# Toward more efficient heuristic construction of Boolean functions 

Domagoj Jakobovic ${ }^{\text {a }}$, Stjepan Picek $^{\text {b }}$, Marcella S. R. Martins ${ }^{\text {c }}$, Markus Wagner ${ }^{\text {d }}$<br>${ }^{a}$ University of Zagreb - Croatia<br>${ }^{b}$ Delft University of Technology - The Netherlands<br>${ }^{c}$ Federal University of Technology - Parana, Brazil<br>${ }^{d}$ University of Adelaide - Australia


#### Abstract

Boolean functions have numerous applications in domains as diverse as coding theory, cryptography, and telecommunications. Heuristics play an important role in the construction of Boolean functions with the desired properties for a specific purpose. However, there are only sparse results trying to understand the problem's difficulty. With this work, we aim to address this issue. We conduct a fitness landscape analysis based on Local Optima Networks (LONs) and investigate the influence of different optimization criteria and variation operators. We observe that the naive fitness formulation results in the largest networks of local optima with disconnected components. Also, the combination of variation operators can both increase or decrease the network size. Most importantly, we observe correlations of local optima's fitness, their degrees of interconnection, and the sizes of the respective basins of attraction. This can be exploited to restart algorithms dynamically and influence the degree of perturbation of the current best solution when restarting.


Keywords:
balancedness, nonlinearity, landscape analysis, local optima networks

[^0]
## 1. Introduction

Boolean functions are mathematical objects that can be uniquely represented in truth tables and they have applications in diverse domains. Not only do they form a core concept in combinatorial optimization, such as in the satisfiability problem, but they are used to construct Hadamard matrices [1], strongly regular graphs [2], and decision diagrams [3]. In coding theory, every binary unrestricted code of length $2^{n}$ can be interpreted as a set of Boolean functions $[4,5]$. In sequences, bent sequences constructed using bent Boolean functions have the lowest value of mutual correlations and autocorrelations, and they are used in communication systems with multiple access [6]. In telecommunications, bent Boolean functions are used in CDMA networks [7]. In cryptography, Boolean functions are used in stream and block ciphers as the source of nonlinearity [8, 9], the design of hash functions [10], or for generating pseudorandom numbers [11]. While various domains have different usages of Boolean functions, some shared characteristics remain. For instance, the ratio between the zeros and ones in the Boolean function's truth table is an important characteristic for many fields. Similarly, the nonlinearity property is not only relevant in cryptography, but also coding theory and sequences. Unfortunately, such widespread use of Boolean functions can also represent a problem since there are numerous scenarios (e.g., considering Boolean function size or relevant properties) for Boolean functions, and it is not always readily available how to construct the required Boolean function.

There are several construction methods to construct Boolean functions: algebraic constructions, random search, heuristics, and combinations of those methods [12]. The advantages of heuristics seem to be (1) the ability to generate many different functions, (2) easy adjustment for different criteria, and (3) very good performance if the size of a Boolean function is not too large. On the other hand, the main drawbacks are (1) no guarantee that optimal solutions will be reached, (2) for every new Boolean function size, new optimization needs to be undertaken, and (3) due to the huge search space size, heuristics are limited in the Boolean function size. In practice, in many domains, the size $n$ of a Boolean function is not very large. For instance, in error-correcting codes, the sizes usually do not surpass 10 since they already give codes of size $2^{n}$ (i.e., codes of length 1024). In cryptography, when used as vectorial Boolean functions, they rarely surpass the size 8, and in the stream ciphers, the size was at most 10 until recent algebraic attacks, and now, the size goes up to 20 inputs. At the same time, already for $n>5$,
the exhaustive search is not possible. Note, that, for a Boolean function with $n$ inputs, there are $2^{2^{n}}$ possible Boolean functions.

Heuristics is applied to evolve Boolean functions for cryptography [13] and combinatorial designs [14, 15]. What is more, some of the common properties of Boolean functions commonly evolved with heuristics are relevant is the telecommunications [7] and sequences [6] domains. Thus, while heuristics has an important role in the design of Boolean functions, there are only sparse results trying to understand the problem's difficulty or when it can reach optimal solutions. Fitness landscape analysis (FLA) studies the influence of representations on the design of such heuristics, addressing the relative importance of features in explaining the algorithm performance [16].

This article investigates how a range of different design decisions can affect the search for Boolean functions. In particular, we conduct the first FLA for Boolean functions considering several function sizes most occurring in the literature, Boolean function properties, and variation operators in isolation as well as in combination. As far as we know, this is also the first time that combined neighborhood strategies are applied (in parallel) and considered in an FLA context in general.

## 2. Boolean Functions and Their Properties

Let $n$ be a positive integer, i.e., $n \in \mathbb{N}^{+}$. The set of all $n$-tuples of elements in the field $\mathbb{F}_{2}$ is denoted as $\mathbb{F}_{2}^{n}$ where $\mathbb{F}_{2}$ is the Galois field with two elements. The inner product of two vectors $a$ and $b$ is denoted by $a \cdot b$ and equals $a \cdot b=\bigoplus_{i=0}^{n-1} a_{i} b_{i}$. Here, " $\oplus$ " represents addition modulo two (bitwise XOR).

An $(n, 1)$-function is any mapping $f$ from $\mathbb{F}_{2}^{n}$ to $\mathbb{F}_{2}$ and such a function is called the Boolean function. A Boolean function $f$ on $\mathbb{F}_{2}^{n}$ can be uniquely represented by a truth table (TT), which is a vector $(f(0), \ldots, f(1))$ that contains the function values of $f$, ordered lexicographically, i.e., $a \leq b$.

The Walsh-Hadamard transform $W_{f}$ is a unique representation of a Boolean function that measures the correlation between $f(x)$ and the linear functions $a \cdot x[17]$ :

$$
\begin{equation*}
W_{f}(a)=\sum_{x \in \mathbb{F}_{2}^{n}}(-1)^{f(x) \oplus a \cdot x} \tag{1}
\end{equation*}
$$

A Boolean function $f$ is balanced if it takes the value 1 exactly the same number $2^{n-1}$ of times as the value 0 when the input ranges over $\mathbb{F}_{2}^{n}$.

| $x_{2}$ | $x_{1}$ | $x_{0}$ | TT |
| :---: | :---: | :---: | :---: |
| 0 | 0 | 0 | 1 |
| 0 | 0 | 1 | 1 |
| 0 | 1 | 0 | 0 |
| 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 0 |
| 1 | 0 | 1 | 0 |
| 1 | 1 | 0 | 1 |
| 1 | 1 | 1 | 0 |

Table 1: Truth table of a Boolean function with 3 inputs.

The minimum Hamming distance between a Boolean function $f$ and all affine functions (in the same number of variables as $f$ ) is called the nonlinearity of $f$. The nonlinearity $N l_{f}$ of a Boolean function $f$ can be expressed in terms of the Walsh-Hadamard coefficients as [17]:

$$
\begin{equation*}
N l_{f}=2^{n-1}-\frac{1}{2} \max _{a \in \mathbb{F}_{2}^{n}}\left|W_{f}(a)\right| . \tag{2}
\end{equation*}
$$

In Table 1, we give an example of a Boolean function with 3 inputs. Clearly, this function is balanced as it has the same number of zeros and ones in the truth table representation (TT column).

In Table 2, we give an example of Walsh-Hadamard calculation of the Boolean function from Table 1. Notice that to conform with Eq. (1), instead of TT, we write $f(x)$. Also, while we write $a$ values as integers, they should be considered as binary values. Finally, from column $W_{f}(a)$, we see that the maximal absolute Walsh-Hadamard spectrum value equals 4, which means that nonlinearity equals 2 as per Eq. (2) $\left(2^{2}-\frac{1}{2} \cdot 4=2\right)$.

