# Multi-layer local optima networks for the analysis of advanced local search-based algorithms

Marcella Scoczynski Ribeiro Martins<sup>1</sup>, Mohamed El Yafrani<sup>2</sup>, Myriam R. B. S. Delgado<sup>1</sup>, and Ricardo Lüders<sup>1</sup>

<sup>1</sup> Federal University of Technology Paraná (UTFPR), Brazil

<sup>2</sup> Operations Research group, Aalborg University, Denmark

Abstract. A Local Optima Network (LON) is a graph model that compresses the fitness landscape of a particular combinatorial optimization problem based on a specific neighborhood operator and a local search algorithm. Determining which and how landscape features affect the effectiveness of search algorithms is relevant for both predicting their performance and improving the design process. This paper proposes the concept of multi-layer LONs as well as a methodology to explore these models aiming at extracting metrics for fitness landscape analysis. Constructing such models, extracting and analyzing their metrics are the preliminary steps into the direction of extending the study on single neighborhood operator heuristics to more sophisticated ones that use multiple operators. Therefore, in the present paper we investigate a twolayer LON obtained from instances of a combinatorial problem using bitflip and swap operators. First, we enumerate instances of NK-landscape model and use the hill climbing heuristic to build the corresponding LONs. Then, using LON metrics, we analyze how efficiently the search might be when combining both strategies. The experiments show promising results and demonstrate the ability of multi-layer LONs to provide useful information that could be used for in metaheuristics based on multiple operators such as Variable Neighborhood Search.

**Keywords:** Local Search  $\cdot$  Local Optima Networks  $\cdot$  Fitness Landscape Analysis

## 1 Introduction

Local Optima Networks (LONs) can be seen as high level models of discrete (combinatorial) fitness landscapes [21]. In the conception of a single layer non-weighted LON, nodes are local optima of the addressed problem instance and edges are search transitions based on a specific neighborhood operator.

These basic models are therefore achievable given a local search algorithm and a set of enumerable instances [23]. Recently, different LON models and metrics have been investigated. Weighted LONs are addressed in [24], while neutral landscapes are considered in [22]. In [16], the authors investigate compressed

LONs. A sampling procedure to extract LONs of larger instances is the focus of [29] while Fractal (self-similarity) measures are used in [26].

Although recently they have been considered to continuous spaces [3,1], the majority of works on LONs reported in the literature are devoted to discrete search spaces and combinatorial optimization [27,9,31,10,11,?,22,16,29,32]. In this case, LON models have been used to capture in detail the number and distribution of local optima in the search space. Nevertheless they are highly dependent on the specific neighborhood operator being addressed, exploring their structures serves as the basis of many theoretical studies on combinatorial optimization.

In this paper we consider the NK-landscape model [18,27,7] to provide combinatorial landscapes. The joint use of LON and NK-landscape models has attracted attention by researchers in Fitness Landscape Analysis (FLA) [21,30,27,24,31]. This is mainly because, by changing the parameters Nand K, it is easy to range from simple to highly complex landscapes and impose different levels of difficulty to the addressed search algorithm.

LONs features are known to be of utmost importance for understanding the search difficulty of the corresponding landscape as they provide useful insights about the landscape of the search space (search difficulty) and what problem properties are most influential, particularly in terms of the local optima distribution.

As discussed in [15], besides other important issues, the search for an optimal (or near-optimal) solution in combinatorial optimization must take into account the following aspects: (i) a local optimum relative to one neighborhood structure is not necessarily a local optimum for another neighborhood structure; (ii) a global optimum is a local optimum with respect to all neighborhood structures. According to [15], the first property suggests using several neighborhoods if local optima found are of poor quality. The second property might be exploited by increasingly using complex moves in order to find local optima with respect to all neighborhood structures used.

Considering all the issues previously discussed (particularly the two aspects pointed out by [15]); and aiming to create the basis for an expansion of FLA to search algorithms that use multiple operators, we propose in this paper the multi-layer local optima network. We analyze LON features extracted from three different landscapes: one obtained using only the bit flip move, another resulted from the 1-swap move and the last one obtained by combining both bit-flip and 1-swap in a two-layer network. The present paper proposes to explore multilayer local optimal networks aiming to evaluate the use of multiple neighborhood operators as occurs in advanced local metaheuristics like Variable Neighborhood Search (VNS).

Therefore, the main contributions of this paper are: (i) Proposing and formalizing the concept of multi-layer optimal networks (MLLONs); (ii) Presenting a methodology for exploring MLLONs and extracting metrics for fitness landscape analysis; (iii) Presenting an analysis of each individual layer in an MLLON as well as their comparison with the whole multi-layer network. Although they are well explored in complex networks [4,8,19], as far as we know, multi-layer networks had never been considered before in the context of FLA for optimization problems. Therefore, we believe that the present paper contributes with both, FLA and optimization areas, by presenting the preliminary steps into the direction of more robust theoretical analyses of sophisticated metaheuristics.

