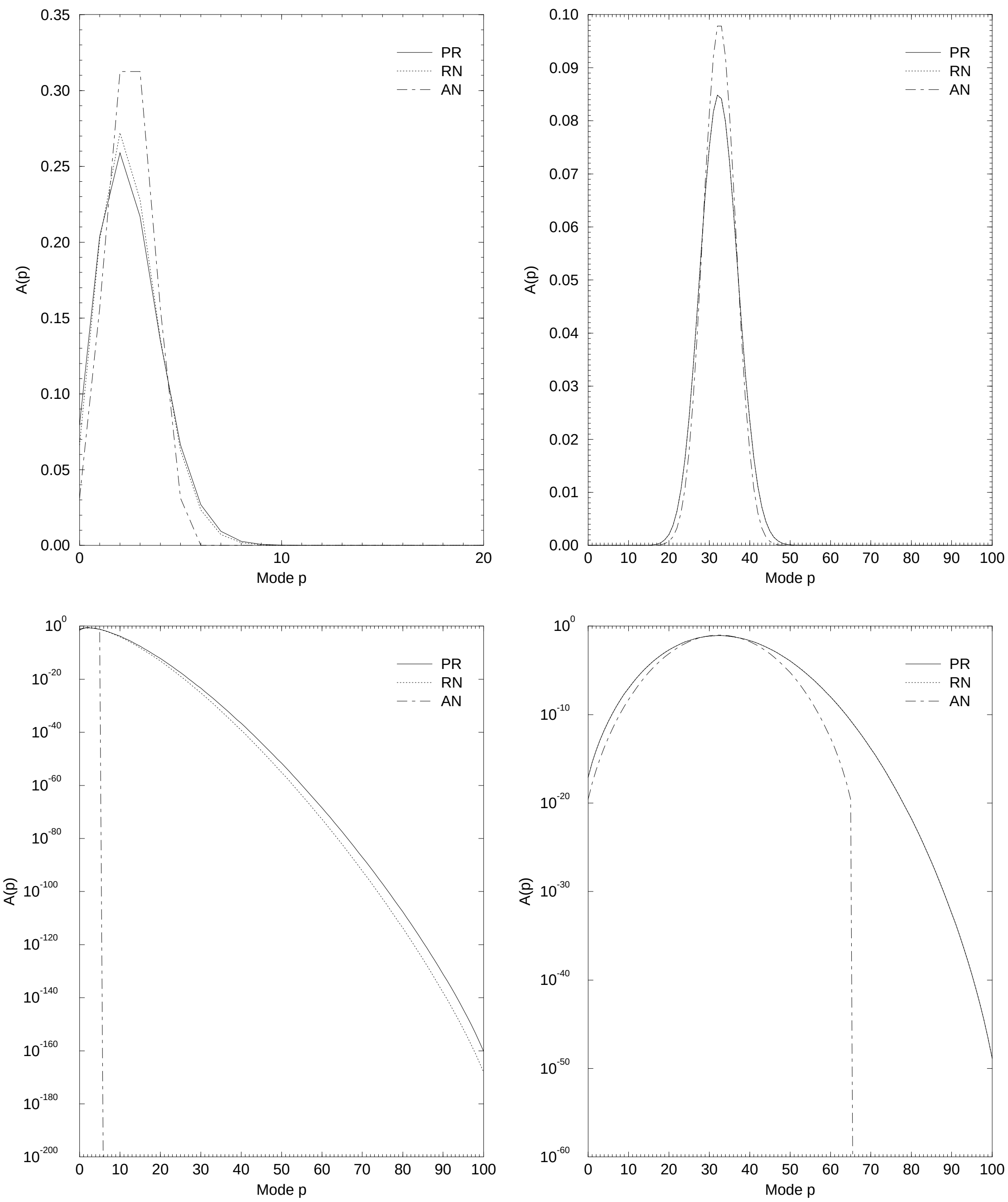


**Figure 2:** Spectral decompositions of Nk models on boolean hypercubes with $n{=}100$.
Left side: $k{=}4$; right side: $k{=}64$.
Numerical data strongly suggest that for the AN model the symmetry relation $\tilde{B}_p = \tilde{B}_{k+1-p}$ holds for all $n$. The logarithmic plots (bottom) emphasize that the two random neighborhood Nk models involve all modes $0 \le p \le n$ for all $k$ while the AN models are superpositions of the modes $0 \le p \le k+1 \le n$.