The maximal value of the Walsh-Hadamard spectrum equals at least $2^{n / 2}$, which occurs in the case of bent Boolean functions [1]. Bent functions cannot be balanced, as their Hamming weight equals $2^{n}-1 \pm 2^{\frac{n}{2}-1}$. Bent functions exist only for $n$ even. The nonlinearity of bent functions equals [1, 18]:

$$
\begin{equation*}
N l_{f}=2^{n-1}-2^{\frac{n}{2}-1} . \tag{3}
\end{equation*}
$$

The nonlinearity of a Boolean function with $n$ variables is bounded above by $2^{n-1}-2^{\frac{n}{2}-1}$ (the Covering Radius Bound). Clearly, this bound cannot be

| $a$ | $f(x)$ | $W_{f}(a)$ |
| :---: | :---: | :---: |
| 0 | 1 | $(-1)^{1}+(-1)^{1}+(-1)^{0}+(-1)^{1}+(-1)^{0}+(-1)^{0}+(-1)^{1}+(-1)^{0}=0$ |
| 1 | 1 | $(-1)^{1}+(-1)^{0}+(-1)^{0}+(-1)^{0}+(-1)^{0}+(-1)^{1}+(-1)^{1}+(-1)^{1}=0$ |
| 2 | 0 | $(-1)^{1}+(-1)^{1}+(-1)^{1}+(-1)^{0}+(-)^{0}+(-1)^{0}+(-1)^{0}+(-1)^{1}=0$ |
| 3 | 1 | $(-1)^{1}+(-1)^{0}+(-1)^{1}+(-1)^{1}+(-1)^{0}+(-1)^{1}+(-1)^{0}+(-1)^{0}=0$ |
| 4 | 0 | $(-1)^{1}+(-1)^{1}+(-1)^{0}+(-1)^{1}+(-1)^{1}+(-1)^{1}+(-1)^{0}+(-1)^{1}=-4$ |
| 5 | 0 | $(-1)^{1}+(-1)^{0}+(-1)^{0}+(-1)^{0}+(-1)^{1}+(-1)^{0}+(-1)^{0}+(-1)^{0}=4$ |
| 6 | 1 | $(-1)^{1}+(-1)^{1}+(-1)^{1}+(-1)^{0}+(-1)^{1}+(-1)^{1}+(-1)^{1}+(-1)^{0}=-4$ |
| 7 | 0 | $(-1)^{1}+(-1)^{0}+(-1)^{1}+(-1)^{1}+(-1)^{1}+(-1)^{0}+(-1)^{1}+(-1)^{1}=-4$ |

Table 2: Calculation of the Walsh-Hadamard spectrum for a Boolean function with 3 inputs.
tight when $n$ is odd, so for Boolean functions with an odd number of inputs, the maximal nonlinearity lies between $2^{n-1}-2^{\frac{n-1}{2}}$ and $2^{n-1}-2^{\frac{n}{2-1}}$.

While we consider here only two properties, balancedness and nonlinearity, they play important roles in different domains. For example, finding the covering radius for the Reed-Muller code of order one is equivalent to finding maximally nonlinear Boolean functions [17]. Note that balanced Boolean functions are used in cryptography and coding theory while bent functions are, for instance, used in sequences and mobile networks.

## 3. Applications of Boolean Functions

In the last few decades, there has been a number of papers considering heuristics and Boolean functions. A more careful study reveals that a large part of those works considers applications in cryptography, and we provide an overview in the following.

To the best of our knowledge, Millan et al. were the first to apply genetic algorithms (GAs) to the evolution of cryptographically suitable Boolean functions [19]. There, the authors experimented with GA to evolve Boolean functions with high nonlinearity. Later, Millan et al. [20] continued to use GA to evolve Boolean functions with high nonlinearity. In conjunction with the GA, they used hill climbing and a resetting step to find Boolean functions with even higher nonlinearity and sizes of up to 12 inputs. Dawson et al. [21] experimented with two-stage optimization to generate Boolean functions. They used a combination of simulated annealing and hill-climbing with a cost function motivated by the Parseval theorem to find functions with high nonlinearity and low autocorrelation. Kavut and Melek [22] developed improved cost functions for a search that combines simulated annealing and hill
climbing. With that approach, the authors were able to find some functions of eight and nine inputs that have a combination of nonlinearity and autocorrelation values previously not obtained. Millan et al. [23] proposed a new adaptive strategy for the local search algorithm for the generation of Boolean functions with high nonlinearity. Hernan et al. [24] were the first to use a multi-objective random bit climber to search for balanced Boolean functions of size up to eight inputs with high nonlinearity. Picek et al. [25] experimented with genetic algorithms and genetic programming to find Boolean functions that possess several cryptographic properties. As far as we are aware, this is the first application of genetic programming to the evolution of Boolean functions with cryptographic properties. Picek at. investigated the symmetries in highly nonlinear balanced Boolean functions with 8 inputs [26]. Mariot and Leporati [27] used Particle Swarm Optimization to find Boolean functions with good trade-offs of cryptographic properties for dimensions up to 12 .

There have been several successful approaches where the authors could find bent Boolean functions for different dimensions. Hrbacek and Dvorak experimented with Cartesian genetic programming to evolve bent Boolean functions of size up to 16 inputs [30]. Picek and Jakobovic used genetic programming to evolve algebraic constructions used to construct bent Boolean functions [31].

When considering combinatorial designs, Mariot et al. used evolutionary algorithms to design binary orthogonal arrays [14] and orthogonal Latin squares [15].

## 4. Analyzing Fitness Landscapes

Fitness landscapes describe the relationship between search and fitness space [33], thus a heuristic strategy can navigate a specific landscape structure searching for optimal solutions.

Several cost models have been used to make specific predictions for combinatorial problems, identifying which features of the fitness landscape contribute more to the problem solving complexity during the search. By identifying these features, some improvements regarding the algorithm performance can be designed.

The Local Optima Network (LON) [34] is a model designed to understand the local optima structure in combinatorial landscapes, incorporating


Figure 1: An example of the connectivity in local optima networks.
network analysis techniques to study fitness landscapes and problem difficulty [35].

The fitness landscape in LON models is modeled as a graph where the local optima represent nodes that can be connected. A local search heuristic $\mathcal{H}$ maps the solution space $S$ to the set of locally optimal solutions $S^{*}$. Given a fitness function $F$, a solution $i$ in the solution space $S$ is a local maximum according to a neighbourhood operator $N$ if $F(i) \geq F(s), \forall s \in N(i)$.

Each local optima $i$ has an associated set of basin of attraction defined by $B_{i}=\{s \in S \mid \mathcal{H}(s)=i\}$. This set contains all the solutions that, after applying a local search starting from each of them, the procedure returns $i$. The cardinality of $B_{i}$ is the size of the basin of attraction of $i$. Given a neighborhood operator, we assume a connection between two local optima if at least one solution in one basin has a neighbor solution in the other basin. This assumption is based on previous basin-edges models, which also do not consider weighted edges [34, 36, 37].

Figure 1 shows a simplified LON for visualization purposes, illustrating the basin of attraction (red circles), their local optima (big blue dots), the solutions that converge to the local optima when applying the local search (small red dots), and the edges between the local optima (black lines) that exist due to neighborhood. Note that sophisticated heuristics might result in many more interconnections between the basin of attraction than what we have presented in the example.

In early works, local optima networks were exhaustively extracted on representative NK landscape instances [38, 34]. Additionally, some works investigated the correlation between LON features and the performance of search heuristics [39, 40, 16].

Permutation-based problems have also been subject to LON analyzes [41]. Besides, [35] extended the LON modeling to neutral fitness landscapes. Neutral networks are connected networks of solutions of equal fitness, with pos-
sibly jumps between them. The authors study two neutral versions of the NK landscape model, tuning the amount of neutrality. The results confirmed that the study of neutrality could improve the heuristic search.

Recently, some works addressed a LON variant called Compressed Local Optima Network. The work proposed in [42] investigated fitness landscape properties for the Number Partitioning Problem, exploring whether the global landscape structure of the number partitioning problem changes with the phase transition. In [43], the authors analyzed the network features to find differences between the landscape structures for the Permutation Flowshop Scheduling Problem (PFSP). The results provided insights into which features impact the performance of an iterated local search heuristic.