This paper is organized as follows. Section 2 provides background information on LONs, the addressed problem (NK Landscape models), standard graph and complex network metrics as well as a brief description of some related approaches. Then, Section 3 describes in detail the proposed approach. Section 4 presents the set up for experiments and obtained results. Finally, Section 5 concludes the paper.

# 2 Background

This section provides basic information necessary to understand LON models (for fitness landscape analysis) and the NK Landscape models (the addressed problem). The section also discusses some related approaches focusing on LON variants and different application problems.

## 2.1 Local Optima Networks

A local optima network (LON) is a graph model used to represent landscape of combinatorial problems [21]. The networks can be explored using a set of metrics to characterize their landscapes and problem difficulty [28].

In combinatorial optimization, the solutions of the addressed instance problem form a set that can be connected according to a given heuristic or move operators. In a LON, the local search heuristic  $\mathcal{H}$  maps a set of local optimum solutions  $S^*$  from a solution space S [21]. Considering a fitness function F, a solution  $s^*$  in the solution space S is a local maximum given a neighbourhood operator of type t  $(Nh_t)$ , iff  $F(s^*) \geq F(s), \forall s \in Nh_t(s)$ . Figure 1 illustrates a LON with two subsets of solutions (small blue circles surrounded by large blue circles), from which two different local optima (red circles) can be reached using a specific  $\mathcal{H}$  and a particular neighborhood operator. These subsets are called basins of attraction and can be connected by weighted or non-weighted edges.

To obtain the LON by enumerating all the solutions and then finding each basis of attraction with its associated local optima,  $\mathcal{H}$  starts from every solution s in the solution space S, constructs the neighborhood structure of s based on the neighborhood operator (bit-flip or swap for example) and using an update strategy (e.g., best improvement) selects one among the neighbors to be the next current solution. The process is repeated until a local optimum is reached. For more details see Algorithm 1 in Section 3.2

The process of finding a local optima from s involves constructing a neighborhood structure to move from s to s' during the search. The total number of solutions in the neighborhood structure of a solution s varies according to

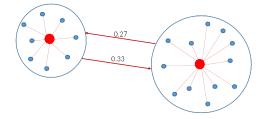


Fig. 1: An example of a Local Optima Network with two basins connected by weighted edges

the neighborhood operator considered. In this paper we address two different operators (bit-flip and swap) resulting in two different neighborhood structures. In the first case  $(Nh_{\rm bf})$ , bit-flip changes a bit of the binary solution from  $0 \rightarrow 1$  and vice-versa. Therefore, for a binary string of size N, there are N neighbors for each solution. In the second case  $(Nh_{\rm sw})$ , the swap operator (more specifically the 1-swap operator) interchanges two randomly chosen bits of the string. Therefore, the total of neighbors  $T_N$  is calculated as the number of ones  $(T_{1s})$  times number of zeros present in s,  $T_N = T_{1s}(N - T_{1s})$ .

For each pair of solutions s and s',  $p(s \rightarrow s')$  is the probability of moving from s to s' with the given neighborhood structure. Assuming the bit-flip neighborhood operator we have:

$$p(s \to s') = \begin{cases} 1/N \text{ if } s' \in Nh_{bf}(s) \\ 0 \text{ otherwise} \end{cases}$$

and for swap:

$$p(s \to s') = \begin{cases} 1/T_N \text{ if } s' \in Nh_{sw}(s)\\ 0 \text{ otherwise} \end{cases}$$

As previously discussed and depicted in Figure 1, the basin of attraction of a local optimum  $LO_j \in S$  is defined as  $B_j = \{s \in S | \mathcal{H}(s) = LO_j\}$ . This set, whose cardinality is given by  $|B_j|$ , contains all the solutions  $s \in S$  from the local optimum  $LO_j$  can be achieved when the local search heuristic  $\mathcal{H}$  is applied. In Figure 1, two basins  $B_1$  and  $B_2$  are shown (large blue circles), each one composed of  $|B_1| = 8$  and  $|B_2| = 12$  solutions s (small blue circles), and their central nodes (red nodes) identify  $LO_1$  and  $LO_2$ , respectively. According to [23], the probability of moving from basin  $B_i$  to  $B_j$  is calculated as:

$$p(B_i \to B_j) = \frac{1}{|B_i|} \sum_{s \in B_i} \sum_{s' \in B_j} p(s \to s') \tag{1}$$

The simplest LON model is built therefore by connecting every two basins of attraction  $B_i$  and  $B_j$ , whenever  $p(B_i \rightarrow B_j) > 0$ . Assuming weighted networks [5] as a useful extensions of basic LONs, weights as those depicted in Figure 1  $(w_{ij} = p(B_i \rightarrow B_j))$  can be also explored using specific FLA metrics [24].

Although basins-transitions edges present a somewhat symmetric structure, when two nodes i and j are connected, both edges  $e_{ij}$  and  $e_{ji}$  are present [28].

#### 2.2 NK-landscape Models

In this paper we consider the NK-landscape model [18] as the application problem. These problems have been designed to explore how the neighbourhood structure and the strength of interactions among neighbouring variables (subfunctions) are related to the search space ruggedness.

