

# Self-adaptation via Multi-objectivisation: A Theoretical Study

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## ABSTRACT

The exploration vs exploitation dilemma is to balance exploring new but potentially less fit regions of the fitness landscape while also focusing on regions near the fittest individuals. For the tunable problem class SPARSELOCALOPT, a non-elitist EA with tournament selection can limit the percentage of “sparse” local optimal individuals in the population using a sufficiently high mutation rate (Dang et al., 2021). However, the performance of the EA depends critically on choosing the “right” mutation rate, which is problem instance-specific. A promising approach is self-adaptation, where parameter settings are encoded in chromosomes and evolved.

We propose a new self-adaptive EA for single-objective optimisation, which treats parameter control from the perspective of multi-objective optimisation: The algorithm simultaneously maximises the fitness and the mutation rates. Since individuals in “dense” fitness valleys survive high mutation rates, and individuals on “sparse” local optima only survive with lower mutation rates, they can co-exist on a non-dominated Pareto front.

Runtime analyses show that this new algorithm (MOSA-EA) can efficiently escape a local optimum with unknown sparsity, where some fixed mutation rate EAs become trapped. Complementary experimental results show that the MOSA-EA outperforms a range of EAs on random NK-LANDSCAPE and  $k$ -SAT instances.

## CCS CONCEPTS

• Theory of computation → Optimisation with randomised search heuristics;

## KEYWORDS

Evolutionary algorithms, self-adaptation, multi-modal functions

### ACM Reference Format:

Per Kristian Lehre and Xiaoyu Qin. 2022. Self-adaptation via Multi-objectivisation: A Theoretical Study. In *Genetic and Evolutionary Computation Conference (GECCO '22)*, July 9–13, 2022, Boston, MA, USA. ACM, New York, NY, USA, 15 pages. <https://doi.org/10.1145/3512290.3528836>

## 1 INTRODUCTION

Evolutionary algorithms (EAs) can be good solvers for multi-modal optimisation problems if they balance exploring new but potential

less fit regions of the fitness landscape while also focusing on the regions near the fittest individuals [28]. In the past decade, several studies in the area of runtime analysis investigated how EAs can cope with *local optima*. In addition to mechanisms like crossover [2, 10], stagnation detection [3, 26] and adapting population size [19], a large mutation rate was shown to help some mutation-EA only escaping certain local optima. For example, the  $(1+1)$  EA can be sped up on  $JUMP_k$  by using the larger mutation rate  $k/n$  rather than  $1/n$  [3]. However, a too large mutation rate may lead to failed optimisation. For non-elitist EAs, there are *error thresholds* of mutation rate values [21], where if the mutation rate is above the error threshold, the runtime of the algorithm is exponential.

Non-elitist EAs can “jump” a large Hamming distance. But they can potentially also maintain less fit individuals in the population, allowing the population to cross a fitness valley. They might keep some currently low but potentially high fitness individuals in the population and optimise them “smoothly”. Recently, a tunable problem class SPARSELOCALOPT was proposed to describe a kind of fitness landscapes with *sparse deceptive regions* (local optima) and *dense fitness valleys* [9]. Informally, every search point in a dense set has many neighbours in that set, and every search point in a sparse set has few members in any direction. Dang et al. [9] show that EAs with a non-linear selection and a sufficiently high mutation rate, i.e., close to the error threshold, can cope with sparse local optima. Non-linear selection is a type of non-elitist selection, in which the probability of each individual to be selected is based on its rank in the population, e.g., tournament and linear ranking selections [23]. Typically, the fitter individual has a higher probability to be selected, but the worse individual still has some chance to be chosen. From their analysis, non-linear selections and sufficiently high mutation rates can limit the percentage of “sparse” local optimal individuals in the population by choosing a sufficiently high mutation rate. The reason is that the sparse local optimal individuals can have a higher chance to be selected but can only survive a small percentage of such individuals after mutation, while the dense fitness valley individuals may have less chance of being selected but can have higher chance of surviving mutation. However, the performance of the EA depends critically on choosing the “right” mutation rate, which should be sufficiently high but below the error threshold. Moreover, finding such a mutation rate might be difficult or infeasible for some problem instances with not too sparse local optima.

The self-adaptive parameter control mechanism is a promising method to configure parameters. It encodes the parameters in each individual and evolves the parameters together with its solution through variation operators. There exist a few theoretical studies of self-adaptation in the decade. Dang and Lehre [12] first present that a self-adaptive population using two mutation rates can perform well on the PEAKEDLO function which is a simple artificial two-peak function. As a comparison, they also proved that the algorithm using neither fixed mutation rate nor uniformly selected

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GECCO '22, July 9–13, 2022, Boston, MA, USA

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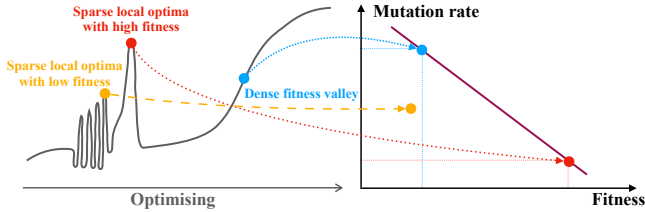
ACM ISBN 978-1-4503-9237-2/22/07...\$15.00

