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# Complex Networks Analysis of Combinatorial Spaces: the NK Landscape Case

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We propose a network characterization of combinatorial fitness landscapes by adapting the notion of inherent networks proposed for energy surfaces. We use the well-known family of  $NK$  landscapes as an example. In our case the inherent network is the graph whose vertices represent the local maxima in the landscape, and the edges account for the transition probabilities between their corresponding basins of attraction. We exhaustively extracted such networks on representative  $NK$  landscape instances, and performed a statistical characterization of their properties. We found that most of these network properties are related to the search difficulty on the underlying  $NK$  landscapes with varying values of  $K$ .

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## I. INTRODUCTION

Difficult combinatorial landscapes are found in many important problems in physics, computing, and in common everyday life activities such as resource allocation and scheduling. For example, spin-glass systems give rise to such energy landscapes which are characterized by many local minima and high energy barriers between them. These landscapes generally show frustration, i.e. frozen disorder where the system is unable to relax into a state in which all constraints are satisfied. In completely different fields, such as combinatorial optimization, similar hard problems also arise, for example the well-known *traveling salesman*

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*problem* and many others.

In order to understand the reasons that make these problems difficult to optimize, a number of model landscapes have been proposed. One of the simplest yet representative example is Kauffman’s family of  $NK$  landscapes [1]. The  $NK$  family of landscapes is a problem-independent model for constructing multimodal landscapes that can gradually be tuned from smooth to rugged, where the term “rugged” is intuitively related to the degree of variability in the objective function value in neighboring positions in configuration space. The more rugged the landscape, the higher the number of local optima, and the landscape becomes correspondingly more difficult to search for the global optimum. The idea of an  $NK$  landscape is to have  $N$  “spins” or “genes”, each with two possible values, 0 or 1. The model is a real stochastic function  $\Phi$  defined on binary strings  $s \in \{0, 1\}^N$  of length  $N$ ,  $\Phi : s \rightarrow \mathbb{R}_+$ . The value of  $K$  determines how many other spin values in the string influence a given spin  $s_i$ ,  $i = 1, \dots, N$ . The value of  $\Phi$  is the average of the contributions  $\phi_i$  of all the spins:

$$\Phi(s) = \frac{1}{N} \sum_{i=1}^N \phi_i(s_i, s_{i_1}, \dots, s_{i_K})$$

By increasing the value of  $K$  from 0 to  $N - 1$ ,  $NK$  landscapes can be tuned from smooth to rugged. For  $K = 0$  all contributions can be optimized independently which makes  $\Phi$  a simple additive function with a single maximum. At the other extreme when  $K = N - 1$  the landscape becomes completely random, the probability of any given configuration of being the optimum is  $1/(N + 1)$ , and the expected number of local optima is  $2^N/(N + 1)$ . Intermediate values of  $K$  interpolate between these two cases and have a variable degree of “epistasis”, i.e. of spin (or gene) interaction [1].

The  $K$  variables that form the context of the fitness contribution of gene  $s_i$  can be chosen according to different models. The two most widely studied models are the *random neighborhood* model, where the  $K$  variables are chosen randomly according to a uniform distribution among the  $N - 1$  variables other than  $s_i$ , and the *adjacent neighborhood* model, in which the  $K$  variables are those closest to  $s_i$  in a total ordering  $s_1, s_2, \dots, s_N$  (using periodic boundaries). No significant differences between the two models were found in terms of global properties of the respective families of landscapes, such as mean number of local optima or autocorrelation length [1, 2]. Similarly, our preliminary studies on the characteristics of the  $NK$  landscape optima networks did not show noticeable differences between the two neighborhood models. Therefore, we conducted our full study on the more general random model.

The  $NK$  model is related to spin glasses, and more precisely to  $p$ -spin models [3, 4], where  $p$  plays a role similar to  $K$ . In spin glasses the function analogous to  $\Phi$  is the energy  $H$  and the stable states are the minima of the energy hypersurface.

In this study we seek to provide fundamental new insights into the structural organization of the local optima in combinatorial landscapes, particularly into the connectivity of their basins of attraction. Combinatorial landscapes can be seen as a graph whose

vertices are the possible configurations. If two configurations can be transformed into each other by a suitable operator move, then we can trace an edge between them. The resulting graph, with an indication of the fitness at each vertex, is a representation of the given problem fitness landscape. A useful simplification of the graphs for the energy landscapes of atomic clusters was introduced in [5, 6]. The idea consists in taking as vertices of the graph not all the possible configurations, but only those that correspond to energy minima. For atomic clusters these are well-known, at least for relatively small assemblages. Two minima are considered connected, and thus an edge is traced between them, if the energy barrier separating them is sufficiently low. In this case there is a transition state, meaning that the system can jump from one minimum to the other by thermal fluctuations going through a saddle point in the energy hyper-surface. The values of these activation energies are mostly known experimentally or can be determined by simulation. In this way, a network can be built which is called the “inherent structure” or “inherent network” in [5, 7].

We propose a network characterization of combinatorial fitness landscapes by adapting the notion of *inherent networks* described above. We use the family of  $NK$  landscapes as an example. In our case the inherent network is the graph where the vertices are all the local maxima and the edges account for transition probabilities between maxima. We exhaustively extract such networks on representative small  $NK$  landscape instances, and perform a statistical characterisation of their properties. Our analysis is inspired, in particular, by the work of [5, 6] on energy landscapes, and in general, by the field of complex networks [8]. A related work can be found in [9], where the case of lattice polymer chains is studied. However, the notion of an edge there is very different, being related to moves that bring a given conformation into an allowed neighboring one. Similar ideas have been put forward in physical chemistry to understand the thermodynamics and kinetics of complex biomolecules through the network study of their free-energy landscapes [10]. It should also be noted that our approach is different from the barrier-tree representations of landscapes proposed by Stadler et al. (see, for example, [11]).

The next section describes how combinatorial landscapes are mapped onto networks, and includes the relevant definitions and algorithms used in our study. The empirical analysis of our selected  $NK$  landscape instances is presented in the following two sections; one devoted to the study of basins, and the other to the network statistical features. Finally, we present our conclusions and ideas for future work.

## II. LANDSCAPES AS NETWORKS

Many natural and artificial systems can be modeled as networks. Typical examples are communication systems (the Internet, the web, telephonic networks), transportation lines (railway, airline routes), biological systems (gene and protein interactions), and social interactions (scientific co-authorship, friendships). It has been shown in recent years that many of these networks

exhibit what has been called a *small-world* topology [8], in which nodes are highly clustered yet the path length between them is small. Additionally, in several of these networks the distribution of the number of neighbours (the degree distribution) is typically right-skewed with a “heavy tail”, meaning that most of the nodes have less-than-average degree whilst a small fraction of hubs have a large number of connections. These topological features are very relevant since they impact strongly on networks’ properties such as their robustness and searchability.