In the NK model, N refers to the number of (binary) variables, i.e. the string/solution length, and K to the strength of interaction, i.e. the number of variables that influence a particular variable. By increasing the value of K from 0 to N-1, the landscapes can be tuned from smooth to rugged. The K variables that contribute to the fitness of a string can be selected according to different models, and the two most widely studied ones are the random neighborhood and the adjacent neighborhood models. In this paper we adopt the general random model due to the fact that no significant differences between the two were found in terms of the landscape global properties [18].

## 2.3 Related works

Local optima networks have been explored on NK landscape problem [27,21], including their extension to neutral fitness landscapes [31]. Neutral networks consider solutions of equal (or quasi equal) objective function values. Besides, several works analyzed the correlation between LON features and the performance of search heuristics in several problems [6,10,23].

In [24] the authors address weighted LONs and consider first-improvement (greedy-ascent) hill-climbing algorithm, instead of a best-improvement (steepest-ascent) one, for the definition and extraction of the basins of attraction of land-scape optima. Results suggest differences with respect to both the network connectivity, and the nature of the basins of attraction. The paper discusses the impact of these structural differences between the two models (first versus best) in the behavior of search heuristics.

Permutation-based problems have also been subject to LON analyses [11]. In [22] the authors considered the LON model to characterize and visualize the global structure of travelling salesperson (TSP) fitness landscapes of different classes, including random and structured real-world instances of realistic size. The authors also investigated how to visualize neutral landscapes featured by the structured TSP instances.

Another LON variant is discussed in [16]. The Compressed Local Optima Network is used to investigate different landscapes for the Permutation Flowshop Scheduling Problem (PFSP), exploring the network features to find differences between the landscape structures. The author analysed which features impact the performance of an iterated local search heuristic.

Recently, the work presented in [32] investigated two hill climbing local searches on a new combinatorial problem. The authors investigated the modeled LONs to explore and understand the difficulty of Travelling Thief Problem (TTP) instances. The results showed that certain operators can provide LONs with disconnected components and sometimes there exist exploitable correlations of node degree, basin size, and fitness.

The authors in [29] addressed the limitation to fully enumerate all local optima, presenting a sampling procedure to extract LONs of larger instances and estimate their metrics without losing much in accuracy. They propose to increase the number of relevant features that could be used for performance prediction of Quadratic Assignment Problem (QAP) algorithms, in order to find whether LON features could be more correlated with performance than basic fitness landscape features. The experiments produced reliable results.

Another recent work in [26] investigated the use of fractal (self-similarity) measures in local optima space in a fitness landscape. The authors applied fractal dimension and associated metrics over NK landscape instances. The results showed a correlation between fractal geometry in the networks and the performance for search algorithms.

## 3 Proposed model

In this section we present the details of the proposed approach, including an overview on its basic concepts, the associated formalism and how to explore it through standard and new FLA metrics.

## 3.1 Multi-layer Local Optima Networks

As a main contribution of the present paper we propose the multi-layer Local Optima Network (MLLON). Figure 2 illustrates an example of an MLLON composed of two layers  $Nh_1$  and  $Nh_2$ , each one obtained using a different neighborhood operator.

LON representations actually focus on local optima and edges only. However, in Figure 2 we also shown the details of each basin of attraction to facilitate the explanation of the proposed model. In the proposed model, connections between basins located at the same layer (the intra-layer connections shown as blue thin edges in Figure 2), represent the usual transitions between pairs of basins as described in Section 2.1. The novelty of this paper is with respect to the possibility of **connecting layers** through **inter-layer** connections. These connections allow one to **interchange** the landscape analysis between different **neighborhood operators**. Inter-layer connections are shown as **red** and **green** edges and can be divided in two main groups: mirror and basin inter-layer connections.

In the first case (mirror inter-layer connections), they appear as red edges and indicate that the local optima are the same. In other words, if a local optimum appears in both layers, there is a red edge connecting them, indicating

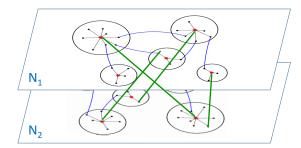


Fig. 2: An example of a Multi-layer Local Optima Network composed of two layers: blue thin edges connect basins at the same layer (the intra-layer connections) while inter-layer connections are shown as red (connecting the same local optima) and green edges (connecting any two solutions). The weights are omitted for simplification and readability purposes.

the possibility of changing the neighborhood operator due to this common local optimum. In the second case (basin inter-layer connections), they appear as green edges and indicate that there is at least one common solution in both basins, which turns possible to the search moving from the other layer (due to the common solution) and using the new corresponding operator. Therefore, in MLLONs, one can navigate from one layer to another whenever a local optimum occurs in both layers or two basins in different layers share solutions.

## 3.2 The MLLON Formalism

When dealing with more than one neighborhood operator as occurs in many search techniques, a fundamental concept is when is the moment to change the operator. In the context of MLLONs, this means changing the layer associated with one particular operator to another layer associated to a different operator. In this paper we consider two different circumstances when the operator can change: when the search achieves a local optimum shared with other layers (called mirror), or when the search achieves a solution that occurs in two or more layers. In the first case we must set the probability of changing the operator due to a mirror  $(P_{co}^m)$ . In the second case we must set the probability of changing the operator due to a common solution in two different layers  $(P_{co}^{\neq})$ .