<https://doi.org/10.1145/3512290.3528836>

**Table 1: Theoretical results of EAs on  $\text{PEAKEDLO}_{m,k}$  (for some constant  $c, \delta > 0$ )**

Algorithm	$\text{PEAKEDLO}_{m,k}$	Runtime $T$	Theorem
$(\mu + \lambda)$ EA	Any $k \leq n$ and $k, m \in \Omega(n)$	$\Pr(T \leq e^{cn}) \leq e^{-\Omega(n)}$	Theorem 2
$(\mu, \lambda)$ EA	Any $k \leq n$ and $k, m \in \Omega(n)$	$\Pr(T \leq e^{cn}) \leq e^{-\Omega(n)}$	Theorem 3
2-tour. EA	Any $k < (\ln(3/2) - \delta)n$ and $k, m \in \Omega(n)$	$\Pr(T \leq e^{cn}) \leq e^{-\Omega(\lambda)}$	Theorem 4
$(\mu, \lambda)$ MOSA-EA	Any $n \geq k \in \Omega(n)$ , $\lceil m \rceil < 2A(1 + \ln(p_{\text{inc}})/\ln(\alpha_0) - o(1))k^2$	$E[T] = O(n^2 \log(n))$	Theorem 5

mutation rate will fail on this problem. Doerr et al. [17] rigorously analysed a self-adaptation mechanism on  $(1, \lambda)$  EA, in which the mutation rate  $r/n$  is mutated multiplying a constant or dividing a constant (uniform random selection) before mutating the solution. They prove that the algorithm optimises ONEMAX in expected time  $O(n \log(n))$  runtime, which is the best possible results for evolutionary algorithms. Another recent rigorous analysis from Case and Lehre [5] showed that the self-adaptation of mutation rate over a continuous interval can be effective on the unknown structure version of LEADINGONES function. Their analysis divides the search space of solution and mutation rate into two-dimensional levels. They then use the level-based theorem [7] to obtain the runtime, which is asymptotically optimal among all unary unbiased black-box algorithms.

**Figure 1: Intuition of MOSA-EA**

Case and Lehre [5] also showed that the self-adaptation can find the (nearly) maximal “right” mutation rate for each search point on some benchmark functions. We say the “right” mutation rate for a search point is below a threshold, where the expected number of non-worse offsprings of an individual with a mutation rate below this threshold is greater than 1. For SPARSELOCALOPT, the maximal “right” mutation rate for dense fitness valleys can be higher, while the maximal “right” mutation rate for sparse local optima may be lower. In self-adaptation, individuals can be configured to different mutation rates. If we maximise the mutation rates for both sparse local optima and dense fitness valleys, then the sparse local optimal individual and the dense fitness valley individual could potentially co-exist in a non-dominated Pareto front (Figure 1). Therefore, we can treat parameter control from the perspective of multi-objective optimisation to find the optimal solution and the maximal “right” mutation rates for each search point simultaneously.

In this paper, we propose the *multi-objective self-adaptive EA* (MOSA-EA) for single-objective optimisation, which treats parameter control from the perspective of multi-objective optimisation: The algorithm simultaneously maximises the fitness and the mutation rates. To present advantages of the MOSA-EA, we first propose the  $\text{PEAKEDLO}_{m,k}$  function, which is a version of  $\text{PEAKEDLO}$  [12] with tunable *sparsity*, where the fitness value is  $m$  if a local optimal individual  $x = 0^k *^{n-k}$  and is LEADINGONES value otherwise, where  $*$  represents an arbitrary bit. The sparsity of the local optima can be tuned by the sparse parameter  $k \in [n]$ . With the  $\text{PEAKEDLO}_{m,k}$

function, we simulate a situation in that algorithms have already been trapped into unknown sparse local optima and estimate the expected time to reach the global optimum. The runtime analyses show that the MOSA-EA can cope with local optima for any  $k \in \Omega(n)$ , while the elitist EA, the  $(\mu, \lambda)$  EA, and the tournament EA fails for some  $k \in \Omega(n)$ . Table 1 demonstrates the theoretical results obtained in this study. The used parameters for the algorithms can be found in the corresponding theorems. The experimental results show that the MOSA-EA can outperform the  $(1+1)$  EA, the non-elitist EAs and the UMDA on two challenging combinatorial optimisation problems, random NK-LANDSCAPE and random  $k$ -SAT instances.

## 2 PRELIMINARIES

We first define some notations which are used later. For any  $n, m \in \mathbb{N}$  satisfying  $n \geq m > 0$ , we define  $[n] := \{1, \dots, n\}$ ,  $[0..n] := \{0\} \cup [n]$ ,  $[-1..n] := \{-1\} \cup [0..n]$  and  $[m..n] := [0..n] \setminus [0..m-1]$ . We use  $H(\cdot, \cdot)$  to denote the Hamming distance. The natural logarithm and the logarithm to the base 2 are denoted by  $\ln(\cdot)$  and  $\log(\cdot)$ , respectively. Let  $f : \mathcal{X} \rightarrow \mathbb{R}$  be any pseudo-Boolean function, where  $\mathcal{X} = \{0, 1\}^n$  is the set of bitstrings of length  $n$ . Define  $\text{LEADINGONES}(x) := \text{LO}(x) := \sum_{i=1}^n \prod_{j=1}^i x_j$ . For self-adapting mutation rate, we are interested in an extended search space of  $\mathcal{Y} := \mathcal{X} \times [\varepsilon, 1/2]$  which includes  $\mathcal{X}$  and the space of mutation rates. Appendices mentioned can be found in the supplementary material.

### 2.1 $\text{PEAKEDLO}_{m,k}$ problems

Dang and Lehre [12] proposed a two-modal function  $\text{PEAKEDLO}_m$  where the fitness value is  $m$  if a peak individual  $x = 0^n$  and  $\text{LO}(x)$  otherwise. The “density” of the fitness valley can be tuned by  $m$ . In this section, we introduce a more general version of  $\text{PEAKEDLO}$ , where the “sparsity” of the peak individual can be tuned by a parameter  $k$ . Let  $*$  represent an arbitrary bit. Then the problem class is defined as  $\text{PEAKEDLO}_{m,k}(x) := \begin{cases} m & \text{if } x = 0^k *^{n-k}, \\ \text{LO}(x) & \text{otherwise,} \end{cases}$  for any  $k \in [n]$  and any  $1 < m \in \mathbb{R}$ . The  $\text{PEAKEDLO}_m$  function [12] is a special case of  $\text{PEAKEDLO}_{m,k}$  where  $k = n$ . Similarly to [12], we assume that the algorithm is initiated from the search points  $0^k *^{n-k}$ . It is unlikely that the algorithm will end up on this particular local optima if the population is initialised uniformly at random. However, here, we are interested in the capability of an algorithm to escape a local optimum, wherever it is encountered. Our assumption is therefore reasonable for the purposes of analysis.