To model a physical energy landscape as a network, Doye [5] needed to decide first on a definition both of a state of the system and how two states were connected. The states and their connections will then provide the nodes and edges of the network. For systems with continuous degrees of freedom, this was achieved through the ‘inherent structure’ mapping. In this mapping each point in configuration space is associated with the minimum (or ‘inherent structure’) reached by following a steepest-descent path from that point. This mapping divides configurations into basins of attraction surrounding each minimum on the energy landscape.

Our goal is to adapt this idea to the context of combinatorial optimization. In our case, the vertices of the graph can be straightforwardly defined as the local maxima of the landscape. These maxima are obtained exhaustively by running a best-improvement local search algorithm (see Fig. 1) from every configuration of the search space. The definition of the edges, however, is a much more delicate matter. In our initial attempt [12] we considered that two maxima  $i$  and  $j$  were connected (with an undirected and unweighed edge), if there exists at least one pair of direct neighbors solutions  $s_i$  and  $s_j$ , one in each basin of attraction ( $b_i$  and  $b_j$ ). We found empirically on small instances of  $NK$  landscapes, that such definition produced densely connected graphs, with very low ( $\leq 2$ ) average path length between nodes for all  $K$ . Therefore, apart from the already known increase in the number of optima with increasing  $K$ , no other network property accounted for the increase in search difficulty. Furthermore, a single pair of neighbours between adjacent basins, may not realistically account for actual basin transitions occurring when using common heuristic search algorithms. These considerations, motivated us to search for alternative definitions of the edges connecting local optima. In particular, we decided to associate weights to the edges that account for the transition probabilities between the nodes (local optima). More details on the relevant algorithms and formal definitions are given below.

### A. Definitions and Algorithms

**Definition:** Fitness landscape [11].

A landscape is a triplet  $(S, V, f)$  where  $S$  is a set of potential solutions i.e. a search space,  $V : S \rightarrow 2^S$ , a neighborhood structure, is a function that assigns to every  $s \in S$  a set of neighbors  $V(s)$ , and  $f : S \rightarrow R$  is a fitness function that can be pictured as the *height* of the corresponding solutions.

In our study, the search space is composed by binary strings of length  $N$ , therefore its size is  $2^N$ . The neighborhood is defined by the minimum possible move on a binary search space, that is, the 1-move or bit-flip operation. In consequence, for any given string  $s$  of length  $N$ , the neighborhood size is  $|V(s)| = N$ .

The *HillClimbing* algorithm to determine the local optima and therefore define the basins of attraction, is given below:

```

Choose initial solution  $s \in S$ 
repeat
choose  $s' \in V(s)$  such that  $f(s') = \max_{x \in V(s)} f(x)$ 
if  $f(s) < f(s')$  then
 $s \leftarrow s'$ 
end if
until  $s$  is a Local optimum

```

FIG. 1: *HillClimbing* algorithm.

**Definition:** Local optimum.

A local optimum is a solution  $s^*$  such that  $\forall s \in V(s^*), f(s) < f(s^*)$ .

The *HillClimbing* algorithm defines a mapping from the search space  $S$  to the set of locally optimal solutions  $S^*$ .

**Definition:** Basin of attraction.

The basin of attraction of a local optimum  $i \in S$  is the set  $b_i = \{s \in S \mid \text{HillClimbing}(s) = i\}$ . The size of the basin of attraction of a local optimum  $i$  is the cardinality of  $b_i$ .

Notice that for non-neutral fitness landscapes, as are  $NK$  landscapes, the basins of attraction as defined above, produce a partition of the configuration space  $S$ . Therefore,  $S = \cup_{i \in S^*} b_i$  and  $\forall i \in S \forall j \neq i, b_i \cap b_j = \emptyset$

**Definition:** Edge weight.

For each pair of solutions  $s$  and  $s'$ , let us define  $p(s \rightarrow s')$  as the probability to pass from  $s$  to  $s'$  with the given neighborhood structure. In the case of binary strings of size  $N$ , and the neighborhood defined by the single bit-flip operation, there are  $N$  neighbors for each solution, therefore:

if  $s' \in V(s)$ ,  $p(s \rightarrow s') = \frac{1}{N}$  and

if  $s' \notin V(s)$ ,  $p(s \rightarrow s') = 0$ .

We can now define the probability to pass from a solution  $s \in S$  to a solution belonging to the basin  $b_j$ , as:

$$p(s \rightarrow b_j) = \sum_{s' \in b_j} p(s \rightarrow s')$$

Notice that  $p(s \rightarrow b_j) \leq 1$ .

Thus, the total probability of going from basin  $b_i$  to basin  $b_j$  is the average over all  $s \in b_i$  of the transition probabilities to solutions  $s' \in b_j$ :

$$p(b_i \rightarrow b_j) = \frac{1}{\#b_i} \sum_{s \in b_i} p(s \rightarrow b_j)$$

$\#b_i$  is the size of the basin  $b_i$ . We are now prepared to define our ‘inherent’ network or network of local optima.

**Definition:** Local optima network.

The local optima network  $G = (S^*, E)$  is the graph where the nodes are the local optima, and there is an edge  $e_{ij} \in E$  with weight  $w_{ij} = p(b_i \rightarrow b_j)$  between two nodes  $i$  and  $j$  if  $p(b_i \rightarrow b_j) > 0$ .

Notice that since each maximum has its associated basin,  $G$  also describes the interconnection of basins.

According to our definition of edge weights,  $w_{ij} = p(b_i \rightarrow b_j)$  may be different than  $w_{ji} = p(b_j \rightarrow b_i)$ . Thus, two weights are needed in general, and we have an oriented transition graph.

The following two definitions are relevant to the discussion of the boundary of basins.

**Definition:** Boundary of a basin of attraction.

The *boundary*  $B(b)$  of a basin of attraction  $b$  can be defined as the set of configurations within a basin that have at least one neighbor’s solution in another basin  $b'$ .

**Definition:** Interior of a basin of attraction.

Conversely, the *interior*  $I(b)$  of a basin is composed by the configurations that have all their neighbors in the same basin.

Formally,

$$B(b) = \{s \in b \mid \exists b' \neq b, \exists s' \in b', \exists e_{ss'} \in E\},$$

$$I(b) = b - B(b)$$

### III. EMPIRICAL ANALYSIS OF BASINS

In order to avoid sampling problems that could bias the results, we used the largest values of  $N$  that can still be analyzed exhaustively with reasonable computational resources. We thus extracted the local optima networks of landscape instances with  $N = 14, 16, 18$ , and  $K = 2, 4, 6, \dots, N - 2, N - 1$ . For each pair of  $N$  and  $K$  values, 30 randomly generated instances were explored. Therefore, the networks statistics reported below represent the average behaviour of 30 independent instances.