The authors in [36] investigated two hill-climbing local search procedures for building their corresponding LONs. The LONs were analyzed to understand the difficulty of Travelling Thief Problem (TTP) instances. Among others, they found that certain operators can result in LONs with disconnected components and that at times potentially exploitable correlations of node degree, basin size, and fitness exist.

Using a similar methodology, the first landscape analysis in the greater field of security investigated cryptographic S-Boxes [37]. For the chosen fitness functions and two neighbourhood operators (considered in isolation), it was observed that the number of local optima is substantial, and a conjecture has been made that links S-Boxes of odd dimensions to their problem difficulty.

Here, we use fitness landscape analysis to study the effects that algorithmic design decisions have on optimizing Boolean functions' two important properties. We consider three fitness functions, two initialization strategies, and three neighborhood operators - the latter in isolation and combination, resulting in seven different neighborhoods.

## 5. Creating Networks with Local Search

In order to obtain LONs of the Boolean function optimization landscape, we use a local search procedure that, starting from a given initial solution, converges to a corresponding local optimum. Along with the initial solution, all the intermediate solutions leading from the initial solution to the local optimum are added as the members of that local optimum's basin of attraction. This procedure is repeated for each solution in the set of initial solutions. After that, we record all unique local optima and reconstruct the connections

```
```

Algorithm 1 A greedy local search heuristic

```
```

Algorithm 1 A greedy local search heuristic
$s \leftarrow$ initial solution
$s \leftarrow$ initial solution
while there is an improvement do
while there is an improvement do
$s^{*}=s$
$s^{*}=s$
for each $s^{* *}$ in $\mathcal{N}(s)$ do
for each $s^{* *}$ in $\mathcal{N}(s)$ do
if $F\left(s^{* *}\right)>F\left(s^{*}\right)$ then
if $F\left(s^{* *}\right)>F\left(s^{*}\right)$ then
$s^{*} \leftarrow s^{* *}$
$s^{*} \leftarrow s^{* *}$
end if
end if
end for
end for
$s=s^{*}$
$s=s^{*}$
end while

```
```