Considering  $p^M(B_i \to B_j)$  as the probability of moving from any basin  $B_i$  to any basin  $B_j$  in the multiple layer network, we can define a more general concept regarding the probability of transition between a pair of basins as:

$$p^{M}(B_{i} \rightarrow B_{j}) = \begin{cases} P_{sl} & \text{if } L_{i} = L_{j}, LO_{i} = LO_{j} \\ P_{co}^{m} & \text{if } L_{i} \neq L_{j}, LO_{i} = LO_{j} \\ p(B_{i} \rightarrow B_{j}) & \text{if } L_{i} = L_{j}, LO_{i} \neq LO_{j} \\ P_{co}^{\neq} p(B_{i} \cap B_{j}) & \text{if } L_{i} \neq L_{j}, LO_{i} \neq LO_{j} \end{cases}$$

$$(2)$$

where  $P_{sl}$  is the probability of a self-loop in a particular layer;  $P_{co}^m \in (0, 1]$  is the probability of changing the operator (co) when we find a mirror, i.e., when the local optima are the same  $(LO_i = LO_j)$  but located at different layers  $(L_i \neq L_j)$ ;  $P_{co}^{\neq} \in [0, 1]$  is the probability of changing the operator when the local optima are different  $(LO_i \neq LO_j)$ , and located at different layers  $(L_i \neq L_j)$ , what means that the two different basins of attraction  $B_i$  and  $B_j$  are also located at different layers.

In an MLLON, when the basins are in the same layer (i.e.,  $L_i = L_j$  for the pair ij), we have the same probability of transition of a LON, what means  $p^M(B_i \to B_j) = p(B_i \to B_j)$  with  $p(B_i \to B_j)$  given by Equation 1.

The novelty in this paper is the possibility of moving between layers due to the change in the neighborhood operator. In this case, we only have to set the value of parameter  $P_{co}^m$  when we have a mirror (same LO located at different layers), otherwise we set  $P_{co}^{\neq}$  and calculate the probability of transition which is given by Equation .

$$p(B_i \bigcap B_j) = \frac{|B_i \bigcap B_j|}{|B_i \bigcup B_j|} \tag{3}$$

where  $|B_i \cap B_j|$  is the cardinality of the set  $B_i \cap B_j = \{s' | s' \in B_i \text{ and } s' \in B_j\}$ and  $|B_i \bigcup B_j|$  is the cardinality of the set  $B_i \bigcup B_j = \{s | s \in B_i \text{ or } s \in B_j\}$ .

Based on the previous discussion, the probability of transition between two different basins can be summarized as shown in Table 1.

Table 1: Probability of transitions between pair of Basins in MLLONs  $(p^M(B_i \rightarrow B_j))$  color-coded based on Figure 2.

Type	Same $LO$	Different $LO$		
Intra-layer	$p^M(B_i \to B_j) = P_{sl}$	$p^M(B_i \to B_j) = p(B_i \to B_j)$		
Inter-layer	$p^M(B_i \to B_j) = P_{co}^m$	$p^{M}(B_{i} \to B_{j}) = P_{co}^{\neq} p(B_{i} \bigcap B_{j})$		

As depicted in Figure 2 and detailed in Table 1, MLLONs encompass different connections between each pair of basins: intra and inter-layers. It is important to point out that edges between basins (blue, red and green) can identify different kinds of connections, whose weights (probabilities) are calculated based on different sources of information (as shown in each cell of Table 1). However, as discussed in the previous section, for sake of simplicity, neither weight values nor directions are presented in Figure 2.

According to the code colors linking Table 1 and Figure 2, the blue cell in Table 1 has a correspondence with blue edges in Figure 2 and identifies the **intra-layer** connections linking two basins whose local optima are different. Notice that in Figure 2, **intra-layer edges** connecting two basins with the same local optima are impossible to occur. This is because although the formalism allows the occurrence of self-loops with probability  $P_{sl}$ , in the model addressed in the experiments there is no duplicated local optimum in the same layer and

no loop is allowed. Therefore, the corresponding cell is grey and the associated probability is set as 0 in the experiments. However, assuming a looping edge as possible, this information could also be considered by the model. The red cell has a correspondence with red edges and identifies the **inter-layer** connections linking two basins with the same local optima (notice that same local optima does not mean the same basins of attraction, since their solutions can be different). The green cell has a correspondence with green edges and identifies the **inter-layer** connections linking two basins with different local optima.

As can be seen in the first line of Table 1, LONs are a special case of MLLOs. Therefore, in the case of a unique layer (LON),  $L_i = L_j$  for all the basins and  $P_{co}^m = P_{co}^{\neq} = 0$ , since there is no mirror or other operator to be considered. Moreover,  $P_{sl} > 0$  indicates the possibility of self-loops in the LON,  $p^M(B_i \rightarrow B_j) = p(B_i \rightarrow B_j)$  and can be calculated as Equation 1.