### 2.2 Non-elitist EAs

Non-elitism means that the fitness individual in a generation is not always copied to the next generation. There exist many studies on non-elitist selection [8, 9, 11, 15, 22]. In this paper, we show that fixed mutation rate non-elitist EAs are inefficient when optimising  $\text{PEAKEDLO}_{m,k}$  when initialised from  $0^k *^{n-k}$ . We take the  $(\mu, \lambda)$  EA

<sup>2</sup>For some constants  $p_{\text{inc}} < 2/5$ ,  $\alpha \geq 4$ ,  $A > 1$  based on restrictions in Theorem 5.

and the 2-tournament EA as examples to show this, which can be described as Algorithm 6 (shown in Appendix C) with “plugging” Algorithms 8 and 9 (shown in Appendix C) into Line 4, respectively. The non-elitist selection mechanisms can also be applied to the self-adaptive EAs which is introduced in the next section.

### 2.3 Level-based theorem

The *level-based theorem* [7, 16] is a runtime analysis tool used to obtain upper bounds on the runtime of population-based EAs on many problems [9, 13, 22]. The theorem applies to algorithms that follow the scheme of Algorithm 7 (shown in Appendix C). Let  $D$  be some mapping from the set of all possible populations  $\mathcal{Z}^\lambda$  into the space of probability distributions over  $\mathcal{Z}$ , where  $\mathcal{Z}$  is a finite state space. Thus, we can consider that each individual in  $P_{t+1}$  is sampled from a distribution  $D(P_t)$  which responds to Lines 4-5 of Algorithm 6.

**THEOREM 1 ([7]).** *Given a partition  $(A_1, A_2, \dots, A_m)$  of a finite state space  $\mathcal{Z}$ , let  $T := \min\{t \mid |P_t \cap A_m| > 0\}$  be the first point in time that the elements of  $A_m$  appear in  $P_t$  of Algorithm 7. If there exist  $z_1, \dots, z_{m-1}, \delta \in (0, 1]$ , and  $\gamma_0 \in (0, 1)$  such that for any population  $P \in \mathcal{Z}^\lambda$ ,*

(G1) *for each level  $j \in [m-1]$ , if  $|P \cap A_{\geq j}| \geq \gamma_0 \lambda$  then*

$$\Pr_{y \sim D(P)}(y \in A_{\geq j+1}) \geq z_j,$$

(G2) *for each level  $j \in [m-2]$ , and all  $\gamma \in (0, \gamma_0]$ , if  $|P \cap A_{\geq j}| \geq \gamma_0 \lambda$  and  $|P \cap A_{\geq j+1}| \geq \gamma \lambda$  then  $\Pr_{y \sim D(P)}(y \in A_{\geq j+1}) \geq (1 + \delta)\gamma$ ,*

(G3) *and the population size  $\lambda \in \mathbb{N}$  satisfies  $\lambda \geq \left(\frac{4}{\gamma_0 \delta^2}\right) \ln \left(\frac{128m}{z_* \delta^2}\right)$ ,*

$$\text{where } z_* := \min_{j \in [m-1]} \{z_j\},$$

*then  $E[T] \leq \left(\frac{8}{\delta^2}\right) \sum_{j=1}^{m-1} \left(\lambda \ln \left(\frac{6\delta\lambda}{4+z_j\delta\lambda}\right) + \frac{1}{z_j}\right)$ .*

## 3 MULTI-OBJECTIVE SELF-ADAPTIVE EA

This section will introduce the multi-objective self-adaptive evolutionary algorithm (MOSA-EA). The basic idea of the MOSA-EA is to treat the parameter optimisation task as another objective, i.e., maximising fitness mutation rate simultaneously. Compared to existing self-adaptive EAs, the MOSA-EA is characterised by the population sorting method. Previous self-adaptive EAs [5, 12, 17] sort the population by considering the fitness of individuals first, then the mutation rate. In contrast, the MOSA-EA sorts the population by a non-dominated sorting (Algorithm 2) where we have adapted from two famous multi-objective EAs [14, 27].

### 3.1 Framework of self-adaptive EAs

There exist three self-adapting mutation rate non-elitist EAs in the theory community. They are the 2-tournament self-adaptive EA using two mutation rates [12], the  $(\mu, \lambda)$  self-adaptive EA [5] and the  $(1, \lambda)$  self-adaptive EA [17]. In each generation  $t$ , they all essentially first sort the population  $P_t$  by some sorting mechanism based on fitness function  $f$  and mutation rate  $\frac{\chi}{n}$ . Then, each individual in the next population  $P_{t+1}$  is produced via selection and mutation. The selection mechanism is based on the order of the sorted population. Then, the selected individual changes its mutation rate based on the same self-adapting mutation rate strategy and is bit-wisely flipped with the probability of a new mutation rate. To describe

the above processes, we summarise a framework of self-adaptive EAs (Algorithm 1). In this framework, we can customise the sorting mechanism *Sort*, the selection mechanism  $P_{\text{sel}}$  and the self-adapting mutation rate strategy  $D_{\text{mut}}$ . The MOSA-EA can also be based on this framework. Similarly to non-elitist EAs, we can also consider that each individual in  $P_{t+1}$  is sampled from a distribution  $D(P_t)$  in Theorem 1 which corresponds to Lines 4-6 of Algorithm 1.