    end while
    ```
```

between their basins of attraction.
The local search is described in Algorithm 1; it can be used with an arbitrary representation and an arbitrary neighborhood relationship, where $\mathcal{N}($.$) represents the neighborhood of the given solution. In the local search,$ a new solution is accepted only if at least one solution with a better fitness value is found within the entire neighborhood. Note that the algorithm is deterministic; if there are multiple solutions with the same fitness value, the algorithm will retain the first one that it encounters, while the ordering of the solutions in the neighborhood depends on the actual neighborhood relation. If no better solution is found in the initial solution neighborhood, the algorithm will not record the initial solution as a local optimum.

### 5.1. Neighborhood Operators

This study considers the truth table representation of Boolean functions, which is encoded as a bitstring. We opted to use the bitstring encoding, even though the related works usually report graph/tree encoding as the best performing one, due to two reasons. First, the properties we consider in our fitness functions are directly connected with the truth table representation. Consequently, exploring neighborhoods in the bitstring encoding gives a direct insight into the difficulty of the problem. Contrary, having a small change in an encoding like the tree encoding, which represents a Boolean function in the form of an expression, can cause a large change in the truth table, thus making the algorithmic design decisions more difficult. Second, we explore Boolean functions up to dimension 7 (i.e., when the search space is $2^{128}$ ) and related works show that for such sizes, the bitstring encoding achieves the same performance [13].

With the bitstring encoding, we use three neighborhood variants within Algorithm 1:

1. The first (denoted "swap") uses the swap operation (also known as "toggle") to generate the neighborhood; the swap operation takes two different positions in the bitstring and exchanges them.
2. The second variant (denoted "flip") flips the selected bit in the bitstring.
3. The third variant (denoted "insert") uses the insertion operator; this operator takes a value out of the bitstring at a random position $i$ and inserts it at another random position $j$, thus pushing the values between $i$ and $j$ by one spot to the right.
Also, to investigate complementary capabilities, we consider the following four combined neighborhoods: (1) swap/flip, (2) swap/insert, (3) flip/insert, and (4) swap/flip/insert. Whenever we consider any of these, e.g., swap/flip, we first construct the neighborhood for each operator in isolation, then merge them in the defined order (e.g., all the swap neighbors first, then all the insert neighbors), and then consider this sorted sequence as the combined neighborhood that is created by considering both operators at the same time. Some authors also considered combined strategies by proposing algorithms that use local search methods based on combined neighborhood operators [44]. However, they apply local search strategies sequentially, differently from our investigation: here, in each algorithm step we merge the solutions obtained simultaneously from all operators separately.

As we always consider the entire neighborhood before selecting the best, the order of the neighborhood-operators in these combinations does not matter, unless - as previously highlighted - the fitness of several solutions is identical. In that case, the algorithm will keep the first solution with the best fitness value it encounters, which favors first neighborhoods in the combination.

### 5.2. Initialization Strategies

In preliminary experiments, we observed that randomly sampled initial solutions for the subsequent hill-climbs result in very few edges in the final LONs. To give us a greater chance of observing connections in the LONs, and also for a more systematic approach, we consider "lexicographic" sampling (abbreviated: "lex"). This also starts with a random sample, but all subsequent samples continue in lexicographic order from the first sample, based on the binary representation.

### 5.3. Fitness Functions for Optimization of Boolean Functions

The first fitness function uses the nonlinearity value where the goal is to maximize it:

$$
\begin{equation*}
\text { fitness }_{1}: N l_{f} . \tag{4}
\end{equation*}
$$

In the second fitness function, we aim to search for balanced, highly nonlinear functions. We use a two-stage fitness in which a fitness bonus equal to the nonlinearity is awarded only to a perfectly balanced function; otherwise, the fitness is only described by the balancedness penalty. The balancedness penalty $B A L$ is defined as the difference up to the balancedness (i.e., the number of bits that need to be changed to reach balancedness) This difference is included in the fitness function with a negative sign to act as a penalty in maximization scenarios. The delta function $\delta_{B A L, 0}$ takes the value one when $B A L=0$ and is zero otherwise.

$$
\begin{equation*}
\text { fitness }_{2}:-B A L+\delta_{B A L, 0} \cdot N l_{f} . \tag{5}
\end{equation*}
$$

Finally, the third fitness function extends the second one to consider the whole Walsh-Hadamard spectrum and not only its extreme value:

$$
\begin{equation*}
\text { fitness }_{3}:-B A L+\delta_{B A L, 0} \cdot\left(N l_{f}+\text { Indicator }\right) . \tag{6}
\end{equation*}
$$

The Indicator property is the normalized number of occurrences of the maximal nonlinearity value in the whole spectrum (denoted \#max_values). Naturally, the smaller the number of such maximal values, the easier it is for the algorithm to reach the next nonlinearity value: Indicator $=2^{n}-\frac{\# \text { max_values }}{2^{n}}$.

## 6. Results and Discussion

This section analyzes the local optima networks obtained using the local search heuristic to reveal insights about the search space structure. Furthermore, we study the basins of attraction and their relationship with some LON properties looking for additional search difficulty information.

In our experiments, we explore the following parameters of the search space, which represent various design decisions that need to be made when setting up a heuristic search for Boolean functions:

- Boolean functions of size $4 \leq n \leq 7$;
- three fitness functions (Equations (4), (5), and (6));
- two initialization strategies;
- seven neighbourhood types (based on swap, flip, and insert);
- number of samples (unique initial solutions).

As it is possible to perform an exhaustive search for problem size $n=$ 4 - because the total number of solutions is $2^{16}$ - we build the LONs by enumerating the search space. In other words, the Algorithm 1 is executed for every possible initial solution (every Boolean function in $n=4$ variables). In larger sizes, we conduct a sampling process using a fixed sample size, which is the number of unique initial solutions: for each solution, we run Algorithm 1 until no further improvements are possible. ${ }^{1}$

Note that, because both our fitness functions (nonlinearity, balancedness, and the Walsh-Hadamard spectrum) and our neighbourhood enumeration here require fully defined functions (so that we can enumerate the complete neighbourhood), small structural changes would be necessary to transfer our approach to partially defined Boolean functions that do not define all $2^{n}$ possible solutions.

### 6.1. Topological Properties of Local Optima Networks

In Tables 3 and 4, we show graph properties that are often used for LON analyses [34]. In particular, we extract the following metrics. $n_{v}$ and $n_{e}$ represent the number of vertices (or nodes) and the number of edges of the generated LON, respectively. As in many other studies, we do not consider weights in the edges. $z$ is the average degree. $C$ is the average clustering coefficient. $C_{r}$ is the average clustering coefficient of corresponding random graphs (i.e., random graphs with the same number of vertices and mean degree). $b$ is the average basin size. $l$ is the average shortest path length between any two local optima. $\pi$ is the connectivity, which indicates if the LON is a connected graph. Finally, $S$ is the number of connected components (sub-graphs).