A particular MNLON model can be achieved considering  $P_{co}^m = 1$  and  $P_{co}^{\neq} = 0$ , when the change in the neighborhood operator occurs only when the search achieves a mirror (i.e., the change occurs only when the search achieves a shared local optimum occurring in both layers).

In the experiments we consider this case, and assume that layer  $Nh_1$  is based on bit-flip and layer  $Nh_2$  is based on 1-swap, both built from NL-landscape models (for N = 18 and K ranging from 2 to 16).

Aiming to build each layer, the Best-improvement - Hill Climbing algorithm, presented in Algorithm 1, is applied to determine the local optima and therefore define the basins of attraction. The entire neighborhood is explored and the best solution is returned as the *LO*.

**Algorithm 1** Algorithm based on Best-improvement - HC for constructing the Basins of attraction

**INPUT:** The complete set of solutions S and the type t of the neighborhood  $Nh_t(.)$ 1: repeat 2: Initial solution  $s_0 \in S$ 3:  $s \leftarrow s_0$ repeat 4: Choose  $s' \in Nh_t(s)$  such that  $F(s') = max_{x \in Nh_t(x)}F(x)$ 5:if F(s) < F(s') then 6:  $s \leftarrow s'$ 7: end if 8: 9: until s is a local optima  $LO = s, s_0$  is part of its basin of attraction 10: 11: **until** all solutions in S have been visited as initial solutions  $s_0$ **OUTPUT:** 

## 3.3 Exploring MLLONs by means of graph theory metrics

In the calculation of MLLON metrics, the multi-layer network can be transformed into a single-layer one using different methods. Aggregation and flattening are the most popular ones [13]. In an aggregated network, nodes from different layers are aggregated in a single node by using different methods while flattening preserve connected nodes from different layers by adding an edge between them. In this paper we flattened the multi-layer network, then LON metrics were straightforwardly applied.

In this paper, we consider four types of metrics to explore LONs and ML-LONs:

- 1. descriptive statistics: number of nodes  $(n_v)$ , number of edges  $(n_e)$ , weighted assortativity or affinity (knn) and the fitness-fitness correlation (fnn);
- 2. local metrics: cumulative degree distribution, correlation between degree and basin of attraction size, and correlation between fitness of local optima and basin of attraction size;
- 3. global metrics: average weighted clustering coefficient ( $\overline{wcc}$ ), average weighted clustering coefficient for a random graph ( $\overline{wcc_r}$ ), average shortest path length ( $\overline{l}$ ), strength ( $\overline{st}$ ), disparity ( $\overline{y_2}$ ), degree of outgoing edges ( $\overline{z_{out}}$ ) and the average shortest path to global optima ( $\overline{l_{GO}}$ ). Apart from ( $\overline{l_{GO}}$ ), that is new in the context of FLA, and has been explored for the first time in this paper, these metrics are significantly related to search performance and have been already considered in other works[6,?].

As performed in [32], in terms of descriptive statistics, we start from the simplest ones, number of nodes and edges  $(n_v \text{ and } n_e, \text{ respectively})$  to analyze the impact of each neighborhood operator in the (ML)LON size. Aiming to evaluate the neighborhood connectivity behavior we consider knn, as it measures the nearest-neighbors degree correlation. In this case, the network is said to show assortative mixing if high degree nodes are supposed to be connected to other high degree nodes [20]. The Pearson correlation coefficient is applied to measure the network assortativity; positive values indicate similarity in pair degrees and negative values represent relationships between nodes of different degree. As an attempt to evaluate the multi-modality degree of the landscape, we consider as the last descriptive statistic the fnn which represents the fitness-fitness correlation and measures the correlation between the fitness values of adjacent local optima. As in the case of knn, it also applies the Pearson correlation coefficient statistic coefficient between the fitness value of a node and the weighted-average of its nearest neighbours fitness [29].

In terms of local metrics, we study the cumulative degree distribution, the correlation between the strength and basin size, and the correlation between fitness and basin size, since analysing the behavior of these distributions is useful to understand complex network structures [2,?,?].

In the context of global features, i.e. those calculated considering the whole network, we consider 8 metrics. We start with the average weighted clustering coefficients ( $\overline{wcc}$ ), that measures cliquishness of a neighborhood [4].  $\overline{wcc_r}$  is

the average clustering coefficients of corresponding random graphs (i.e. random graphs with the same number of vertices and mean degree). The average shortest path lengths between any two local optima is defined as  $\bar{l}$ . The strength  $\bar{st}$  for outgoing edges measures the network weighted connectivity, while  $\bar{y}_2$  is the average disparity for outgoing edges which gauges the heterogeneity of the contributions of the edges of each node to the total weight [5].  $\bar{z}_{out}$  is the average out degree, i.e., the total number of outgoing edges. Besides these usual metrics, we consider the average shortest path to global optima ( $\bar{l}_{GO}$ ), measured according to the neighborhood operator applied to generate the corresponding LON.