#### Algorithm 1 Framework of self-adaptive EAs

**Require:** Fitness function  $f$ . Population sizes  $\lambda \in \mathbb{N}$ . Sorting mechanism *Sort*. Selection mechanism  $P_{\text{sel}}$ . Self-adapting mutation rate strategy  $D_{\text{mut}}$ . Initial population  $P_0 \in \mathcal{Y}^\lambda$ .

```

1: for  $t$  in  $0, 1, 2, \dots$  until termination condition met do
2:   Sort( $P_t, f$ )
3:   for  $i = 1, \dots, \lambda$  do
4:     Sample  $I_t(i) \sim P_{\text{sel}}([ \lambda ])$ ; set  $(x, \chi/n) := P_t(I_t(i))$ .
5:     Sample  $\chi' \sim D_{\text{mut}}(\chi)$ .
6:     Create  $x'$  by independently flipping each bit of  $x$  with
       probability  $\chi'/n$ .
7:     Set  $P_{t+1}(i) := (x', \chi'/n)$ .
```

### 3.2 Sorting mechanism

The MOSA-EA aims to maximise fitness and mutation rates simultaneously. To achieve this goal, we apply a multi-objective sorting mechanism to sort the population before producing the next population, as shown in Algorithm 2. Specifically, the multi-objective sorting mechanism uses the strict non-dominated sorting (Algorithm 3) based on maximising two objective functions, i.e., the fitness value of the solution  $f_1(x, \chi) := f(x)$  and the mutation rate of the individual  $f_2(x, \chi) := \chi$ .

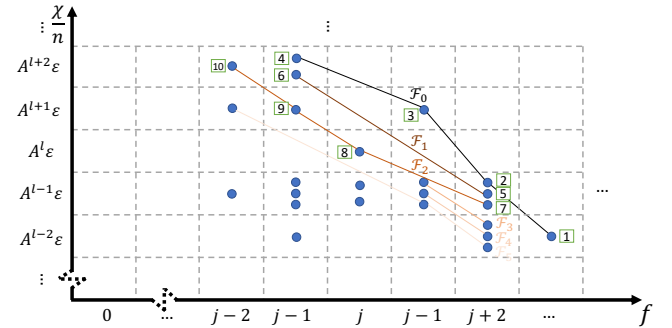


Figure 2: Illustration of multi-objective sorting

After multi-objective sorting described in Algorithm 2, we can get a series of strict non-dominated fronts  $\mathcal{F}_0^t, \mathcal{F}_1^t, \dots$  of  $P_t$ . In each strict non-dominated Pareto front, Algorithm 3 guarantees that there do not exist two individuals with the same fitness value and mutation rate, and individuals are put in a fitness increasing sequence. Note that we assume that the aim is to maximise all objectives in Algorithm 3, and we say an individual  $a$  dominates another individual  $b$ , written as  $a < b$  if (1) the objective values of  $a$  are no lower than  $b$  for all functions, and (2) at least one objective value of  $a$  is strictly higher than that objective value in  $b$ . Figure 2 illustrates an example of the order of a population after multi-objective sorting. Note that the points in the same cell have the same fitness value and the same mutation rate.

The main difference between the fast non-dominated sorting algorithm used in NSGA-II [14] and the strict non-dominated sorting algorithm shown in Algorithm 3 is that the latter can avoid too many similar or copies of the same individual, i.e., same objective values in all functions, in one front, by Lines 9-11. This characteristic can avoid the situation that some individuals dominate the population, i.e., occupying the top positions of the sorted population. In other words, the strict non-dominated sorting algorithm can increase the diversity of the population.

After calculating the strict non-dominated fronts, we sort the individuals in each front based on the fitness function  $f$  (Line 3 in Algorithm 2), since the priority of optimisation is to find better solutions. Then we get a sorted population, in which any individual  $a$  is ranked before an individual  $b$  if  $a$  has a higher fitness value or a higher mutation rate than  $b$ .

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**Algorithm 2** Multi-objective sorting mechanism

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**Require:** Population sizes  $\lambda \in \mathbb{N}$ . Population  $P_t \in \mathcal{Y}^\lambda$ . Fitness function  $f$ .

- 1: Sort  $P_t$  into strict non-dominated fronts  $\mathcal{F}_0^t, \mathcal{F}_1^t, \dots$  based on  $f_1(x, \chi) := f(x)$  and  $f_2(x, \chi) := \chi$
- 2: **for**  $\mathcal{F} = \mathcal{F}_0^t, \mathcal{F}_1^t, \dots$  **do**
- 3:     Sort  $\mathcal{F}$  such that  $f_1(\mathcal{F}(1)) > f_1(\mathcal{F}(2)) > \dots$
- 4:  $P_t := (\mathcal{F}_0^t, \mathcal{F}_1^t, \dots)$ .
- 5: **return**  $P_t$ .

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**Algorithm 3** Strict non-dominated sorting

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**Require:** Population sizes  $\lambda \in \mathbb{N}$ . Population  $P \in \mathcal{Z}^\lambda$ , where  $\mathcal{Z}$  is a finite state space. Objective functions  $f_1, f_2, \dots : \mathcal{Z} \rightarrow \mathbb{R}$  (assume to maximise all objective functions).

- 1: **for** each individual  $P(i)$  **do**
- 2:     Set  $S_i := \emptyset$  and  $n_i := 0$
- 3: **for**  $i = 1, \dots, \lambda$  **do**
- 4:     **for**  $j = 1, \dots, \lambda$  **do**
- 5:         **if**  $P(i) < P(j)$  based on  $f_1, f_2, \dots$  **then**
- 6:              $S_i := S_i \cup \{P(i)\}$ ,
- 7:         **else if**  $P(j) < P(i)$  based on  $f_1, f_2, \dots$  **then**
- 8:              $n_i := n_i + 1$ ,
- 9:         **else if**  $f_\ell(P(i)) = f_\ell(P(j))$  where  $\ell = 1, 2, \dots$  **then**
- 10:             **if**  $P(i) \notin S_j$  **then**  $S_i := S_i \cup \{P(i)\}$  **else**  $n_i := n_i + 1$ .
- 11:     **if**  $n_i = 0$  **then**  $\mathcal{F}_0 = \mathcal{F}_0 \cup \{P(i)\}$ .
- 12: Set  $k := 0$ .
- 13: **while**  $\mathcal{F}_k \neq \emptyset$  **do**
- 14:      $Q := \emptyset$ .
- 15:     **for** each individual  $P(i) \in \mathcal{F}_k$  and  $P(j) \in S_i$  **do**
- 16:         Set  $n_j := n_j - 1$ .
- 17:         **if**  $n_j = 0$  **then**  $Q := Q \cup \{P(j)\}$ .
- 18:     Set  $k := k + 1$ ,  $\mathcal{F}_k := Q$ .
- 19: **return**  $\mathcal{F}_0, \mathcal{F}_1, \dots$

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**Algorithm 4** Self-adapting mutation rate strategy

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**Require:** Parameters  $A > 1$ ,  $\varepsilon > 0$  and  $p_{\text{inc}} \in (0, 1)$ . Mutation parameter  $\chi$ .