In Table 3, we report on the exhaustive search for Boolean functions with size $n=4$. We compare the three fitness functions fitness $_{1}$, fitness $_{2}$, and fitness $_{3}$ using the seven neighborhood operators. We find that the number of vertices $\left(n_{v}\right)$ for flip, swap is the same for the three functions, and this behavior also occurs with swapflip and swapflipinsert, which indicates that

[^1]the local optima and the distinct starting points are the same for these operators. However, except for flip and swap on the three functions, the actual LONs are quite different, with the number of edges $\left(n_{e}\right)$ ranging between about 14000 and 650000 .

The average degrees $(z)$ are higher for combined neighborhoods than for the isolated operators. A higher number of edges $\left(n_{e}\right)$ can also be noted for the combined neighborhoods on fitness $_{2}$ and fitness $_{3}$. Besides, the fitness ${ }_{1}$ function results in greater average degree than fitness $_{2}$ and fitness $_{3}$. Interestingly, the LON consists of only one component for almost all instances for fitness $_{2}$ and fitness $_{3}$ (with the exception of flip and swap for fitness ${ }_{2}$ function). In combination with the observed high mean degree and small minimum distances between nodes, this can mean that a Tabu Search [45, 46] with restarts or a Memetic Algorithm [47] with built-in local searches, or even an approach with explicit niching might be able to perform well and explore the entire network.

Table 4 shows the results using 10000 lexicographic-ordered samples (i.e., for $n \geq 5$ ), where a "sample" refers to a sampled starting point and a subsequent deterministic hill-climb. We typically find several hundreds of local optima. This indicates that there is a very large number of local optima in the landscape. ${ }^{2}$

Next, with the clustering coefficient $(C)$ of a node $i$, we measure how close its neighbors are to being a clique, and it characterizes the extent to which nodes adjacent to node $i$ are connected to each other. This determines, together with $l$, whether a graph is a small-world network (in which nodes are highly clustered yet the path length between them is small). We can observe in both tables that the LONs show a significantly higher degree of local clustering than their corresponding random graphs $\left(C_{r}\right)$. This means that the local optima are connected in two ways: dense local clusters and sparse interconnections, which can be difficult to find and exploit for all operators. Besides this, all connected LONs in both tables have a small minimal path length $l$ on average, i.e., any pair of local optima can be connected by traversing only a few other local optima. 5 mm ]

Additionally, for $n=4$, we briefly investigate the extent to which sampled

[^2]landscapes are representative of the entire problem. To do so, we sample the landscapes, extract the graph properties, and calculate the correlations. The resulting graph properties can be seen in Table .6 in the Appendix. Table 5 reports the Spearman correlation coefficient between the sampled landscapes and the completely enumerated landscapes. When the correlation is higher than 0.4 , then we highlight it in light blue. As one might expect, random initialization can be used to roughly estimate of the number of components $(S)$. Generally, for the lex initialization, the 10000 samples results in higher correlations than for the 1000 case; in some of the later experiments, we still consider 1000 samples due to the size of the neighborhood. In detail, lex shows a high correlation coefficient (with the complete enumeration) for the degree, and it ranges between 0.4 and 0.5 for both clustering coefficient $(C)$ and number of components $(S)$.

Table 3: General LON and basins' statistics for Boolean functions size 4. In each row, we show the LON that is the result of conducting a hill-climb from each of the possible $2^{16}$ unique solutions in the search space. A dash is shown when $l$ cannot be computed as multiple disconnected components exist.

| Size | Initialization | Function | Operator | $n_{v}$ | $n_{e}$ | $z$ | C | $C_{r}$ | $b$ | $l$ | $\pi$ | $S$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 5 | lex | fitness $_{2}$ | flip | 730 | 6272 | 17.1836 | 0.3022 | 0.0221 | 13.6356 | 3.0883 | 1 | 1 |
|  |  |  | insert | 260 | 4377 | 33.6692 | 0.4909 | 0.1296 | 3.8577 | 2.0222 | 1 | 1 |
|  |  |  | swap | 145 | 1960 | 27.0345 | 0.5687 | 0.1888 | 6.1172 | 1.9519 | 1 | 1 |
|  |  |  | flipinsert | 382 | 9569 | 50.0995 | 0.5323 | 0.1324 | 27.0969 | 1.9449 | 1 | 1 |
|  |  |  | swapflip | 193 | 2948 | 30.5492 | 0.5772 | 0.1610 | 52.6528 | 1.9664 | 1 | 1 |
|  |  |  | swapflipinsert | 280 | 7000 | 50.0000 | 0.5756 | 0.1784 | 36.6464 | 1.8604 | 1 | 1 |
|  |  |  | swapinsert | 240 | 5373 | 44.7750 | 0.5505 | 0.1862 | 4.1458 | 1.8633 | 1 | 1 |
|  |  | fitness $_{3}$ | flip | 813 | 8055 | 19.8155 | 0.3190 | 0.0238 | 12.3456 | 2.9684 | 1 | 1 |
|  |  |  | insert | 251 | 4355 | 34.7012 | 0.4918 | 0.1413 | 4.4542 | 1.9452 | 1 | 1 |
|  |  |  | swap | 183 | 3238 | 35.3880 | 0.5245 | 0.1972 | 5.3497 | 1.8835 | 1 | 1 |
|  |  |  | flipinsert | 414 | 11849 | 57.2415 | 0.5437 | 0.1395 | 25.8527 | 1.8909 | 1 | 1 |
|  |  |  | swapflip | 277 | 6554 | 47.3213 | 0.5370 | 0.1714 | 37.6570 | 1.8891 | 1 | 1 |
|  |  |  | swapflipinsert | 352 | 12190 | 69.2614 | 0.5584 | 0.1978 | 30.1477 | 1.8096 | 1 | 1 |
|  |  |  | swapinsert | 255 | 6363 | 49.9059 | 0.5292 | 0.1951 | 4.3451 | 1.8267 | 1 | 1 |
| 6 | lex | fitness $_{2}$ | flip | 363 | 3025 | 16.6667 | 0.3863 | 0.0450 | 27.5840 | 3 | 1 | 1 |
|  |  |  | insert | 236 | 3536 | 29.9661 | 0.4187 | 0.1277 | 2.3136 | 2.1369 | 1 | 1 |
|  |  |  | swap | 62 | 487 | 15.7097 | 0.4982 | 0.2505 | 5.9677 | 1.9334 | 1 | 1 |
|  |  |  | flipinsert | 314 | 6550 | 41.7197 | 0.4724 | 0.1327 | 32.7229 | 2.0490 | 1 | 1 |
|  |  |  | swapflip | 128 | 1698 | 26.5313 | 0.5045 | 0.2089 | 78.8047 | 1.9382 | 1 | 1 |
|  |  |  | swapflipinsert | 221 | 4404 | 39.8552 | 0.5305 | 0.1815 | 46.0905 | 1.9461 | 1 | 1 |
|  |  |  | swapinsert | 156 | 2608 | 33.4359 | 0.5128 | 0.2163 | 3.0128 | 1.8864 | 1 | 1 |
|  |  | fitness $_{3}$ | flip | 595 | 4822 | 16.2084 | 0.3481 | 0.0280 | 17.2185 | 3.1043 | 1 | 1 |
|  |  |  | insert | 163 | 2283 | 28.0123 | 0.5252 | 0.1816 | 4.4479 | 1.9076 | 1 | 1 |
|  |  |  | swap | 113 | 1396 | 24.7080 | 0.5608 | 0.2219 | 5.9735 | 1.8254 | 1 | 1 |
|  |  |  | flipinsert | 422 | 9640 | 45.6872 | 0.4684 | 0.1076 | 26.3436 | 2.0016 | 1 | 1 |
|  |  |  | swapflip | 249 | 4420 | 35.5020 | 0.4949 | 0.1437 | 43.8153 | 1.9196 | 1 | 1 |
|  |  |  | swapflipinsert | 348 | 9459 | 54.3621 | 0.5046 | 0.1572 | 32.0920 | 1.8754 | 1 | 1 |
|  |  |  | swapinsert | 177 | 3389 | 38.2938 | 0.5402 | 0.2185 | 4.7345 | 1.8073 | 1 | 1 |
| 7 | lex | fitness $_{2}$ | flip | 512 | 4223 | 16.4961 | 0.3550 | 0.0329 | 19.3516 | - | 0 | 2 |
|  |  |  | insert | 513 | 7742 | 30.1832 | 0.3696 | 0.0592 | 2.3294 | - | 0 | 2 |
|  |  |  | swap | 30 | 154 | 10.2667 | 0.5846 | 0.3326 | 21.9333 | 2 | 1 | 1 |
|  |  | fitness $_{3}$ | flip | 639 | 5212 | 16.3130 | 0.3201 | 0.0250 | 15.7042 | - | 0 | 2 |
|  |  |  | insert | 465 | 7152 | 30.7613 | 0.3926 | 0.0659 | 6.2839 | 3 | 1 | 1 |
|  |  |  | swap | 75 | 610 | 16.2667 | 0.6362 | 0.2105 | 14.6267 | 2 | 1 | 1 |

Table 4: General LON and basins' statistics for 10000 samples, with the lex initialization. We omit the random initialization, as the LONs always consisted of hundred to thousands of disconnected components. We also omit fitness $s_{1}$ here as it has also resulted in disconnected components. For $n=7$ the results for the combined neighborhoods are missing as they were
 exist.

| Samples | Initialization | $n_{v}$ | $n_{e}$ | $z$ | $C$ | $C_{r}$ | $b$ | 1 | $\pi$ | $S$ |
| ---: | :--- | :--- | :--- | :--- | :--- | :--- | ---: | :--- | :--- | :--- |
| 1,000 | lex | -0.0623 | 0.1891 | 0.8638 | 0.1670 | 0.0675 | 0.2181 | -0.2018 | 0.2582 | 0.3173 |
|  | random | -0.0172 | 0.2468 | 0.1955 |  |  | -0.2335 |  | 0.2709 |  |
| 10,000 | lex | -0.1807 | 0.2073 | 0.9210 | 0.5187 | 0.2338 | 0.4150 | 0.1632 | 0.3920 | 0.3738 |
|  | random | -0.0046 | 0.3290 | 0.3451 | -0.3966 |  | -0.2441 |  | 0.4353 |  |

Table 5: Spearman correlation coefficient between exhausted and sampled landscapes for $n=4$ for both lex and random initialization with 1000 and 10000 samples. Highlighted values present correlation higher than 0.4

Figures 2 to 7 present the obtained networks for Boolean functions with size $n=4$ to $n=7$.