## 4 Experiments and Results

In the experiments conducted here we address the NK-landscape model [18], with N = 18 variables,  $K \in \{2, 4, 6, 8, 10, 12, 14, 16\}$  and uniformly distributed subfunctions. This combination of parameters allows computing optimal solutions by exhaustively enumerating the solution space using reasonable computational resources.

This paper aims to investigate how efficiently is combining neighborhood moving operators (which can be accomplished by moving between multiple landscapes) when compared with each operator used in a stand-alone mode (ie. moving on one specific layer only).

In the experiments, we generate therefore a multi-layer network composed of two layers corresponding to the LONs using bit-flip and 1-swap operators respectively. To navigate in this multi-layer network, edges inter-connecting two layers whose basins have the same local optima have weight values set as  $w_{ij} = p^M(B_i \to B_j) = P_{co}^m = 1$ . This assumption, imposes no difficulty to jump from one layer to another, whenever the same local optima is identified in both layers. Intra-layer edges, on the other hand, present weights according to their neighbourhood type (e.g. bit-flip for layer  $N_1$  and 1-swap for layer  $N_2$ ), whose values are defined as  $w_{ij} = p(B_i \to B_j)$ , with  $p(B_i \to B_j)$  given by Equation 1. Therefore, low values indicate the difficulty to navigate through basin pairs. The exception occurs in the calculation of the shortest path to the global optimum  $(\overline{l_{GO}})$ . This metric requires complement values since lower values indicate better paths, then we consider  $w_{ij} = 1 - p(B_i \to B_j)$ .

Moreover, particularly for the multi-layer network we store the weighted edges, nodes and the corresponding layers as a supra-adjacent matrix [12]. Therefore the multi-layer network can be flattened, preserving more information [13], and standard and complex metrics can be applied.

The networks are implemented and analyzed using Py3Plex [25] and NetworkX [14] from Python. Dijkstra's algorithm is applied to calculate the shortest path length.

#### 4.1 Descriptive Statistics

Table 2 presents descriptive statistics for a particular landscape. We can observe that when K increases, the number of local optima  $(n_v)$  and edges connections

Table 2: Descriptive statistics

4         240         22280         -0.106         -0.60           6         1080         199648         -0.122         -0.60           8         2035         409390         -0.105         -0.64           10         3593         687398         -0.075         -0.63           12         5592         935578         -0.051         -0.63           14         8313         116560         -0.042         -0.58           16         11383         1343544         -0.036         -0.56           16         11383         1343544         -0.036         -0.56           16         11383         1343544         -0.036         -0.56           16         19894         2442764         -0.058         -0.55           6         20720         2499472         -0.064         -0.56           10         22906         2622780         -0.059         -0.66           12         23489         2618234         -0.059         -0.66           12         23489         2618234         -0.059         -0.66           14         23734         2628042         -0.059         -0.66           14         20134	Network type	K	$n_v$	$n_e$	knn	fnn
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		2	32	370	-0.019	-0.356
$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$		4	240	22280	-0.106	-0.604
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		6	1080	199648	-0.122	-0.603
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Dit flip	8	2035	409390	-0.105	-0.649
	Dit-mp	10	3593	687398	-0.075	-0.632
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		12	5592	935578	-0.051	-0.616
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		14	8313	1165660	-0.042	-0.587
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		16	11383	1343544	-0.036	-0.569
$ {\rm Swap} \qquad \begin{array}{ccccccccccccccccccccccccccccccccccc$		2	19317	2432458	-0.023	-0.562
$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$		4	19894	2442764	-0.058	-0.521
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		6	20720	2499472	-0.064	-0.584
	Swap	8	22046	2589536	-0.061	-0.603
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Swap	10	22906	2622780	-0.059	-0.617
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		12	23489	2618234	-0.063	-0.612
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		14	23734	2628042	-0.059	-0.611
		16	24441	2653482	-0.059	-0.604
		2	19349	2432888	-0.023	0.006
$ \begin{array}{rllllllllllllllllllllllllllllllllllll$		4	20134	2465462	-0.051	0.006
$\begin{array}{cccccccc} \text{Multi-layer} & 10 & 26499 & 3316056 & -0.049 & 0.005 \\ 12 & 29081 & 3562612 & -0.023 & 0.004 \\ 14 & 32047 & 3806266 & -0.031 & 0.004 \end{array}$		6	21800	2700928	-0.054	0.006
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Multi lavor	8	24081	3002288	-0.058	0.005
$14 \ \ 32047 \ \ 3806266 \ \ -0.031 \ \ 0.004$	mum-rayer	10	26499	3316056	-0.049	0.005
		12	29081	3562612	-0.023	0.004
$16 \ 35824 \ 4013332 \ -0.084 \ 0.003$		14	32047	3806266	-0.031	0.004
		16	35824	4013332	-0.084	0.003

 $(n_e)$  increases accordingly. The increase in  $n_v$  and  $n_e$  is more significant for the bit-flip than the swap operator. Additionally, the value of these metrics is always higher for the swap operator. This shows that the search difficulty naturally increases when the ruggedness of the instance increases. However, the search difficulty using swap, although high, remains stable regardless of the ruggedness of the instances.