Besides the maxima network, it is useful to describe the associated basins of attraction as these play a key role in search algorithms. Furthermore, some characteristics of the basins can be related to the optima network features. The notion of the basin of attraction of a local maximum has been presented before. We have exhaustively computed the size and number of all the basins of attraction for  $N = 16$  and  $N = 18$  and for all even  $K$  values plus  $K = N - 1$ . In this section, we analyze the basins of attraction from several points of view as described below.

### A. Global optimum basin size versus $K$

In Fig. 2 we plot the average size of the basin corresponding to the global maximum for  $N = 16$  and  $N = 18$ , and all values of  $K$  studied. The trend is clear: the basin shrinks very quickly with increasing  $K$ . This confirms that the higher the  $K$  value, the more difficult for a stochastic search algorithm to locate the basin of attraction of the global optimum

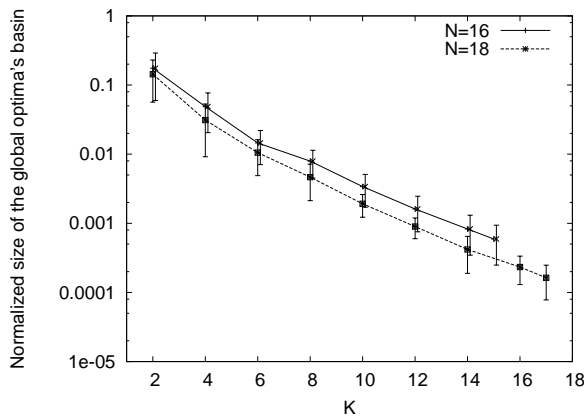


FIG. 2: Average of the relative size of the basin corresponding to the global maximum for each  $K$  over 30 landscapes.

### B. Number of basins of a given size

Fig. 3 shows the cumulative distribution of the number of basins of a given size (with regression line) for a representative instances with  $N = 18$ ,  $K = 4$ . Table I shows the average (of 30 independent landscapes) correlation coefficients and linear regression coefficients (intercept ( $\bar{\alpha}$ ) and slope ( $\bar{\beta}$ )) between the number of nodes and the basin sizes for instances with  $N = 16, 18$  and all for all the studied values of  $K$ . Notice that distribution decays exponentially or faster for the lower  $K$  and it is closer to exponential for the higher  $K$ . This observation is relevant to theoretical studies that estimate the size of attraction basins (see for example [13]). These studies often assume that the basin sizes are uniformly distributed, which is not the case for the  $NK$  landscapes studied here. From the slopes  $\bar{\beta}$  of the regression lines (table I) one can see that high values of  $K$  give



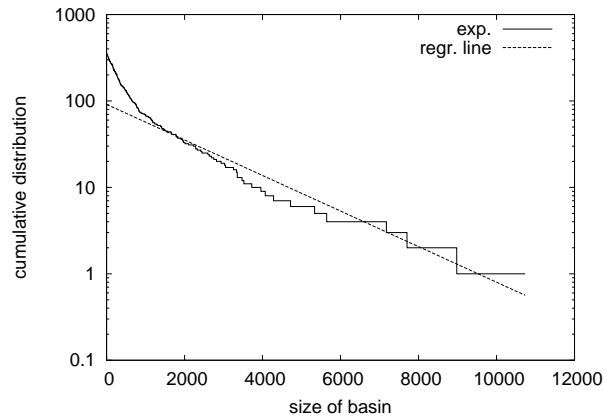


FIG. 3: Cumulative distribution of the number of basins of a given size with regression line. A representative landscape with  $N = 18$ , and  $K = 4$  is visualized. A lin-log scale is used.

rise to steeper distributions (higher  $\bar{\beta}$  values). This indicates that there are less basins of large size for large values of  $K$ . In consequence, basins are broader for low values of  $K$ , which is consistent with the fact that those landscapes are smoother.

### C. Fitness of local optima versus their basin sizes

The scatter-plots in Fig. 4 illustrate the correlation between the basin sizes of local maxima (in logarithmic scale) and their fitness values. Two representative instances for  $N = 18$  and  $K = 4, 8$  are shown. Notice that there is a clear positive correlation between the fitness values of maxima and their basins' sizes. In other words, the higher the peak the wider tend to be its basin of attraction. Therefore, on average, with a stochastic local search algorithm, the global optimum would be easier to find than any other local optimum. This may seem surprising. But, we have to keep in mind that as the number of local optima increases (with increasing  $K$ ), the global optimum basin is more difficult to reach by a stochastic local search algorithm (see Fig. 2). This observation offers a mental picture of  $NK$  landscapes: we can consider the landscape as composed of a large number of mountains (each corresponding to a basin of attraction), and those mountains are wider the taller the hilltops. Moreover, the size of a mountain basin grows exponentially with its height.

## IV. GENERAL NETWORK STATISTICS

We now briefly describe the statistical measures used for our analysis of maxima networks.

The standard clustering coefficient [8] does not consider weighted edges. We thus use the *weighted clustering* measure proposed by [14], which combines the topological information with the weight distribution of the network:

TABLE I: Correlation coefficient ( $\bar{\rho}$ ), and linear regression coefficients (intercept ( $\bar{\alpha}$ ) and slope ( $\bar{\beta}$ )) of the relationship between the basin size of optima and the cumulative number of nodes of a given (basin) size ( in logarithmic scale:  $\log(p(s)) = \alpha + \beta s + \epsilon$ ). The average and standard deviation values over 30 instances, are shown.

$N = 16$			
$K$	$\bar{\rho}$	$\bar{\alpha}$	$\bar{\beta}$
2	-0.944 <sub>0.0454</sub>	2.89 <sub>0.673</sub>	-0.0003 <sub>0.0002</sub>
4	-0.959 <sub>0.0310</sub>	4.19 <sub>0.554</sub>	-0.0014 <sub>0.0006</sub>
6	-0.967 <sub>0.0280</sub>	5.09 <sub>0.504</sub>	-0.0036 <sub>0.0010</sub>
8	-0.982 <sub>0.0116</sub>	5.97 <sub>0.321</sub>	-0.0080 <sub>0.0013</sub>
10	-0.985 <sub>0.0161</sub>	6.74 <sub>0.392</sub>	-0.0163 <sub>0.0025</sub>
12	-0.990 <sub>0.0088</sub>	7.47 <sub>0.346</sub>	-0.0304 <sub>0.0042</sub>
14	-0.994 <sub>0.0059</sub>	8.08 <sub>0.241</sub>	-0.0508 <sub>0.0048</sub>
15	-0.995 <sub>0.0044</sub>	8.37 <sub>0.240</sub>	-0.0635 <sub>0.0058</sub>
$N = 18$			
2	-0.959 <sub>0.0257</sub>	3.18 <sub>0.696</sub>	-0.0001 <sub>0.0001</sub>
4	-0.960 <sub>0.0409</sub>	4.57 <sub>0.617</sub>	-0.0005 <sub>0.0002</sub>
6	-0.967 <sub>0.0283</sub>	5.50 <sub>0.520</sub>	-0.0015 <sub>0.0004</sub>
8	-0.977 <sub>0.0238</sub>	6.44 <sub>0.485</sub>	-0.0037 <sub>0.0007</sub>
10	-0.985 <sub>0.0141</sub>	7.24 <sub>0.372</sub>	-0.0077 <sub>0.0011</sub>
12	-0.989 <sub>0.0129</sub>	7.98 <sub>0.370</sub>	-0.0150 <sub>0.0019</sub>
14	-0.993 <sub>0.0072</sub>	8.69 <sub>0.276</sub>	-0.0272 <sub>0.0024</sub>
16	-0.995 <sub>0.0056</sub>	9.33 <sub>0.249</sub>	-0.0450 <sub>0.0036</sub>
17	-0.992 <sub>0.0113</sub>	9.49 <sub>0.386</sub>	-0.0544 <sub>0.0058</sub>