We can see in Figures 2, 4, and 6 that swap and insert LONs, for example, present local dense connected components for fitness $_{1}$ function, while, in Figures 3, 5, and 7 for flipinsert, swapflipinsert, swapflip, and swapinsert, for examples, LONs are connected graphs for almost all fitness functions (except in swapinsert for fitness $_{1}$ ). The LONs for $n=5, n=6$, and $n=7$ with lex initialization using 10000 samples are connected graphs for almost all fitness functions and operators. For this reason, we suppressed them in this paper.


Figure 2: LON graphs on exhaustive $n=4$ with the three fitness functions for operators flip, insert, swap.


Figure 3: LON graphs on exhaustive $n=4$ with the three fitness functions for combination using operators flipinsert, swapflipinsert, swapflip, and swapinsert.

### 6.2. Distribution of Degree

To characterize the networks visually, we provide three types of plots for our search space: (1) the cumulative degree distribution; (2) the correlation between the degree of local optima and their corresponding basin sizes; and (3) the correlation between the fitness of local optima and their corresponding basin sizes.

For the first one, the cumulative degree distribution function represents the probability $P(k)$ that a random node has a degree larger than $k$.

Let us start with $n=4$. In the left columns of Figure 8 (for neighborhoods in isolation) and of Figure 9 (for neighborhoods in combination), we can see that the degree distributions hardly decay for small degrees for all the three single operators type and fitness functions, while their dropping rate is very high for high degrees, presenting short tails to the right. This behavior shows that there are few nodes with a large number of neighbors. However, most parts of the local optima have a small number of connections. A benefit of these few nodes with high connectivity is that these efficiently connect the entire landscape: a search at a random node has more chances to move to


Figure 4: LON graphs for lex initialization on $n=5$ with fitness functions fitness ${ }_{1}$, fitness $_{2}$ and fitness $_{3}$ using 1000 samples for all three operators: flip, insert, swap.
one of these high degree nodes, and then to another node, which can be an efficient way to search the entire network.

Local search strategies on networks have been investigated according to the degree distribution [48], particularly because some real-world network present properties in the topological structure that can be described by a power-law, or a scale-free degree distribution $P(k)=k^{-\alpha}$, where $\alpha \in[2,3]$ is a scaling parameter.

Aiming to study the cumulative degree distribution more strictly, we use the Kolmogorov-Smirnov test to investigate the adequacy of power-law [49] and exponential models $[50]^{3}$. The test is performed on all distributions shown with a significance level of 0.1 . When the $p$-value $>0.1$, the test fails to reject power-law and exponential as plausible distribution models.

Considering the distributions reported in Figure 8 for $n=4$, none of them fits power-law nor exponential models. For Figures $.13, .14, .15$, and .16 (see Appendix) with 1000 samples, the $n=6$ instances using lexicographic

[^3]

Figure 5: LON graphs for lex initialization on $n=5$ with fitness functions fitness $_{1}$, fitness $_{2}$ and fitness $3_{3}$ using 1000 samples for combination using operators flipinsert, swapflipinsert, swapflip, and swapinsert.
sampling (lex) and fitness $_{2}$ function type for flip operator, and fitness ${ }_{1}$ function type for swap operator, fit a power-law. For Figures .17, .18, .19, and .20 (see Appendix) with 10000 samples the $n=5$ instances for fitness $_{2}$ function type using lexicographic sampling (lex) for flip operator fit a powerlaw, as well as for the same instance considering the fitness $_{3}$ function type. The remaining instances do not fit a power-law nor an exponential model.

The degree distribution contributes to search a power-law graph more rapidly, assuming that the number of edges per node varies from node to node, i.e., its edges do not allow us uniformly sample the graph, but they preferentially lead to high degree nodes [36]. This means that a landscape with few nodes and a high degree enables that a search at a given node chosen at random presents more chances to move to one of these high degree nodes instead to another node, which can efficiently search the entire network.

To summarize our analyzes of degree distributions, as most instances cannot be represented with the straightforward interpretation from powerlaw models, another way to analyze the difficulty of the search space for the heuristics is to consider the size of the basins of attraction - which we will


Figure 6: LON graphs for lex initialization on $n=6$ with fitness functions fitness ${ }_{1}$, fitness $_{2}$ and fitness ${ }_{3}$ using 1000 samples for all three operators: flip, insert, swap.
explore next.

### 6.3. Basin Size Correlation

Our "matrices of plots" present the basin correlation in the middle and right columns, i.e., Figure 8 and Figure 9 show this for $n=4$, and Figures 10,11 , and 12 show these for the larger values of $n$. A particular focus of the last three mentioned figures is the difference of 1000 samples to 10000 samples.

Let us again start with $n=4$ in Figures 8 and 9. Firstly, flips and swaps seem to result in almost perfectly identical LONs. This is interesting, as the flips generate neighbors with the same Hamming distance to the original, and swaps generate neighbors with the Hamming distances 0 or 2.

Secondly, the swapinsert (green) neighborhood typically results in very different LONs, as we have already seen in the earlier tables: the local optima are significantly less interconnected. This might result from using two operators that result in neighbors with the Hamming distance 0 or 2 in combination with the lexicographic sampling. Also, it appears that the use of the flip operator results in significantly greater basins of attraction - however, as


Figure 7: LON graphs for lex initialization on $n=6$ with fitness functions fitness $_{1}$, fitness $_{2}$ and fitness $3_{3}$ using 1000 samples for combination using operators flipinsert, swapflipinsert, swapflip, and swapinsert.
we are using the lexicographic sampling of the initial solutions, this comes to no big surprise.

Thirdly, we can observe that the three different fitness functions resulted in quite different landscapes, and in particular, fitness ${ }_{1}$ is quite different from the other two. We can see some correlations for fitness $s_{1}$ of basin size with degree and fitness. At first sight, it is not clear how this information can be used in a heuristic. However, if techniques like self-adaptation and restarts are used in combination with fitness $_{1}$, then the progress achieved over time can be used in online control to indicate the expected achievable solution quality. Moreover, it should be possible to estimate this characteristic in a search heuristic with restarts to influence the amount of perturbation that is performed on the current best solution (i.e., to provide the first solution for the next hill-climb): if a solution resulted after a local search presents poor fitness, then a not-too-small perturbation should be applied to determine the initial point for the next run, aiming to increase chances to escape the small, bad basin of attraction. Note that the opposite does not hold, meaning that a large perturbation does not guarantee success. For fitness $s_{2}$ and fitness ${ }_{3}$,
however, the correlation is a lot weaker and hence might be difficult to exploit.
Lastly, let us highlight a few interesting aspects of the landscapes when $n$ is larger, i.e., in Figures 10, 11, and 12. For example, we can observe (except in the case of $n=6$ ) that the distance from the black distributions to the blue ones (factor 10 increase in samples) is roughly the same across all experiments - - in particular, this applies (roughly) to both dimensions in all three figures. If the increase would be limited to a shift in the y-axis, then this would mean that the 10 -fold increase in samples does not uncover different structures (as expressed in different degree distributions) in the landscape. However, the increase along the x -axis means that the rate of uncovering new structures is relatively stable. We believe that the number of samples has yet to be further increased as the degree distributions do not show signs of convergence yet. $n=6$ with swaps or inserts shows significantly different behavior, and it might be the case that substructures have not been discovered during a local search that resulted in interconnections between the local optima. This warrants additional future research.