The coefficients $\tilde{B}_p$ of the spectrum can be obtained explicitly for sequence spaces, if the correlation function $R(d)$ is known as we have seen in section 8.1. For Nk models $\tilde{B}_p = \langle R;\omega_p\rangle \,/\, \langle\omega_p;\omega_p\rangle$ has been evaluated using `Mathematica` and `Reduce`. The results are shown in Figure 2. In particular, in case of the AN-version the data suggest the following

**Conjecture.** The coefficients $\tilde{B}_p$ of the AN-Nk model are independent of the system size $n$, and fulfill the symmetry relation

$$\tilde{B}_p = \tilde{B}_{k+1-p} \qquad \text{for all} \quad 0 \le p \le k+1\,,$$

and $i < j$ implies $\tilde{B}_i < \tilde{B}_j$ provided $j < (k+1)/2$ and $\tilde{B}_i > \tilde{B}_j$ provided $i > (k+1)/2$.

We have checked this conjecture for a large number of special cases in the range $n \le 200$ and $0 \le k < n$ using `Mathematica`.

Based on a comparison of correlation lengths it has been suggested [26] that Nk models roughly resemble $p$-spin models with $2p = k+1$. This assumption is supported by the $\tilde{B}_p$-spectra of the Nk models showing that the dominating modes are those centered around $(k+1)/2$ for all three versions of the Nk model, see Figure 2.

The major difference between the different versions of Nk models is that for the AN model only the first $k+1$ coefficients play a role, while for the other two models all modes of the Fourier expansion contribute. An interesting observation in this context [61] is the following: The Nk decision problem *"Is the global optimum of a given Nk model larger than some specified value $M$?"* can be solved in $\mathcal{O}(2^{k+1}n)$-time for the AN version, while the RN and PR versions are NP-complete for $k \ge 3$.

### 8.5. Superposition of Nk Models

We have seen that all isotropic random fields on the Boolean hypercube can be constructed by superpositions of $p$-spin models. In the following we will show that Nk-models *cannot* be used for this purpose. Let $\{\mathcal{N}_k(x)\}$ denote a set of Nk models with different parameters $k$, such that

$$\mathcal{E}[\mathcal{N}_i(x)\mathcal{N}_j(y)] - \mathcal{E}[\mathcal{N}_i(x)]\mathcal{E}[\mathcal{N}_j(y)] = 0$$

whenever $i \neq j$. That is, we assume that the entries in the fitness tables are uncorrelated also between different Nk random fields. Given the construction of the Nk model this seems to be a very natural assumption. Then we have

**Theorem 14.** Denote by $\tilde{B}_p$ the spectrum of the correlation function of a random field of the form $\Xi = \sum_{k=0}^{k_{\max}} \beta_k \mathcal{N}_k$, i.e., $\Xi$ is a superposition of Nk models. Then $\tilde{B}_p > 0$ for all $p \leq k_{\max} + 1$. Furthermore $\tilde{B}_p > 0$ for all $p \leq n$ if at least one of the Nk models $\mathcal{N}_k$ is an RN or a PR version of the Nk model.

**Proof.** We have

$$\mathcal{E}[f(x)f(y)] - \mathcal{E}[f(x)]\mathcal{E}[f(y)] = \sum_{i,j} \beta_i\beta_j \mathcal{E}[\mathcal{N}_i(x)\mathcal{N}_j(y)] - \mathcal{E}[\mathcal{N}_i(x)]\mathcal{E}[\mathcal{N}_j(y)]$$

$$= \sum_{k=0}^{k_{\max}} \beta_k^2 \left\{\mathcal{E}[\mathcal{N}_k(x)\mathcal{N}_k(y)] - \mathcal{E}[\mathcal{N}_k(x)]\mathcal{E}[\mathcal{N}_k(y)]\right\} .$$

Now let $\overline{c}_k$ denote the covariance function $\mathcal{N}_k$. Thus

$$\overline{c}(\mathcal{X}) = \sum_{k=0}^{m_{\max}} \beta_k^2 \overline{c}_k(\mathcal{X}) = \sum_{k=0}^{m_{\max}} \beta_k^2 \sum_{p=0}^{n} A_p^{(k)} \omega_p(\mathcal{X}) = \sum_{p=0}^{n} \left[\sum_{k=0}^{m_{\max}} \beta_k^2 A_p^{(k)}\right] \omega_p(\mathcal{X})$$