$$c^w(i) = \frac{1}{s_i(k_i - 1)} \sum_{j,h} \frac{w_{ij} + w_{ih}}{2} a_{ij} a_{jh} a_{hi}$$

where  $s_i = \sum_{j \neq i} w_{ij}$ ,  $a_{nm} = 1$  if  $w_{nm} > 0$ ,  $a_{nm} = 0$  if  $w_{nm} = 0$  and  $k_i = \sum_{j \neq i} a_{ij}$ .

For each triple formed in the neighborhood of the vertex  $i$ ,  $c^w(i)$  counts the weight of the two participating edges of the vertex  $i$ .  $C^w$  is defined as the weighted clustering coefficient averaged over all vertices of the network.

The standard topological characterization of networks is obtained by the analysis of the probability distribution  $p(k)$  that a

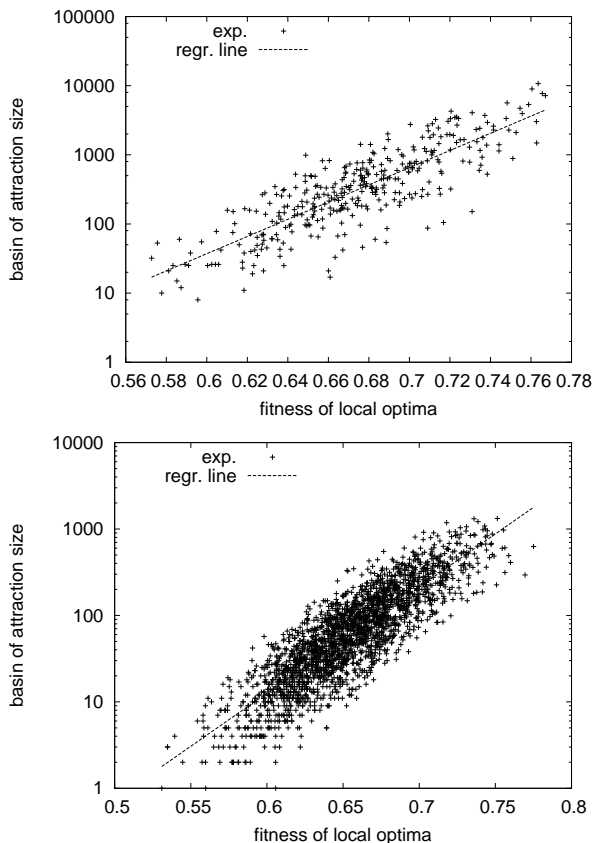


FIG. 4: Correlation between the fitness of local optima and their corresponding basin sizes, for two representative instances with  $N = 18$ ,  $K = 4$  (top) and  $K = 8$  (bottom).

randomly chosen vertex has degree  $k$ . For our weighted networks, a characterization of weights is obtained by the *connectivity and weight distributions*  $p_{in}(w)$  and  $p_{out}(w)$  that any given edge has incoming or outgoing weight  $w$ .

In our study, for each node  $i$ , the sum of outgoing edge weights is equal to 1 as they represent transition probabilities. So, an important measure is the weight  $w_{ii}$  of self-connecting edges (remaining in the same node). We have the relation:  $w_{ii} + s_i = 1$ . The vertex *strength*,  $s_i$ , is defined as  $s_i = \sum_{j \in \mathcal{V}(i) - \{i\}} w_{ij}$ , where the sum is over the set  $\mathcal{V}(i) - \{i\}$  of neighbors of  $i$  [14]. The strength of a node is a generalization of the node's connectivity giving information about the number and importance of the edges.

Another network measure we report here is *disparity* [14]  $Y_2(i)$ , which measures how heterogeneous are the contributions of the edges of node  $i$  to the total weight (strength):

$$Y_2(i) = \sum_{j \neq i} \left( \frac{w_{ij}}{s_i} \right)^2$$

The disparity could be averaged over the node with the same degree  $k$ . If all weights are nearby of  $s_i/k$ , the disparity for nodes of degree  $k$  is nearby  $1/k$ .

Finally, in order to compute the average shortest path between two nodes on the optima network of a given landscape, we considered the expected number of bit-flip mutations to pass from one basin to the other. This expected number can be computed by considering the inverse of the transition probabilities between basins. In other words, if we attach to the edges the inverse of the transition probabilities, this value would represent the average number of random mutations to pass from one basin to the other. More formally, the distance (expected number of bit-flip mutations) between two nodes is defined by  $d_{ij} = 1/w_{ij}$  where  $w_{ij} = p(b_i \rightarrow b_j)$ . Now, we can define the length of a path between two nodes as being the sum of these distances along the edges that connect the respective basins.

TABLE II:  $NK$  landscapes network properties. Values are averages over 30 random instances, standard deviations are shown as subscripts.  $n_v$  and  $n_e$  represent the number of vertexes and edges (rounded to the next integer),  $\bar{C}^w$ , the mean weighted clustering coefficient.  $\bar{Y}$  represent the mean disparity coefficient,  $\bar{d}$  the mean path length (see text for definitions).