Besides this, we can generally observe good correlations of degrees and basin sizes when inserts or swaps are used for $n=5$ and $n=6$. We can also observe that for $n=7$ only inserts seem to provide a decent correlation of degrees and basin sizes that might be exploitable, as mentioned above. Also, as before, the fitness of local optima seems to only carry some possibly exploitable information in the case of flips.

These experimental results can summarize some insights regarding the search improvements. The topological properties for fitness ${ }_{2}$ and fitness $_{3}$ are LON of only one component for almost all instances, presenting high mean degree and small minimum distances between nodes. Besides, the local optima are connected as dense local clusters and sparse interconnections, which can be difficult to exploit. Some heuristics such as Tabu Search with restarts or a Memetic Algorithm with built-in local searches, or even an approach with explicit niching might be able to explore the entire network searching for promising solutions. According to the basin distribution there are few nodes with a large number of neighbors connecting the entire landscape: a search at a random node has more chances to move to one of these high degree nodes, and then to another node, which can be an efficient way to search the entire network. Moreover flip operator seems to provide more information using basin size and fitness of local optima correlation than the others operators.


Figure 8: Statistical measures on exhaustive $n=4$ with the three fitness functions for operators flip (black), insert (blue), swap (red): Cumulative degree distribution in a loglog scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and their corresponding basin sizes (right).

## 7. Conclusions

Boolean functions are interesting mathematical objects that are widely used in many domains. Heuristics play an important role in their construction. However, little is known about the actual problem difficulty and the effect of various design decisions. This paper conducted a fitness landscape analysis (FLA) to study the effect of various decisions on the optimization of cryptographic properties. We investigated Boolean functions considering a different number of function sizes, three fitness functions, seven neighborhood operators used in isolation as well as in combination, and two initialization strategies.

We presented and analyzed the local optima networks (LONs) obtained


Figure 9: Statistical measures on exhaustive $n=4$ with the three fitness functions for combination using operators flipinsert (black), swapflipinsert (blue), swapflip (red), and swapinsert (green): Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and their corresponding basin sizes (right).
using a local search heuristic to investigate the search space structure. Furthermore, we studied the degree distribution and the correlation between the basins of attraction with some LON properties looking for additional information about the search difficulty, considering scenarios (e.g., combinations of neighborhoods) not investigated before.

We have observed (1) that the naive fitness function results in LONs with disconnected components, (2) which can typically be avoided by moving to other fitness functions. However, (3) we then appear to lose a correlation of basin size and LON degrees. (4) For our largest $n=7$ (i.e., when the search space is $2^{128}$ ), inserts appear to provide the largest possible exploitable correlation of basin sizes, local optima degrees, and local optima fitness.

In this paper, we concentrated on Boolean functions with 4 to 7 variables. In future work, we plan to extend our analysis up to 10 variables (i.e., up
flip


Figure 10: Statistical measures for lex initialization on $n=5$ with fitness functions fitness $_{2}$ and fitness $_{3}$ using 1000 (black) and 10000 (blue) samples for all three operators: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and their corresponding basin sizes (right).


Figure 11: Statistical measures for lex initialization on $n=6$ with fitness functions fitness $_{2}$ and fitness $_{3}$ using 1000 (black) and 10000 (blue) samples for all three operators: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and their corresponding basin sizes (right). Note that, in a few cases in the left column, no black line can be drawn as not enough points exist for a $\log -\log$ plot.


Figure 12: Statistical measures for lex initialization on $n=7$ with fitness functions fitness $_{2}$ and fitness $_{3}$ using 1000 (black) and 10000 (blue) samples for all three operators: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and their corresponding basin sizes (right).

536 to 1024 bits), which will require new approaches for evaluating complete 537 neighborhoods.

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## Appendix with Supplemental Material

We make use of the appendix in order to provide additional visualizations of the results. In particular:

1. $n=4$ : Table .6 shows the metrics when considering the sample process for $n=4$ for both lex and random initialization with 1000 and 10000 samples.
2. $n=5$ : Figure .13 shows the difference between the two initialization strategies, which we had not visualized before. Figure .14 shows the complex neighborhoods for 1000 samples.
3. $n=6$ : Figure .15 shows the individual neighborhoods for 1000 samples. Figure . 16 shows the complex neighborhoods for 1000 samples.
4. Figures $.17-.20$ show, for 10000 samples, the results for the neighborhoods in isolation and in combination for fitness $_{2}$ and fitness $_{3}$.

| Samples | Initialization | Function | Operator | $n_{v}$ | $n_{e}$ | $z$ | C | $C_{r}$ | $b$ | $l$ | $\pi$ | $S$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1000 | lex | fitness $_{1}$ | flip | 121 | 520 | 8.5950 | 0.3526 | 0.0858 | 9.0000 | - | 0 | 2 |
|  |  |  | insert | 438 | 3363 | 15.3562 | 0.5590 | 0.0381 | 2.8607 | - | 0 | 13 |
|  |  |  | swap | 306 | 1948 | 12.7320 | 0.6407 | 0.0424 | 4.7516 | - | 0 | 14 |
|  |  |  | flipinsert | 182 | 2494 | 27.4066 | 0.5753 | 0.1508 | 6.6374 | 2.0764 | 1 | 1 |
|  |  |  | swapflip | 306 | 3514 | 22.9673 | 0.4806 | 0.0763 | 4.7516 | 3.0680 | 1 | 1 |
|  |  |  | swapflipinsert | 363 | 5279 | 29.0854 | 0.4869 | 0.0807 | 4.3140 | 2.9272 | 1 | 1 |
|  |  |  | swapinsert | 363 | 3325 | 18.3196 | 0.6810 | 0.0492 | 4.3140 | - | 0 | 11 |
|  |  | fitness $_{2}$ | flip | 185 | 849 | 9.1784 | 0.3165 | 0.0494 | 5.2973 | - | 0 | 2 |
|  |  |  | insert | 626 | 5660 | 18.0831 | 0.4115 | 0.0297 | 2.0272 | - | 0 | 11 |
|  |  |  | swap | 379 | 2236 | 11.7995 | 0.5123 | 0.0292 | 4.3140 | - | 0 | 20 |
|  |  |  | flipinsert | 185 | 2132 | 23.0486 | 0.4563 | 0.1244 | 5.4216 | - | 0 | 2 |
|  |  |  | swapflip | 379 | 3416 | 18.0264 | 0.4235 | 0.0458 | 4.3140 | - | 0 | 2 |
|  |  |  | swapflipinsert | 382 | 4208 | 22.0314 | 0.4484 | 0.0578 | 4.2749 | - | 0 | 2 |
|  |  |  | swapinsert | 382 | 3005 | 15.7330 | 0.5823 | 0.0392 | 4.2749 | - | 0 | 19 |
|  |  | fitness $_{3}$ | flip | 173 | 802 | 9.2717 | 0.3259 | 0.0588 | 5.5954 | - | 0 | 2 |
|  |  |  | insert | 630 | 5630 | 17.8730 | 0.4157 | 0.0301 | 2.0397 | - | 0 | 9 |
|  |  |  | swap | 387 | 2334 | 12.0620 | 0.5106 | 0.0333 | 4.2765 | - | 0 | 19 |
|  |  |  | flipinsert | 173 | 2054 | 23.7457 | 0.4820 | 0.1400 | 5.7977 | - | 0 | 2 |
|  |  |  | swapflip | 387 | 3650 | 18.8630 | 0.4224 | 0.0459 | 4.2765 | - | 0 | 2 |
|  |  |  | swapflipinsert | 390 | 4470 | 22.9231 | 0.4484 | 0.0600 | 4.2385 | - | 0 | 2 |
|  |  |  | swapinsert | 390 | 3131 | 16.0564 | 0.5924 | 0.0409 | 4.2385 | - | 0 | 19 |
| 1000 | random | fitness $_{1}$ | flip | 972 | 1 | 0.0021 | 0.0000 | 0.0000 | 3.1173 | - | 0 | 971 |
|  |  |  | insert | 835 | 0 | 0.0000 | 0.0000 | 0.0000 | 2.1449 | - | 0 | 835 |
|  |  |  | swap | 972 | 1 | 0.0021 | 0.0000 | 0.0000 | 2.6173 | - | 0 | 971 |
|  |  |  | flipinsert | 987 | 0 | 0.0000 | 0.0000 | 0.0000 | 2.5502 | - | 0 | 987 |
|  |  |  | swapflip | 972 | 1 | 0.0021 | 0.0000 | 0.0000 | 2.6173 | - | 0 | 971 |
|  |  |  | swapflipinsert | 987 | 3 | 0.0061 | 0.0000 | 0.0000 | 2.5380 | - | 0 | 984 |
|  |  |  | swapinsert | 987 | 2 | 0.0041 | 0.0000 | 0.0000 | 2.5380 | - | 0 | 985 |
|  |  | fitness $_{2}$ | flip | 803 | 0 | 0.0000 | 0.0000 | 0.0000 | 2.9178 | - | 0 | 803 |
|  |  |  | insert | 692 | 0 | 0.0000 | 0.0000 | 0.0000 | 2.2934 | - | 0 | 692 |