- 1:  $\chi' = \begin{cases} \min(A\chi, \varepsilon n A^{\lfloor \log_A(\frac{1}{2\varepsilon}) \rfloor}) & \text{with probability } p_{\text{inc}}, \\ \max(\chi/A, \varepsilon n) & \text{otherwise.} \end{cases}$
- 2: **return**  $\chi'$ .

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**Algorithm 5** Self-adapting mutation rate strategy (theoretical)

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**Require:** Parameters  $A > 1$ ,  $\varepsilon > 0$ ,  $p_{\text{inc2}} > 0$ ,  $p_{\text{inc}} > 0$  and  $p_{\text{inc}} + p_{\text{inc2}} < 1$ . Mutation parameter  $\chi$ .

- 1:  $\chi' = \begin{cases} \min(A\chi, \varepsilon n A^{\lfloor \log_A(\frac{1}{2\varepsilon}) \rfloor}) & \text{with probability } p_{\text{inc}}, \\ \varepsilon n A^{\lfloor \log_A(\frac{1}{2\varepsilon}) \rfloor} & \text{with probability } p_{\text{inc2}}, \\ \max(\chi/A, \varepsilon n) & \text{otherwise.} \end{cases}$
- 2: **return**  $\chi'$ .

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### 3.3 Self-adapting mutation rate

Self-adapting mutation rate is the key step of self-adaptive EAs. Case and Lehre [5] and Doerr et al. [17] use a strategy to increase the mutation rate by a multiplicative factor  $A > 1$  with some probability  $p_{\text{inc}}$ , decrease otherwise. We apply a similar strategy in Algorithm 4 on the MOSA-EA in experiments (Section 6), where adapting mutation rate from  $\varepsilon$  to nearly  $1/2$ . To make theoretical analysis easier, we adopt Algorithm 5 on the MOSA-EA in Theorem 5. The difference is that Algorithm 5 has an additional tiny probability  $p_{\text{inc2}}$  to increase the mutation rate to the highest of possible mutation rates.

Finally, we say the MOSA-EA is Algorithm 1 using the multi-objective sorting mechanism (Algorithm 2). In this paper, we only consider the  $(\mu, \lambda)$  MOSA-EA with using comma selection (Algorithm 8). For self-adapting mutation rate strategy, we apply Algorithms 4 and 5 in Sections 6 and 5, respectively.

## 4 INEFFICIENCY OF FIXED MUTATION RATE

The  $(\mu + \lambda)$  EA and the  $(\mu, \lambda)$  EA are proved inefficient when optimising the BBFNNEL function which belongs to the SPARSE-LOCALOPT problem class [8, 9]. We use similar proof ideas to prove the inefficiency on PEAKEDLO $_{m,k}$  for  $(\mu + \lambda)$  EA and  $(\mu, \lambda)$  EA, which is shown in Theorems 2 and 3, respectively. Furthermore, the tournament EA can solve SPARSELOCALOPT problems with very “sparse” local optima [8, 9]. In Theorem 4, we show the 2-tournament EA with any fixed mutation rate cannot handle a too sparse local optimum on PEAKEDLO $_{m,k}$ . Due to the page limit, the proofs in this section are omitted and can be found in Appendix D.

**THEOREM 2.** *The expected runtime of the  $(\mu + \lambda)$  EA with  $\lambda, \mu \in \text{poly}(n)$ ,  $\lambda/\mu \geq 1$ , initial population  $P_0 = \{0^k *^{n-k}\}^\mu$ , and mutation parameter  $\chi \in O(1)$  on PEAKEDLO $_{m,k}$  with any  $k \leq n$  and  $k, m \in \Omega(n)$  satisfies  $\Pr(T \leq e^{cn^d}) \leq e^{-\Omega(n)}$  for some constants  $c, d > 0$ .*

**THEOREM 3.** *For any constant  $\delta > 0$ , the  $(\mu, \lambda)$  EA with  $\lambda, \mu \in \text{poly}(n)$ ,  $\lambda/\mu = \alpha_0$  where  $\alpha_0 > 1$  is a constant, mutation parameter  $0 < \chi \notin [\ln(\lambda/\mu) - \delta, \ln(\lambda/\mu) + \delta]$ , and initial population  $P_0 = \{0^k *^{n-k}\}^\lambda$  has runtime  $\Pr(T \leq e^{cn}) \leq e^{-\Omega(n)}$  on PEAKEDLO $_{m,k}$  with any  $k \leq n$  and  $k, m \in \Omega(n)$  for some constant  $c > 0$ .*

**THEOREM 4.** For some constant  $\xi \in (0, 2/3)$ , any  $k \leq an$  where  $a = \ln(3(1 - \xi)/2)$  is a constant and  $m \in \Omega(n)$ , the runtime of the 2-tournament EA with population size  $\lambda \in \text{poly}(n)$  on  $\text{PEAKEDLO}_{m,k}$  with the initial population  $P_0 = \{0^k *^{n-k}\}^\lambda$  and any fixed mutation rate satisfies  $\Pr(T \leq e^{cn}) = e^{-\Omega(\lambda)}$  for a constant  $c > 0$ .

## 5 EFFICIENCY OF MOSA-EA

We now analyse the runtime of the MOSA-EA on  $\text{PEAKEDLO}_{m,k}$  (Theorem 5). In a previous study, Case and Lehre [5] derived an upper bound on the runtime of the  $(\mu, \lambda)$  self-adaptive EA on an unknown structure version of  $\text{LEADINGONES}$  function via the level-based theorem [7]. They first divide the search space  $\mathcal{Y}$  into a two-dimensional level partition including fitness levels and mutation rate sub-levels. Then they define two threshold values  $\theta_1(j)$  and  $\theta_2(j)$  which is an ideal range of mutation rate to improve the solution for each fitness level. Informally, they count the number of generations to increase the mutation rate to enter this ideal mutation rate range, and the number of generations to improve the solution to the next fitness level if with an ideal mutation rate.