Furthermore, there is a weak negative correlation for knn for all values of K (specially for the bit-flip), indicating smooth relationships between nodes of different degrees for the three cases. In other words, part of local optima with a large number of connections are connected to local optima with a low number of connections, which might provide a smooth navigation of the overall network [10].

The metric fnn is particularly relevant for algorithms like VNS where fitness is applied as the acceptance criteria, as it measures correlation between the fitness values of adjacent local optima. In general, it is expected that a positive correlation contributes to the search process [10]. For both bit-flip and swap, the fnn values are negative, indicating low connectivity between local optima with similar fitness value. However, this negative correlation becomes weak positive when combining the two landscapes using the multi-layer network. This can be explained by the addition of connections between two landscapes by linking local optima of same fitness with high weight values. We believe that using an aggregation method instead of flattening the multi-layer network could mitigate this effect, however, comparing these methods is out of the scope of this paper.

## 4.2 Global Metrics

Table 3 summarizes the results for global metrics averaged for one landscape. For the bit-flip operator, the average shortest path length is small and proportional to  $log(n_v)$  with mostly high clustering coefficients compared to an equivalent random graph. Therefore, the resulting graph is compatible with small-world networks.

On the other hand, despite its proportionality to  $log(n_v)$ , l is larger for the swap operator than the corresponding values for the bit-flip with significantly small clustering coefficients. This typically indicates that the resulting graph does not fit properly in a small-world network model, yielding to a difficult in the network navigation. This phenomenon naturally extends to the multi-layer network, but it is slightly alleviated thanks to the combination with the bitflip-based LON. The small clustering coefficient can be explained by the large number of local optima (number of nodes in Table 2) which yields to small basins and thus a small probability of neighborhood connections. In fact, in contrast to the bit-flip operator which gives a more connected network, the swap operator add the constraint of needing two unequal decision variable to apply the move, resulting in a possible not connected graph. It is worth noting that similar results were obtained for the swap operator in some graphs when applied to the S-BOX problem [17].

Table 3: Global Metrics

LON type	K	$\overline{wcc}$	$\overline{wcc_r}$	$\overline{l}$	$\overline{st}$	$\overline{y_2}$	$\overline{z_{out}}$	$\overline{l_{GO}}$
bit-flip	2	0.524	0.752	1.67	11.12	0.09	11.56	1.13
	4	0.641	0.777	1.61	92.17	0.01	92.83	1.07
	6	0.489	0.343	1.83	184.08	0.01	184.86	1.41
	8	0.406	0.198	1.92	200.36	0.01	201.17	1.53
	10	0.317	0.107	2.02	190.47	0.01	191.32	1.80
	12	0.256	0.060	2.17	166.44	0.01	167.31	1.89
	14	0.210	0.034	2.37	139.34	0.01	140.22	2.15
	16	0.181	0.021	2.55	117.15	0.02	118.03	2.46
	2	0.000	0.013	3.41	124.96	0.03	125.92	3.71
swap	4	0.000	0.012	3.41	121.84	0.03	122.79	3.10
	6	0.000	0.012	3.42	119.69	0.03	120.63	2.90
	8	0.000	0.011	3.43	116.53	0.03	117.46	3.75
	10	0.000	0.010	3.44	113.58	0.03	114.50	3.73
	12	0.000	0.009	3.46	110.55	0.03	111.47	3.10
	14	0.000	0.009	3.46	109.82	0.04	110.73	3.01
	16	0.000	0.009	3.47	107.66	0.04	108.57	3.44
mult: lawan	2	0.001	0.013	3.39	124.65	0.03	125.74	1.12
multi-layer	4	0.007	0.012	3.33	121.37	0.03	122.45	1.06
	6	0.024	0.011	3.31	122.77	0.03	123.90	1.39
	8	0.034	0.010	3.30	123.51	0.03	124.67	1.53
	10	0.042	0.009	3.30	123.90	0.03	125.14	1.80
	12	0.048	0.008	3.31	121.20	0.03	122.51	1.88
	14	0.054	0.007	3.31	117.38	0.03	118.77	2.15
	16	0.056	0.006	3.33	110.57	0.03	112.03	2.31

The metric  $\overline{l_{GO}}$  shows that the bit-flip operator ensures reaching a global optimum in a small number of steps. While the cost of finding a global optimum significantly increases in the swap-based LON. This is consistent with the  $\overline{l}$  results. Interestingly, combining both landscapes results in a network requiring less steps to find a global optimum. This means that, although using only bit-flip might be more efficient than using swap all the time, the search seems to benefit from the combination of both as swap may provide 'jumps' that are not available when using only bit-flip.

The metric  $z_{out}^i$  counts the number of outgoing edges of node i (i.e., a local optimum LO in the respective LON). According to [10] it is relevant to know whether all transitions have the same weight, or if there is a preferred direction. The disparity  $y_2^i = \sum_{j \neq i} \left(\frac{w_{ij}}{st_i}\right)$  of node i indicates the weight heterogeneity of outgoing edges [5]. It is related to the strength  $st^i$ : when all edges leaving a node i have the same probabilities, the disparity is the inverse of the out-degree  $1/z_{out}^i$ . Therefore, a low disparity indicates equally likely transitions, with no guidance in the search trajectory. This behavior seems to be present in the three network models since similar  $\overline{y_2}$  values were found independently of ruggedness.