$K$	$\bar{n}_v$	$\bar{n}_e$	$\bar{C}^w$	$\bar{Y}$	$\bar{d}$
$N = 14$					
2	14 <sub>6</sub>	200 <sub>131</sub>	0.98 <sub>0.0153</sub>	0.367 <sub>0.0934</sub>	76 <sub>194</sub>
4	70 <sub>10</sub>	3163 <sub>766</sub>	0.92 <sub>0.0139</sub>	0.148 <sub>0.0101</sub>	89 <sub>6</sub>
6	184 <sub>15</sub>	12327 <sub>1238</sub>	0.79 <sub>0.0149</sub>	0.093 <sub>0.0031</sub>	119 <sub>3</sub>
8	350 <sub>22</sub>	25828 <sub>1801</sub>	0.66 <sub>0.0153</sub>	0.070 <sub>0.0020</sub>	133 <sub>2</sub>
10	585 <sub>22</sub>	41686 <sub>1488</sub>	0.54 <sub>0.0091</sub>	0.058 <sub>0.0010</sub>	139 <sub>1</sub>
12	896 <sub>22</sub>	57420 <sub>1012</sub>	0.46 <sub>0.0048</sub>	0.052 <sub>0.0006</sub>	140 <sub>1</sub>
13	1085 <sub>20</sub>	65287 <sub>955</sub>	0.42 <sub>0.0045</sub>	0.050 <sub>0.0006</sub>	139 <sub>1</sub>
$N = 16$					
2	33 <sub>15</sub>	516 <sub>358</sub>	0.96 <sub>0.0245</sub>	0.326 <sub>0.0579</sub>	56 <sub>14</sub>
4	178 <sub>33</sub>	9129 <sub>2930</sub>	0.92 <sub>0.0171</sub>	0.137 <sub>0.0111</sub>	126 <sub>8</sub>
6	460 <sub>29</sub>	41791 <sub>4690</sub>	0.79 <sub>0.0154</sub>	0.084 <sub>0.0028</sub>	170 <sub>3</sub>
8	890 <sub>33</sub>	93384 <sub>4394</sub>	0.65 <sub>0.0102</sub>	0.062 <sub>0.0011</sub>	194 <sub>2</sub>
10	1, 470 <sub>34</sub>	162139 <sub>4592</sub>	0.53 <sub>0.0070</sub>	0.050 <sub>0.0006</sub>	206 <sub>1</sub>
12	2, 254 <sub>32</sub>	227912 <sub>2670</sub>	0.44 <sub>0.0031</sub>	0.043 <sub>0.0003</sub>	207 <sub>1</sub>
14	3, 264 <sub>29</sub>	290732 <sub>2056</sub>	0.38 <sub>0.0022</sub>	0.040 <sub>0.0003</sub>	203 <sub>1</sub>
15	3, 868 <sub>33</sub>	321203 <sub>2061</sub>	0.35 <sub>0.0022</sub>	0.039 <sub>0.0004</sub>	200 <sub>1</sub>
$N = 18$					
2	50 <sub>25</sub>	1579 <sub>1854</sub>	0.95 <sub>0.0291</sub>	0.307 <sub>0.0630</sub>	73 <sub>15</sub>
4	330 <sub>72</sub>	26266 <sub>7056</sub>	0.92 <sub>0.0137</sub>	0.127 <sub>0.0081</sub>	174 <sub>9</sub>
6	994 <sub>73</sub>	146441 <sub>18685</sub>	0.78 <sub>0.0155</sub>	0.076 <sub>0.0044</sub>	237 <sub>5</sub>
8	2, 093 <sub>70</sub>	354009 <sub>18722</sub>	0.64 <sub>0.0097</sub>	0.056 <sub>0.0012</sub>	273 <sub>2</sub>
10	3, 619 <sub>61</sub>	620521 <sub>20318</sub>	0.52 <sub>0.0071</sub>	0.044 <sub>0.0007</sub>	292 <sub>1</sub>
12	5, 657 <sub>59</sub>	899742 <sub>14011</sub>	0.43 <sub>0.0037</sub>	0.038 <sub>0.0003</sub>	297 <sub>1</sub>
14	8, 352 <sub>60</sub>	1163640 <sub>11935</sub>	0.36 <sub>0.0023</sub>	0.034 <sub>0.0002</sub>	293 <sub>1</sub>
16	11, 797 <sub>63</sub>	1406870 <sub>6622</sub>	0.32 <sub>0.0012</sub>	0.032 <sub>0.0001</sub>	283 <sub>1</sub>
17	13, 795 <sub>77</sub>	1524730 <sub>4818</sub>	0.30 <sub>0.0009</sub>	0.032 <sub>0.0001</sub>	277 <sub>1</sub>

## A. Detailed Study of Network Features

In this section we study in more depth some network features which can be related to stochastic local search difficulty on the underlying fitness landscapes. Table II reports the average (over 30 independent instances for each  $N$  and  $K$ ) of the network properties described.  $\bar{n}_v$  and  $\bar{n}_e$  are, respectively, the mean number of vertices and the mean number of edges of the graph for a given  $K$  rounded to the next integer.  $\bar{C}^w$  is the mean weighted clustering coefficient.  $\bar{Y}$  is the mean disparity, and  $\bar{d}$  is the mean path length.

### 1. Clustering Coefficients

The fourth column of table II lists the average values of the weighted clustering coefficients for all  $N$  and  $K$ . It is apparent that the clustering coefficients decrease regularly with increasing  $K$  for all  $N$ . For the standard unweighed clustering, this would mean that the larger  $K$  is, the less likely that two maxima which are connected to a third one are themselves connected. Taking weights, i.e. transition probabilities into account this means that either there are less transitions between neighboring basins for high  $K$ , and/or the transitions are less likely to occur. This confirms from a network point of view the common knowledge that search difficulty increases with  $K$ .

### 2. Shortest Path to the Global Optimum

The average shortest path lengths  $\bar{d}$  are listed in the sixth column of table II. Fig. 5 (top) is a graphical illustration of the average shortest path length between optima for all the studied  $NK$  landscapes. Notice that the shortest path increases with  $N$ , this is to be expected since the number of optima increases exponentially with  $N$ . More interestingly, for a given  $N$  the shortest path increases with  $K$ , up to  $K = 10$ , and then it stagnates and even decreases slightly for the  $N = 18$ . This is consistent with the well known fact that the search difficulty in  $NK$  landscapes increases with  $K$ . However, some paths are more relevant from the point of view of a stochastic local search algorithm following a trajectory over the maxima network. In order to better illustrate the relationship of this network property with the search difficulty by heuristic local search algorithms, Fig. 5 (bottom) shows the shortest path length to the global optimum from all the other optima in the landscape. The trend is clear, the path lengths to the optimum increase steadily with increasing  $K$ .