**THEOREM 5.** For some constant  $\delta \in (0, 1)$ , Algorithm 1 using the multi-objective sorting mechanism (Algorithm 2), self-adapting mutation rate strategy described in Algorithm 5 and the  $(\mu, \lambda)$  selection (Algorithm 8) with  $\frac{\lambda}{\mu} = \alpha_0 \geq 4$  and  $c \log^2(n) \leq \lambda \in \text{poly}(n)$  where  $\alpha_0$  is a constant and  $c$  is a large enough constant, has expected runtime  $O(n \lambda \log(n) \log(\log(n)) + n^2 \log(n))$  on  $\text{PEAKEDLO}_{m,k}$  started with any initial population, if satisfying

- $p_{\text{inc}} \in \left(\frac{1+\delta}{\alpha_0}, \frac{2}{5}\right)$ ,  $A > (1 + \sqrt{1/(\alpha_0(1 - p_{\text{inc}}))})$  are constants,
- $\varepsilon = \frac{b}{n}$ ,  $p_{\text{inc}2} = \frac{d}{n}$  for any small constants  $b, d > 0$ ,
- $\lceil m \rceil < \left(\ln\left(\frac{\alpha_0 p_{\text{inc}}}{1+\delta}\right)\right) / \left(2A \ln\left(\frac{\alpha_0}{1-\delta}\right)\right) k - \ln\left(\frac{\alpha_0 p_{\text{inc}}}{1+\delta}\right) + 1$ , where  $k = an$  for any constant  $a \in (0, 1]$ .

Although the MOSA-EA analysed in Theorem 5 is significantly different from the  $(\mu, \lambda)$  self-adaptive EA, e.g., different sorting mechanisms and different self-adapting mutation rate strategies, we can use a similar proof idea for these two varieties of  $\text{LEADINGONES}$ . We first divide the search space  $\mathcal{Y}$  into regions based on  $k$  and  $m$  of  $\text{PEAKEDLO}_{m,k}$ . Then we partition each region into fitness levels and mutation rate sub-levels. We formally define these in Section 5.1. Section 5.2 defines some threshold values and functions, similarly to [5], and we also introduce some useful lemmas. Finally, in Section 5.3, we apply the level-based theorem (Theorem 1) to the level partition to get an upper bound of runtime on  $\text{PEAKEDLO}_{m,k}$ .

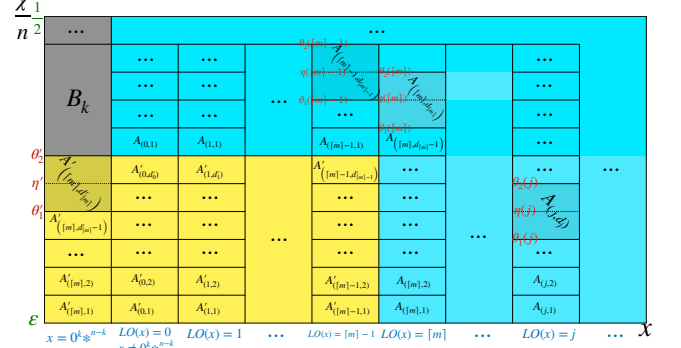
### 5.1 Partitioning the search space into levels

We partition the two-dimensional search space  $\mathcal{Y} = X \times [\varepsilon, 1/2]$  into “levels”. We first divide the search space  $\mathcal{Y}$  into three parts  $A'$ ,  $A$  and  $B_k$  based on fitness value and mutation rate, which are coloured by yellow, blue and grey in Figure 3, respectively. Note that Figure 3 is an informal illustration since the formal definitions are complicated. Formally, we define the regions with the  $\text{PEAKEDLO}_{m,k}$  parameters  $k, m$  and a threshold value  $\theta'_2$  as

- $A'_j := \{(x, \chi) \mid \text{LO}(x) = j \text{ and } x \neq 0^k *^{n-k} \text{ and } \chi < \theta'_2\}$  for  $j \in [0.. \lceil m \rceil - 1]$ ;
- $A'_{\lceil m \rceil} := \{(x, \chi) \mid x = 0^k *^{n-k} \text{ and } \chi < \theta'_2\}$ ;

- $A_j := \{(x, \chi) \in X \mid \text{LO}(x) = j \text{ and } x \neq 0^k *^{n-k} \text{ and } \chi \geq \theta'_2\}$  for  $j \in [0.. \lceil m \rceil - 1]$ ;
- $A_j := \{(x, \chi) \mid \text{LO}(x) = j\}$ , for  $j \in [\lceil m \rceil..n]$ ;
- $B_k := \{(x, \chi) \mid x = 0^k *^{n-k} \text{ and } \chi \geq \theta'_2\}$ .

We will define  $\theta'_2$  in the next subsection. Note that  $B_k$  contains no level which is applied in the level-based theorem, and we will prove



**Figure 3: Informal illustration of the level partition on  $\text{PEAKEDLO}_{m,k}$  function (Regions  $A'$ ,  $A$ ,  $B_k$  are coloured by yellow, blue, grey, respectively)**

To describe the ranking of sub-levels, we define that any level in  $A$  is higher than all levels in  $A'$ , any sub-level in  $A_j$  is higher than all sub-levels in  $A_{j-1}$ , and any sub-level in  $A'_j$  is higher than all sub-levels in  $A'_{j-1}$  for  $j \geq 1$ .