Therefore we have $\overline{c}(\mathcal{X}) = \sum_{p=0}^{n} A_p \omega_p(\mathcal{X})$ with $A_p \stackrel{\text{def}}{=} \sum_{k=0}^{m_{\max}} \beta_k^2 A_p^{(k)} \geq 0$. The coefficients $A_p$ are strictly positive as long as $A_p^{(k)} > 0$, which is true for all $p \leq k_{\max} + 1$ in the AN case, and for all $p$ in the other two versions of the Nk-model. The definition of the coefficients $\tilde{B}_p$ completes the proof. ∎

**Corollary.** A $p$-spin model cannot be represented as a superposition of Nk models for all $p \geq 1$. $\mathcal{E}[\chi(\mathcal{X})]$ coincides for the Nk models with $k = 0$ and the 1-spin model $\mathcal{H}_1$.

An obvious consequence is then the following

**Corollary.** An Nk model with $k > 0$ is not elementary.

## 9. Discussion

We have developed a mathematical framework for a detailed analysis of random field models of fitness landscapes. The two basic ingredients are partitions $\mathfrak{R}$ of $V \times V$ which exhibit sufficient algebraic regularity and the expansion of the random field $\Xi$ in terms of a Fourier basis, i.e., with respect to an orthonormal basis of eigenfunctions of the graph Laplacian $-\Delta$. The most useful results are obtained when $\mathfrak{R}$ is at least a coherent configuration or even a symmetric association scheme. The most important examples of regular configuration spaces lead in a very natural way to such highly regular partitions: The distance partition of distance regular graphs, such as the Hamming graphs (sequence spaces) and the Johnson graphs, form a symmetric association scheme [45].

Isotropy is an important property of a random field as it has become clear in computer simulations [3, 62] that plateaus, ridges, and other anisotropies strongly influence adaptation on a landscape [14, 15]. Isotropic random fields are characterized by their Fourier coefficients. In particular, on a boolean hypercube all isotropic random fields are superpositions of Derrida's $p$-spin models.

The autocorrelation function of the random field $R$ and the expected correlation function $\rho$ of a single instance can be expressed in terms of the Fourier expansion of the random field itself. On finds that the correlation functions are in general expansions in terms of the correlation functions $\omega_p$ of elementary random fields on the configuration space under consideration. These functions $\omega_p$ can be computed analytically for a number of problems, since they are the left eigenvectors of the collapsed adjacency matrix of the underlying configuration space. They only depend on the graph structure of the configuration space but not on the fitness function. For sequence spaces (Hamming graphs) they are suitably normalized Krawtchouk polynomials. The coefficients $B_p$ and $\tilde{B}_p$, resp., of such an expansion are sums of squares of the Fourier coefficients and measure the relative importance of the different "modes". Instead of the correlation function we can then use the "spectrum", that is the coefficients of this decomposition, as a means of specifying the random field. On a boolean hypercube, for instance, the $\tilde{B}_p$-spectrum can be interpreted directly as the relative importance of $p$-ary (spin) interactions.

We have shown that for a number of examples, notably for $p$-spin Hamiltonians the expected correlation function $\rho$ within a single landscapes (instance) coincides with the correlation function $R$ of the random field itself. This is not true in general. A comparison of the definition of the coefficients $B_p$ and $\tilde{B}_p$ reveals that a non-zero value of the average correlation $w$ of the random field will cause the two correlation measures to be different. For instance, the correlation functions $R$ of the Nk models yield a non-zero coefficient $\tilde{B}_0$ and therefore $w \neq 0$.

The formalism derived in this contribution suggests to approximate a given landscape by a superposition of statistical models that are elementary random fields. The coefficients of such a superposition can be obtained by observing that the correlation function is a superposition of the correlation functions of the individual elementary random fields under consideration. An application of this technique to RNA free energy landscapes is reported in [63]. In this contribution we have computed the $\tilde{B}_p$-spectrum of Kauffman's Nk models in order to illustrate this idea.

As a practical application of these results we suggest to replace a computationally expensive landscapes (such as the RNA landscapes in [3, 62, 50, 25, 64, 48]) by simpler statistical models with the same correlation function. The $B_p$-spectrum of the given landscape provides an efficient means for fitting a superposition of elementary random fields to the desired correlation structure.

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