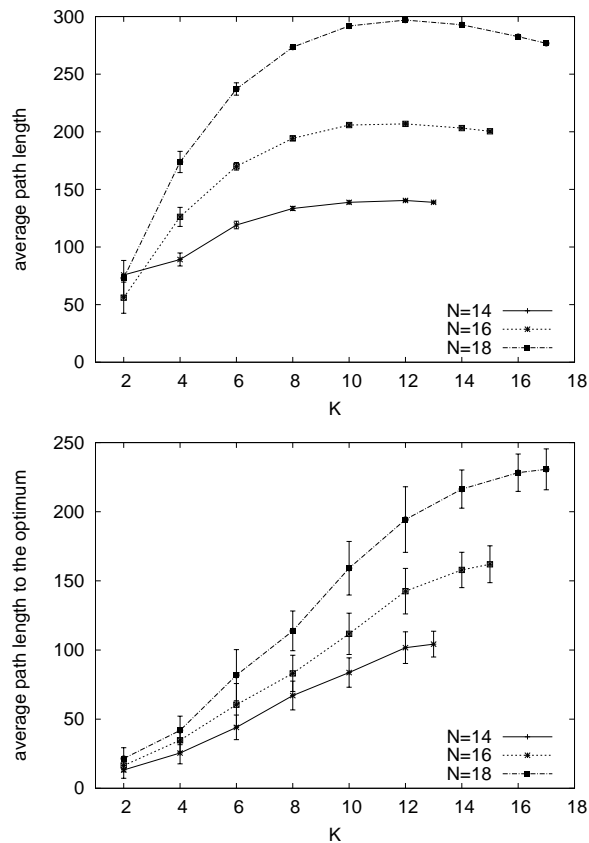


FIG. 5: Average distance (shortest path) between nodes (top), and average path length to the optimum from all the other basins (bottom).

### 3. Outgoing Weight Distribution

Here we report on the outgoing weight distributions  $p_{out}(w)$  of the maxima network edges. Fig. 6 shows the empirical probability distribution function for the cases  $N = 16$  and  $N = 18$  (logarithmic scale has been used on the x-axis). The case  $N = 14$  is similar but is not reported here because it is much more noisy for  $K = 2$  and 4 due to the small size of the graphs in these cases (see table II). One can see that the weights, i.e. the transition probabilities to neighboring basins are small. The distributions are far from uniform and, for both  $N = 16$  and  $N = 18$ , the low  $K$  have longer tails. For high  $K$  the decay is faster. This seems to indicate that, on average, the transition probabilities are higher for low  $K$ .

We have already remarked that the approach taken in [5, 6, 9] is different in that edges between two optima either exist or not; in other words the notion of transition probability is absent. However, it is worth recalling that Doye et al. [5, 6] found that their inherent networks were of the scale-free type with the global minimum being often the most connected node. The landscape is thus essentially a “funnel” meaning that the system can relax to the global minimum from almost any other local minimum. In our language, we would say that this kind of landscape is an ‘easy’ one to search. In contrast, the inherent networks found by

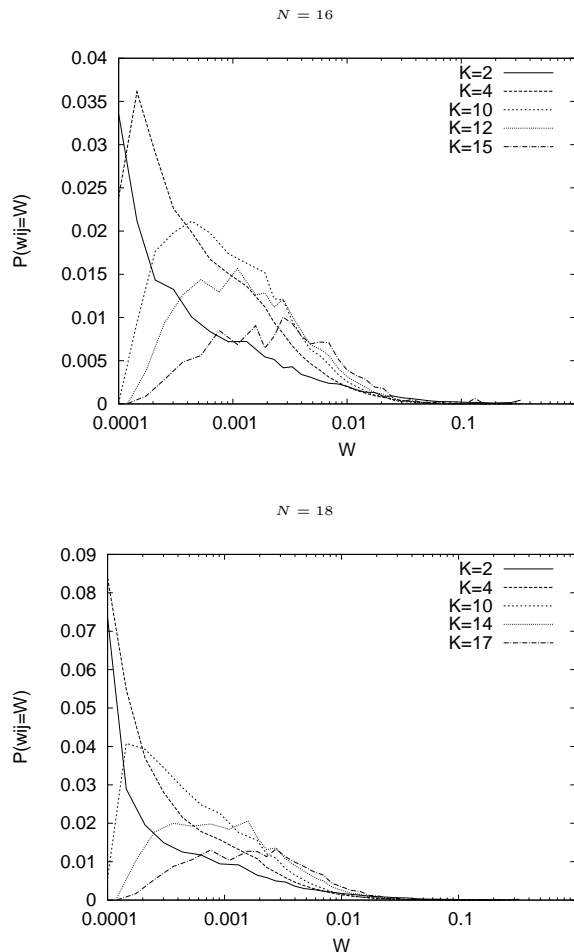


FIG. 6: Probability distribution of the network weights  $w_{ij}$  for outgoing edges with  $j \neq i$  in log-scale on x-axis. Averages of 30 instances for each  $N$  and  $K$  are reported.

Scala et al. [9] for lattice polymer chains are of the small-world type but they show a fast-decaying degree distribution function.

#### 4. Disparity

Fig. 7 depicts the disparity coefficient as defined in the previous section for  $N = 16, 18$ . An interesting observation is that the disparity (i.e. inhomogeneity) in the weights of a node's out-coming links tends to decrease steadily with increasing  $K$ . This reflects that for high  $K$  the transitions to other basins tend to become equally likely, which is another indication that the landscape, and thus its representative maxima network, becomes more random and difficult to search.

When  $K$  increases, the number of edges increases and the number of edges with a weight over a certain threshold increases too (see fig. 6). Therefore, for small  $K$ , each node is connected with a small number of nodes each with a relative high weight. On the other hand, for large  $K$ , the weights become more homogeneous in the neighbourhood, that is, for each node, all the

neighboring basins are at similar distance.

If we make the hypothesis that edges with higher weights are likely to be connected to nodes with larger basins (an intuition that we need to confirm in future work) then, as the larger basins tend to have higher fitness (see Fig. 4), the path to higher fitness values would be easier to find for lower  $K$  than for larger  $K$ .

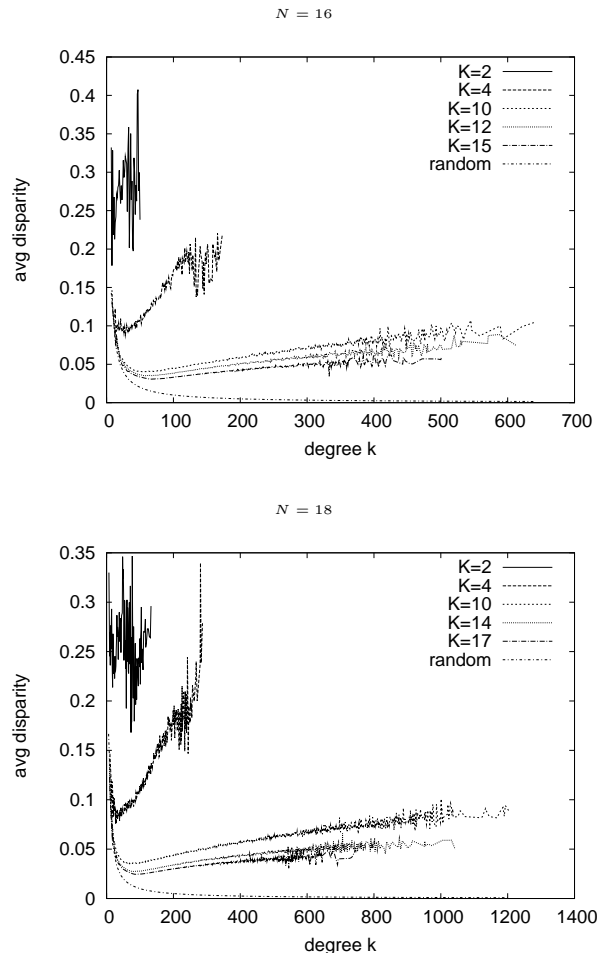


FIG. 7: Average disparity,  $Y_2$ , of nodes with a given degree  $k$ . Average of 30 independent instances for each  $N$  and  $K$  are reported. The curve  $1/k$  is also reported to compare to random case.