Now, we define sub-levels in regions  $A'$  and  $A$ . For region  $A'$ , we first define the *depth*  $d'_j$  of levels  $A'_j$ :

- For  $j \in [0.. \lceil m \rceil - 1]$ ,  $d'_j := \min\{\ell \in \mathbb{N} \mid \varepsilon A^\ell \geq \theta'_2\}$ ;
- For  $j = \lceil m \rceil$ ,  $d'_{\lceil m \rceil} := \min\{\ell \in \mathbb{N} \mid \varepsilon A^\ell \geq \theta'_1\}$ .

The depth of level in  $A'$  implies the number of sub-levels to enter higher region, i.e.,  $A$ . Then,

- For  $j \in [0.. \lceil m \rceil - 1]$ , we define the sub-levels for  $\ell \in [d'_j]$  as  $A'_{(j,\ell)} := A'_j \times [\varepsilon A^{\ell-1}, \min(\varepsilon A^\ell, \theta'_2))$ ,
- For  $j = \lceil m \rceil$ , we define the *low levels* for  $\ell \in [d'_{\lceil m \rceil} - 1]$  as  $A'_{(\lceil m \rceil,\ell)} := A'_{\lceil m \rceil} \times [\varepsilon A^{\ell-1}, \min(\varepsilon A^\ell, \theta'_1))$ , and we define the *edge level* as  $A'_{(\lceil m \rceil,d'_{\lceil m \rceil})} := A'_{\lceil m \rceil} \times [\theta'_1, \min(\frac{1}{2}, \theta'_2)]$ .

To define sub-levels in region  $A_j$ , we use two threshold values  $\theta_1(j)$  and  $\theta_2(j)$  which will be defined in the following subsection. Similarly to [5],  $\theta_1(j)$  and  $\theta_2(j)$  imply the ideal range of mutation rate to mutate the solution to level  $A_j$ . We also begin at defining the *depth*  $d_j$  of levels  $A_j$ .

- For  $j \in [0.. \lceil m \rceil - 1]$ ,  $d_j := \min\{\ell \in \mathbb{N} \mid \theta'_2 A^\ell \geq \theta_1(j)\}$ ;
- For  $j \in [\lceil m \rceil..n - 1]$ ,  $d_j := \min\{\ell \in \mathbb{N} \mid \varepsilon A^\ell \geq \theta_1(j)\}$ .

The depth of level implies the number of sub-levels to tune the mutation rate from the lowest to an ideal mutation rate.

- For  $j \in [0.. \lceil m \rceil - 1]$ , we define the *low levels* as  $A_{(j,\ell)} := A_j \times [\theta'_2 A^{\ell-1}, \min(\theta'_2 A^\ell, \theta_1(j))]$ , for  $\ell \in [d_j - 1]$ , and define the *edge levels* as  $A_{(j,d_j)} := A_j \times [\theta_1(j), \min(\frac{1}{2}, \theta_2(j))] \cup A_{>j} \times (\min(\frac{1}{2}, \theta_2(j+1)), \min(\frac{1}{2}, \theta_2(j)))$ .
- For  $j \in [\lceil m \rceil..n - 1]$ , we define the *low levels* as  $A_{(j,\ell)} := A_j \times [\varepsilon A^{\ell-1}, \min(\varepsilon A^\ell, \theta_1(j))]$ , and we define the *edge levels* as  $A_{(j,d_j)} := A_j \times [\theta_1(j), \min(\frac{1}{2}, \theta_2(j))] \cup A_{>j} \times (\min(\frac{1}{2}, \theta_2(j+1)), \min(\frac{1}{2}, \theta_2(j)))$ .



- We let  $A_n$  contain only one sub-level  $A_{(n,1)} := A_j \times [\varepsilon, 1/2]$ .

## 5.2 Definitions and useful lemmas

We now define the functions  $\theta_1$ ,  $\eta$  and  $\theta_2$  for levels  $A_j$  where  $j \in [0..n-1]$ , and the values  $\theta'_1$ ,  $\eta'$  and  $\theta'_2$  for levels  $A'_{[m]}$ , which use in the levels definitions above.

- For  $A_j$  where  $j \in [n-1]$ , let

$$\eta(j) := \frac{1}{2A} \left( 1 - \left( \frac{1+\delta}{\alpha_0 p_{\text{inc}}} \right)^{\frac{1}{j}} \right), \theta_1(j) := \frac{\eta(j)}{A}, \theta_2(j) := 1 - q^{\frac{1}{j}}, \text{ where}$$

$$q := \frac{1-\zeta}{\alpha_0}, r_0 := \frac{1+\delta}{\alpha_0(1-p_{\text{inc}}-p_{\text{inc}2})}, \zeta := 1 - \alpha_0(r_0)^{1+\sqrt{r_0}}$$

- For  $A_0$ , let  $\eta(0)$  be any function such that  $\eta(0) = \frac{\eta(1)}{A} - o(1)$ , and we define  $\theta_1(0) := \frac{\eta(0)}{A}$ , and  $\theta_2 := \frac{\theta_2(1)}{A}$ .
- For  $A'_{[m]}$ , we define  $\eta' := \eta(k)$ ,  $\theta'_1 := \theta_1(k)$  and  $\theta'_2 := \theta_2(k)$ .

For convenience, let  $x' \sim p_{\text{mut}}(x, \chi)$  denote that individual  $x'$  is sampled by independently flipping each bit of  $x$  with probability  $\chi/n$ , which is another expression of Line 6 in Algorithm 1. Then, for all individuals  $(x, \chi)$  in  $A_j$  where  $j \in [0..n-1]$  and  $\chi \in [\varepsilon n, n/2]$ , we define the *survival probability* as  $r(j, \chi) := \min_{x \in A_j} \Pr_{x' \sim p_{\text{mut}}(x, \chi)}(x' \in A_{\geq j})$ , and for all individuals  $(x, \chi)$  in  $A'_j$ , where  $j \in [0..[m]]$  and  $\chi \in [\varepsilon n, n/2]$ , we define the *survival probability* as  $r'(j, \chi) := \min_{x \in A'_j} \Pr_{x' \sim p_{\text{mut}}(x, \chi)}(x' \in A'_{\geq j})$ .