|  |  |  | swap | 832 | 6 | 0.0144 | 0.0000 | 0.0000 | 2.9075 | - | 0 | 826 |
|  |  |  | flipinsert | 832 | 0 | 0.0000 | 0.0000 | 0.0000 | 2.9014 | - | 0 | 832 |
|  |  |  | swapflip | 832 | 8 | 0.0192 | 0.0000 | 0.0000 | 2.9123 | - | 0 | 824 |
|  |  |  | swapflipinsert | 832 | 10 | 0.0240 | 0.0000 | 0.0000 | 2.9038 | - | 0 | 822 |
|  |  |  | swapinsert | 832 | 8 | 0.0192 | 0.0000 | 0.0000 | 2.8990 | - | 0 | 824 |
|  |  | fitness $_{3}$ | flip | 803 | 0 | 0.0000 | 0.0000 | 0.0000 | 2.9178 | - | 0 | 803 |
|  |  |  | insert | 704 | 0 | 0.0000 | 0.0000 | 0.0000 | 2.2884 | - | 0 | 704 |
|  |  |  | swap | 844 | 6 | 0.0142 | 0.0000 | 0.0000 | 2.8945 | - | 0 | 838 |
|  |  |  | flipinsert | 844 | 0 | 0.0000 | 0.0000 | 0.0000 | 2.8886 | - | 0 | 844 |
|  |  |  | swapflip | 844 | 8 | 0.0190 | 0.0000 | 0.0000 | 2.8993 | - | 0 | 836 |
|  |  |  | swapflipinsert | 844 | 12 | $0.0284$ | 0.0000 | $0.0000$ | 2.8910 | - | 0 | 832 |
|  |  |  | swapinsert |  | $10$ | $0.0237$ | $0.0000$ | $0.0000$ | $2.8863$ | - | 0 | 834 |
| 10000 | lex | fitness $_{1}$ | flip | 732 | 6286 | 17.1749 | 0.3105 | 0.0233 | 14.2514 | 2.9103 | 1 | 1 |
|  |  |  | insert | 3574 | 71540 | 40.0336 | 0.3816 | 0.0113 | 3.3898 | - | 0 | 11 |
|  |  |  | swap | 1785 | 32130 | 36.0000 | 0.4864 | 0.0199 | 7.3647 | - | 0 | 14 |
|  |  |  | flipinsert | 938 | 37871 | 80.7484 | 0.4886 | 0.0855 | 11.9872 | 2.1088 | 1 | 1 |
|  |  |  | swapflip | 1785 | 52112 | 58.3888 | 0.3814 | 0.0326 | 7.3647 | 3.1423 | 1 | 1 |
|  |  |  | swapflipinsert | 2035 | 88221 | 86.7037 | 0.3988 | 0.0429 | 6.8590 | 3.0030 | 1 | 1 |
|  |  |  |  | 2035 | 62664 | 61.5862 | 0.5420 | 0.0302 | 6.8590 | - | 0 | 14 |
|  |  | fitness $_{2}$ | flip | 1835 | 13696 | 14.9275 | 0.2121 | 0.0085 | 5.3232 | - | 0 | 2 |
|  |  |  | insert | 5289 | 99516 | 37.6313 | 0.2836 | 0.0072 | 2.1624 | - | 0 | 8 |
|  |  |  | swap | 3797 | 56380 | 29.6971 | 0.3364 | 0.0078 | 4.3303 | - | 0 | 14 |
|  |  |  | flipinsert | 1812 | 48743 | 53.8002 | 0.2743 | 0.0299 | 5.5425 | 2.9435 | 1 |  |
|  |  |  | swapflip | 3796 | 75460 | 39.7576 | 0.2920 | 0.0105 | 4.3314 | 4.2448 | 1 | 1 |
|  |  |  | swapflipinsert | 3840 | 107445 | 55.9609 | 0.2797 | 0.0147 | 4.2745 | 3.8454 | 1 | 1 |
|  |  |  |  | 3841 | 87823 | 45.7292 | 0.3417 | 0.0118 | 4.2734 | - | 0 | 14 |
|  |  | fitness $_{3}$ | flip | 1707 | 13253 | 15.5278 | 0.2230 | 0.0082 | 5.6473 | - | 0 | 2 |
|  |  |  | insert | 5281 | 99007 | 37.4956 | 0.2841 | 0.0070 | 2.1888 | - | 0 | 9 |
|  |  |  | swap | 3777 | 58117 | 30.7742 | 0.3377 | 0.0079 | 4.3818 | - | 0 | 14 |
|  |  |  | flipinsert | 1683 | 47481 | 56.4242 | 0.2861 | 0.0336 | 5.9673 | 2.8311 | 1 | 1 |
|  |  |  | swapflip | 3776 | 78943 | 41.8130 | 0.2926 | 0.0110 | 4.3829 | 4.1114 | 1 | 1 |
|  |  |  | swapflipinsert | 3819 | 111198 | 58.2341 | 0.2819 | 0.0153 | 4.3263 | 3.7668 | 1 | 1 |
|  |  |  | swapinsert | 3820 | 89878 | 47.0565 | 0.3470 | 0.0123 | 4.3251 | - | 0 | 14 |
|  | random | fitness $_{1}$ | flip | 9698 | 11 | 0.0023 | 0.0000 | 0.0000 | 3.1448 | - | 0 | 9687 |
| 10000 |  |  | insert | 8335 | 29 | 0.0070 | 0.0000 | 0.0000 | 2.1445 | - | 0 | 8306 |
|  |  |  | swap | 9698 | 93 | 0.0192 | 0.0003 | 0.0000 | 2.6172 | - | 0 | 9606 |
|  |  |  | flipinsert | 9831 | 88 | 0.0179 | 0.0000 | 0.0000 | 2.5442 | - | 0 | 9743 |
|  |  |  | swapflip | 9697 | 130 | 0.0268 | 0.0005 | 0.0000 | 2.6176 | - | 0 | 9569 |
|  |  |  | swapflipinsert | 9828 | 194 | 0.0395 | 0.0002 | 0.0000 | 2.5308 | - | 0 | 9635 |
|  |  |  | swapinsert | 9829 | 153 | 0.0311 | 0.0000 | 0.0000 | 2.5305 | - | 0 | 9676 |
|  |  | fitness $_{2}$ | flip | 8033 | 5 28 | 0.0012 | 0.0000 | 0.0000 | 2.9512 | - | 0 | 8028 |
|  |  |  | insert | 6848 | 28 | 0.0082 | 0.0000 | 0.0000 | 2.3112 | - | 0 | 6820 |
|  |  |  | swap flipinsert | 8332 8353 | 534 43 | 0.1282 0.0103 | 0.0061 0.0000 | 0.0000 0.0000 | 2.9399 2.9251 | - | 0 0 | 7881 8310 |
|  |  |  | swapflip | 8326 | 744 | 0.1787 | 0.0084 | 0.0000 | 2.9455 | - | 0 | 7774 |
|  |  |  | swapflipinsert | 8325 | 1108 | 0.2662 | 0.0115 | 0.0000 | 2.9348 | - | 0 | 7559 |
|  |  |  | swapinsert | 8331 | 881 | 0.2115 | 0.0108 | 0.0000 | 2.9292 | - | 0 | 7648 |
|  |  | fitness $_{3}$ | flip | 8033 | 4 | 0.0010 | 0.0000 | 0.0000 | 2.9512 | - | 0 | 8029 |
|  |  |  | insert | 6963 | 29 | 0.0083 | 0.0000 | 0.0000 | 2.3078 | - | 0 | 6934 |
|  |  |  | swap | 8445 | 505 | 0.1196 | 0.0065 | 0.0000 | 2.9275 | - | 0 | 8010 |
|  |  |  | flipinsert | 8468 | 40 | 0.0094 | 0.0000 | 0.0000 | 2.9127 | - | 0 | 8428 |
|  |  |  | swapflip | 8438 | 690 | 0.1635 | 0.0082 | 0.0000 | 2.9333 | - | 0 | 7899 |
|  |  |  | swapflipinsert | 8437 | 1058 | 0.2508 | 0.0102 | 0.0000 | 2.9230 | - | 0 | 7679 |
|  |  |  | swapinsert | 8444 | 853 | 0.2020 | 0.0097 | 0.0000 | 2.9172 | - | 0 | 7769 |

Table .6: General LON and basins' statistics for $n=4$ with 1000 and 10000 samples, considering lex and random initialization. A dash is shown when $l$ cannot be computed as multiple disconnected components exist.

[^4]
random





Figure .14: Statistical measures for lex initialization on $n=5$ with the three fitness functions for combination using operators flipinsert (black), swapflipinsert (blue), swapflip (red), and swapinsert (green) using 1000 samples: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and corresponding basin sizes (right).


Figure .15: Statistical measures for lex initialization on $n=6$ with the three fitness functions for operators flip (black), insert (blue), swap (red) using 1000 samples: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and corresponding basin sizes (right).


Figure .16: Statistical measures for lex initialization on $n=6$ with fitness functions fitness $_{2}$ and fitness $_{3}$ for combination using operators flipinsert (black), swapflipinsert (blue), swapflip (red), and swapinsert (green) using 1000 samples: Cumulative degree distribution in a $\log$-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and corresponding basin sizes (right).


Figure .17: Statistical measures for lex initialization on $n=5$ with fitness functions fitness $_{2}$ and fitness $_{3}$ for operators flip (black), insert (blue), swap (red) using 10000 samples: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and corresponding basin sizes (right).


Figure .18: Statistical measures for lex initialization on $n=5$ with fitness functions fitness $_{2}$ and fitness $_{3}$ for combination using operators flipinsert (black), swapflipinsert (blue), swapflip (red), and swapinsert (green) using 10000 samples: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and corresponding basin sizes (right).


Figure .19: Statistical measures for lex initialization on $n=6$ with fitness functions fitness $_{2}$ and fitness $_{3}$ for operators flip (black), insert (blue), swap (red) using 10000 samples: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and corresponding basin sizes (right).


Figure .20: Statistical measures for lex initialization on $n=6$ with fitness functions fitness $_{2}$ and fitness $_{3}$ for combination using operators flipinsert (black), swapflipinsert (blue), swapflip (red), and swapinsert (green) using 10000 samples: Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and corresponding basin sizes (right).


[^0]:    Email addresses: domagoj.jakobovic@fer.hr (Domagoj Jakobovic), s.picek@tudelft.nl (Stjepan Picek), marcella@utfpr.edu.br (Marcella S. R. Martins), markus.wagner@adelaide.edu.au (Markus Wagner)

[^1]:    ${ }^{1}$ While it is possible to calculate the fitness values of all $2^{32}$ solutions in case of $n=5$, it is not possible to conduct this many hill-climbs, including all neighborhood calculations, which are needed to create the networks.

[^2]:    ${ }^{2}$ We do not report on the results of the LONs based on random initial solutions (and the subsequent hill-climbs), as these consisted of hundreds or even thousands of disconnected components.

[^3]:    ${ }^{3}$ originally proposed by [34] to describe the degree distributions for NK models

[^4]:    Figure .13: Statistical measures for lex (left) and random (right) initialization on $n=5$ with the three fitness functions for operators flip (black), insert (blue), swap (red) using 1000 samples (within each block of three): Cumulative degree distribution in a log-log scale (left), Correlation between the degree of local optima and their corresponding basin sizes (middle), and Correlation between the fitness of local optima and corresponding basin sizes (right). The forth column is blank, as nodes are of degree $0(z=0)$ (see fifth column).