### 5. Boundary of basins

Fig. 8 shows the averages, over all the nodes in the network, of the weights  $w_{ii}$  (i.e. the probabilities of remaining in the same basin after a bit-flip mutation). Notice that the weights  $w_{ii}$  are much higher when compared to those  $w_{ij}$  with  $j \neq i$  (see Fig. 6). In particular, for  $K = 2$ , 50% of the random bit-flip mutations will produce a solution within the same basin of attraction. These average probabilities of remaining within the same basin, are above 12% for the higher values of  $K$ . Notice that the averages



are nearly the same regardless the value of  $N$ , but decrease with the epistatic parameter  $K$ .

The exploration of new basins with the random bit-flip mutation seems to be, therefore, easier for large  $K$  than for low  $K$ . But, as the number of basins increases, and the fitness correlation between neighboring solutions decreases with increasing  $K$ , it becomes harder to find the global maxima for large  $K$ . This result suggests that the dynamic of stochastic local search algorithms on  $NK$  landscapes with large  $K$  is different from that with lower values of  $K$ , with the former engaging in more random exploration of basins.

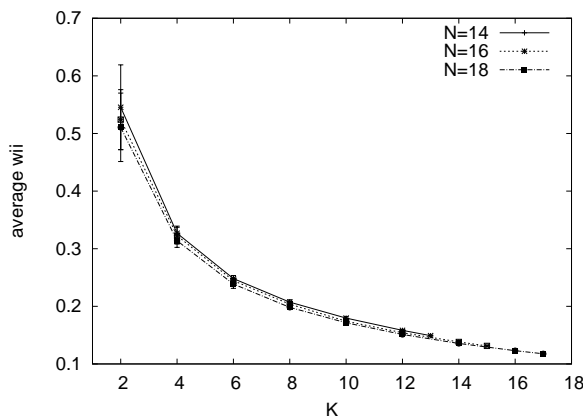


FIG. 8: Average weight  $w_{ii}$  according to the parameters  $N$  and  $K$ .

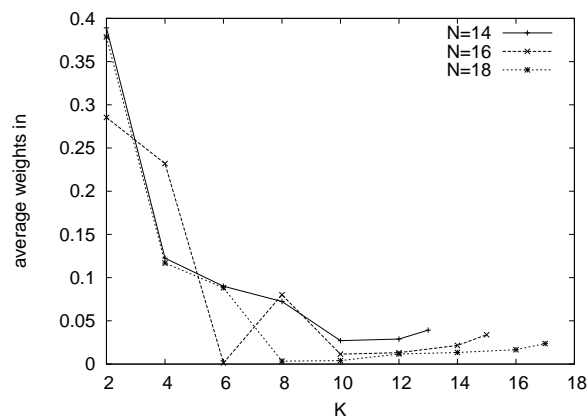
Table III gives the average number of configurations in the interior of basins (this statistic is computed on 30 independent landscapes). Notice that the size of the basins' interior is below 1% (except for  $N = 14, K = 2$ ). Surprisingly, the size of the basins' boundaries is nearly the same as the size of the basins themselves. Therefore, the probability of having a neighboring solution in the same basin is high, but nearly all the solutions have a neighbor solution in another basin. Thus, the interior basins seem to be “*hollow*”, a picture which is far from the smooth standard representation of landscapes in 2D with real variables where the basins of attraction are visualized as real mountains.

### 6. Incoming Weights Distribution

It is also of interest to study the distribution of the weights of edges impinging into a given node  $p_{in}(w)$ . However, a plot of this quantity is not very informative. We prefer to show in Fig. 9 the average values over 30 independent landscapes for each value of  $N$  and for the whole interval of  $K$ . The general trend for all values of  $N$  is that the average weight of the incoming transitions into a node quickly decreases with increasing  $K$ . This means that it is more difficult to make a transition to a local maximum when  $K$  is large. This agrees with the fact that the relative basins' size is a rapidly decreasing function of  $K$  (see Fig. 2). In fact, there is a strong positive correlation between the basins' size and the weights of the transitions into the corresponding maximum,

TABLE III: Average (on 30 independent landscapes for each  $N$  and  $K$ ) of the mean relative sizes of the basins interiors.

$K$	$N = 14$	$N = 16$	$N = 18$
2	0.0167 <sub>0.02478</sub>	0.0050 <sub>0.00798</sub>	0.0028 <sub>0.00435</sub>
4	0.0025 <sub>0.00065</sub>	0.0012 <sub>0.00025</sub>	0.0006 <sub>0.00010</sub>
6	0.0029 <sub>0.00037</sub>	0.0014 <sub>0.00015</sub>	0.0007 <sub>0.00009</sub>
8	0.0043 <sub>0.00045</sub>	0.0022 <sub>0.00012</sub>	0.0011 <sub>0.00006</sub>
10	0.0055 <sub>0.00041</sub>	0.0031 <sub>0.00015</sub>	0.0018 <sub>0.00006</sub>
12	0.0061 <sub>0.00041</sub>	0.0040 <sub>0.00014</sub>	0.0025 <sub>0.00007</sub>
13	0.0059 <sub>0.00029</sub>		
14		0.0045 <sub>0.00012</sub>	0.0031 <sub>0.00004</sub>
15		0.0044 <sub>0.00014</sub>	
16			0.0035 <sub>0.00005</sub>
17			0.0034 <sub>0.00006</sub>

FIG. 9: Average value of the weights of incoming transitions into maxima nodes for  $N = 14, 16, 18$  and for whole  $K$  interval.

i.e. as the basin becomes larger, the number of transitions into it increases too. This is shown on the scatter-plots (Fig. 10). The correlation follows approximately a power-law, the regression lines are also visualized. The correlation coefficient for all plots is high (above 0.97). If we hypothesize that the incoming weights are proportional to the size of the basin, i.e. that edges between nodes are randomly distributed over the search space, the sum of the incoming weights for a basin  $b_i$  should be  $\frac{\#b_i}{2N} \#S^*$ . This theoretical line is visualized on the scatter-plots (Fig. 10). Notice that the difference between the theoretical and regression lines, is higher for low values of  $K$ . For large  $K$ , the weights are given almost only by the size of basins. This is not the case for small  $K$  values, where the fitness correlation between neighboring solutions is high [2]. This explains why the hypothesis does

not hold in this case. So, the incoming weights could be deduced from the size of basins and the fitness of solutions belonging to the basin.