### 4.3 Local Metrics

Complex networks are also characterized by degree distributions [2]. Therefore, in this paper we show the cumulative degree distribution besides scatter plots presenting the correlations between size of basin of attraction, degree and fitness. Herein, we consider the strength distribution (instead of degree distribution) as weighted networks are addressed.

Comparing all local metrics in Figure 3, we notice that, differently from the descriptive statistics and global metrics, bit-flip predominates most of time, although the multi-layer network inherits behaviors from both layers in some particular cases.

Figures 3a, 3d and 3g show the cumulative strength distribution, in loglog scale, considering a particular landscape for bit-flip, swap and multi-layer networks, respectively. In each figure, one curve is shown for each value of K. The cumulative strength distribution function represents the probability P(st = c)that a randomly chosen node has a strength larger than or equal to c. For all the K values, the cumulative strength distributions decay slowly for small strength values, with a faster dropping rate for high values of strength. Moreover, for bitflip, the curves for distinct K values differentiate from each other more than for swap and multi-layer. This behavior is not inherit by multi-layer since its curves seem more impacted by the swap LON. The curves indicate that the most part of the nodes have low strength connections, while few nodes present connections with significantly higher values of strength. This behaviour can be observed for the bit-flip, swap and the multi-layer networks.

Figures 3b, 3e and 3h present the correlation between the strength and the size of basins of attraction in a semi-logy scale. Analyzing the bit-flip landscape, we observe that their basin sizes are greater than the swap ones showing a slightly

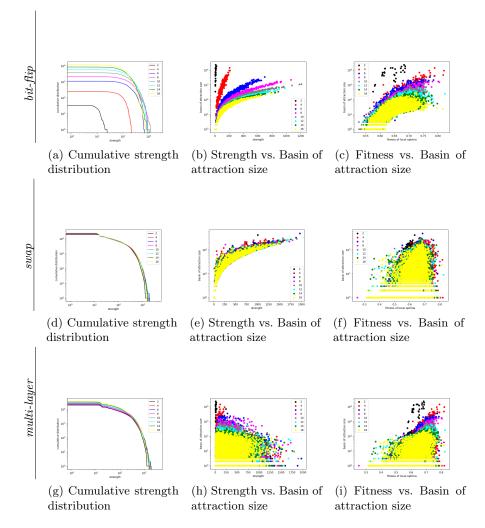


Fig. 3: Local metrics for bit-flip, swap, and multi-layer for each value of K. Figures a, d and g are in log-log scale; Figures b, e, h, c, f and i are in a semilogy scale.

positive correlation with strength for some values of K. However this behavior seems to be different in swap, that presents a high positive correlation for any value of K, corroborating with the stable results presented in Table 2. Moreover, we notice that in this case, bit-flip influences much more the multi-layer than swap.

From Figures 3c, 3f and 3i, which present the correlation between the fitness and the basin of attraction size in a semi-logy scale, a low correlation between these metrics for bit-flip while a non-linear correlation, tending to lie near a smooth curve, can be observed for swap. In this case multi-layer seems to mix the behavior of both operators, in spite of reducing the correlation levels observed for both. In the case of swap, we observe a slightly better behavior since positive correlation between fitness and sizes of basins of attraction would be interesting as lots of solutions would be eventually attracted to good local optima or even the global optimum.

# 5 Conclusions and future directions

Local Optima Networks (LONs) are graph models used in fitness landscape analysis for understanding the search difficulty, studying metaheuristics and extracting representative characteristics from problem instances. In this paper we analyzed LON features extracted from three different landscapes all of built from NK-landscape instances. The first landscape uses the bit-flip, the second one uses 1-swap moves and the third was obtained by combining both operators in a two-layer network. In this way we proposed a new model called multi-layer local optimal network (MLLON). In addition, formal concepts of MLLONs have been presented, including important aspects of the methodology to explore the model and extract FLA metrics from it.

The MLLON analysis showed how properties are shared from both network layers. Depending on the network metric considered, the swap operator introduces properties which are invariant with K. This is the case for global metrics in general. However, the bit-flip operator introduces shortcuts evidenced by high clustering coefficients and short paths to the global optimum, giving characteristics of small-world network models.

In the future, we intend to study how the proposed multi-layer model can lead to making specific design decision in the context of VNS and other metaheuristics alike. To achieve this, we aim at using more local search operators and efficiently connecting basins of attraction belonging to different landscapes. Particularly, considering the edges between basins with different local optima (which can be accomplished by setting  $P_{co}^{\neq} > 0$ ). In addition, we plan to explore other characteristics of the multi-layer networks that we did not consider in this paper, as neutrality, and exploring other forms of calculating metrics for multi-layer networks (e.g. by layer aggregation instead of flattening).

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