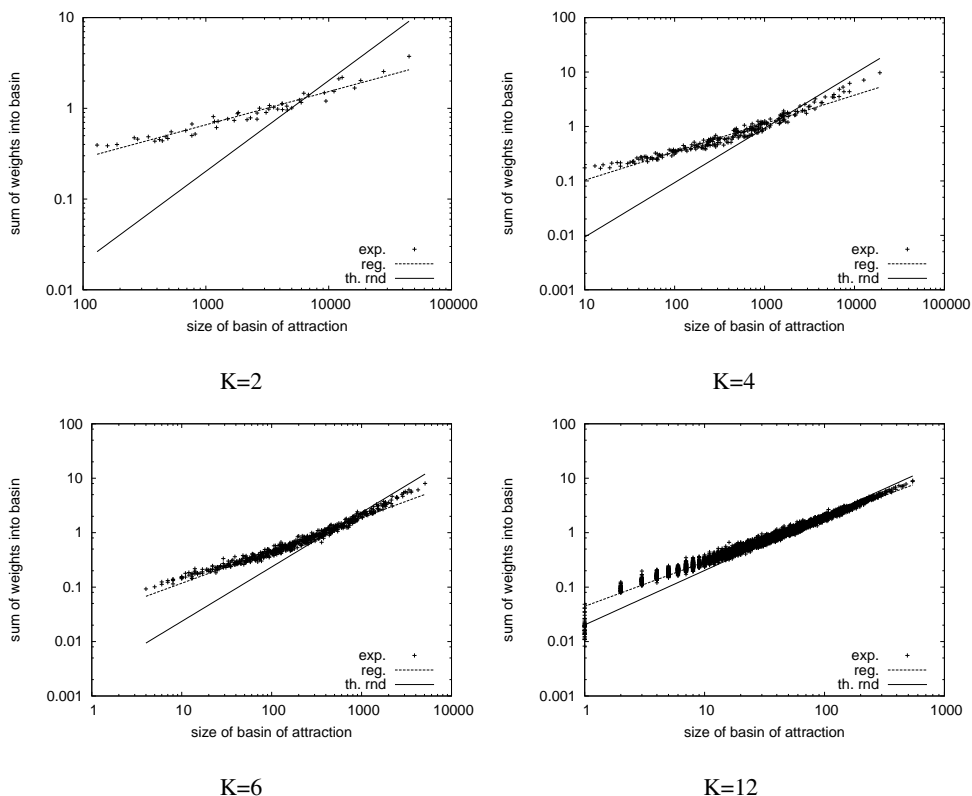


FIG. 10: Scatter-plots of the sum of weights into basins vs. the basin size for  $N = 18$  and various  $K$  values. Log-log scale. The regression line of each scatter-plot is shown. The theoretical curves, under the hypothesis that the weights are proportional, to the size of basin are also given.

## V. CONCLUSIONS

We have proposed a new characterization of combinatorial fitness landscapes using the well-known family of  $NK$  landscapes as an example. We have used an extension of the concept of inherent networks proposed for energy surfaces [5] in order to abstract and simplify the landscape description. In our case the inherent network is the graph where the nodes are all the local maxima and the edges accounts for transition probabilities (using the 1-flip operator) between the local maxima basins of attraction. This mapping leads to oriented weighted graphs, instead of the more commonly used unordered and unweighed ones [5]. We believe that the present representation is closer to the view offered by a Monte Carlo search heuristic such as simulated annealing which produces a trajectory on the configuration space based on transition probabilities according to a Boltzmann equilibrium distribution[15]. We have exhaustively obtained these graphs for  $N = \{14, 16, 18\}$ , and for all even

values of  $K$ , plus  $K = N - 1$ , and conducted a network analysis on them. The network representation of the  $NK$  fitness landscapes has proved useful in characterizing the topological features of the landscapes and gives important information on the structure of their basins of attraction. In fact, our guiding motivation has been to relate the statistical properties of these networks, to the search difficulty of the underlying combinatorial landscapes when using stochastic local search algorithms (based on the bit-flip operator) to optimize them. We have found clear indications of such relationships, in particular:

**The clustering coefficients:** suggest that, for high values of  $K$ , the transition between a given pair of neighboring basins is less likely to occur.

**The shortest paths to the global optimum:** become longer with increasing  $N$ , and for a given  $N$ , they clearly increase with higher  $K$ .

**The outgoing weight distribution:** indicate that, on average, the transition probabilities from a given node to neighbor nodes are higher for low  $K$ .

**The incoming weight distribution:** indicate that, on average, the transition probabilities from the neighborhood of a node become lower with increasing  $K$ .

**The disparity coefficients:** reflect that for high  $K$  the transitions to other basins tend to become equally likely, which is an indication of the randomness of the landscape.

The previous results clearly confirm and justify from a novel network point of view the empirically known fact that  $NK$  landscapes become harder to search as they become more and more random with increasing  $K$ .

The construction of the maxima networks requires the determination of the basins of attraction of the corresponding landscapes. We have thus also described the nature of the basins, and found that the size of the basin corresponding to the global maximum becomes smaller with increasing  $K$ . The distribution of the basin sizes is approximately exponential for all  $N$  and  $K$ , but the basin sizes are larger for low  $K$ , another indirect indication of the increasing randomness and difficulty of the landscapes when  $K$  becomes large. Furthermore, there is a strong positive correlation between the basin size and the degree of the corresponding maximum, which confirms that the synthetic view provided by the maxima graph is a useful. Finally, we found that the size of the basins boundaries is roughly the same as the size of basins themselves. Therefore, nearly all the configurations in a given basin have a neighbor solution in another basin. This observation suggests a different landscape picture than the smooth standard representation of 2D landscapes where the basins of attraction are visualized as real mountains. Some of these results on basins in  $NK$  landscapes were previously unknown [1].

This study represents our first attempt towards a topological and statistical characterization of easy and hard combinatorial landscapes, from the point of view of complex networks analysis. Much remains to be done. First of all, the results found should be confirmed for larger instances of  $NK$  landscapes. This will require good sampling techniques, or theoretical studies since exhaustive sampling becomes quickly impractical. Other landscape types should also be examined, such as those containing neutrality, which are very common in real-world applications, and especially the landscapes generated by important hard combinatorial problems such as the traveling salesman problem and other resource allocation problems. Work is in progress for neutral versions of  $NK$  landscapes and for knapsack problems. Finally, the landscape statistical characterization is only a step towards implementing good methods for searching it. We thus hope that our results will help in designing or estimating efficient search techniques and operators.

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