We then explain that condition  $[m] < \left( \ln \left( \frac{\alpha_0 p_{\text{inc}}}{1+\delta} \right) \right) / \left( 2A \ln \left( \frac{\alpha_0}{1-\delta} \right) \right) k - \ln \left( \frac{\alpha_0 p_{\text{inc}}}{1+\delta} \right) + 1$  in Theorem 5 essentially implies  $\theta'_2 < \theta_1(j)$  for all  $j \in [0..[m]-1]$  by Lemma 1 (the proof can be found in Appendix D.4). Informally, it means that the local optima is “sparse” and the fitness valley is “dense”.

**LEMMA 1.** *Assume that the parameters  $A$ ,  $\alpha_0$  and  $p_{\text{inc}}$  satisfy the constraints in Theorem 5. For any constant  $\delta \in (0, 1)$ , if  $[m] < \left( \ln \left( \frac{\alpha_0 p_{\text{inc}}}{1+\delta} \right) \right) / \left( 2A \ln \left( \frac{\alpha_0}{1-\delta} \right) \right) k - \ln \left( \frac{\alpha_0 p_{\text{inc}}}{1+\delta} \right) + 1$ , where  $k = an$  for any constant  $a \in (0, 1)$ , then  $\theta'_2 < \theta_1(j)$  for all  $j \in [0..[m]-1]$ .*

Then we introduce three lemmas to support the proofs for conditions (G2) and (G1) of Theorem 1. Due to the page limit, the lemmas and their proofs can be found in Appendices D.5, D.6 and D.7. Lemma 6 presents some useful inequalities, and Lemmas 7 and 8 can be used to prove conditions (G2) and (G1), respectively. The lemmas and the proofs may look similar to [5], but they are separate statements since different algorithms and level partitions are considered in Theorem 5 and [5].

Too many individuals with high fitness but incorrect mutation rate would ruin the progress of the population. We therefore need to prove that there are not too many such “bad” individuals in the population. We first define a “bad” region  $B \subset \mathcal{Y}$  containing search points with a mutation rate that is too high, and we say an individual  $(x, \chi/n) \in B$  has too high mutation rate. For the constant  $\zeta \in (0, 1)$ , let

$$B := \{(x, \chi/n) \in A_j \times [\varepsilon, 1/2] \mid$$

$$(j \in [0..n-1] \wedge \forall y \in X \setminus \{0^k * n^{-k}\} \Pr_{x' \sim p_{\text{mut}}(y, \chi)}(x' \in A_{\geq j}) < \frac{1-\zeta}{\alpha_0})$$

$$\vee (\forall y = 0^k * n^{-k} \Pr_{x' \sim p_{\text{mut}}(y, \chi)}(x' = 0^k * n^{-k}) < \frac{1-\zeta}{\alpha_0})\}. \quad (1)$$

By  $\theta_2(j)$ ,  $\theta'_2$  and  $B_k$ , the region  $B$  can also be expressed as

$$B = \bigcup_{j=0}^{n-1} A_{>j} \times (\min(1/2, \theta_2(j+1)), \min(1/2, \theta_2(j))) \cup B_k. \quad (2)$$

We show that too many such individuals in the population is rare by Lemma 9 (shown in Appendix D.8).

## 5.3 Applying the level-based theorem

Now, we use Lemmas 6, 7, 8 and 9 to prove Theorem 5 via Theorem 1.

**PROOF (THEOREM 5).** We say that a generation  $t$  is “failed” if the population  $P_t$  contains more than  $(1 - \zeta/2)\mu$  individuals in region  $B$ . We will optimistically assume that no generation fails. Under this assumption, we will prove that the conditions of Theorem 1 hold, leading to an upper bound on the expected number of function evaluations  $t_0(n)$  until a search point in  $A_{(n,1)}$  is created. In the end we will use a restart argument to account for failed generations.

Each strict non-dominated front has at most  $\lceil \log_A(1/2\varepsilon) \rceil = c' \log(n)$  individuals where  $c' > 0$  is some constant, so there are at least  $\lambda/(c' \log(n)) \in \Omega(\log(n))$  fronts. Let  $c' := \lceil \log_A(\frac{n}{2\varepsilon}) \rceil / \log(n)$ , where  $c' \log(n)$  is the maximal number of individuals in a front. Let  $\gamma_0 := b'/\log(n)$  for some constant  $0 < b' < \zeta/(2\alpha_0 c')$ . By the assumption, the number of individuals are not in region  $B$  and have chance to be selected is at least  $\zeta\mu/2$ . Since  $\gamma_0\lambda = b'\lambda/\log(n) < \zeta\lambda/(2\alpha_0 c' \log(n)) = \zeta\mu/(2 \log(n)) < \zeta\mu/2$ , therefore any individual ranked in the first  $\gamma_0\lambda$  positions will be selected with probability  $\frac{1}{\mu}$  by the  $(\mu, \lambda)$  selection.

By the ranking mechanism, if an individual  $(x, \chi)$  ranked in the first  $\gamma\lambda$  positions where  $\gamma \in (0, \gamma_0]$ , then any individual  $(x', \chi')$  where either  $f(x') > f(x)$  or  $\chi' > \chi$  will be ranked in the first  $\gamma\lambda$  positions, which guarantees individuals in  $A'_{>(j,\ell)}$  are ranked in the first  $\gamma\lambda$  positions if there are at least  $\gamma\lambda$  individuals in  $A'_{\geq(j,\ell)}$ , and guarantees individuals in  $A_{>(j,\ell)}$  are ranked in the first  $\gamma\lambda$  positions if there are at least  $\gamma\lambda$  individuals in  $A_{\geq(j,\ell)}$ .

Now we consider (G1)-(G2) of Theorem 1 in regions  $A'$  and  $A$ .

**Region  $A'$ :** For  $\gamma \in (0, \gamma_0]$ , if there are  $\gamma\lambda$  individuals in level  $A'_{>(j,\ell)}$  for some  $j \in [0..[m]]$  and  $\ell \in [d'_j]$ , then the probability of selecting an individual from  $A'_{>(j,\ell)}$  is  $\gamma\alpha_0$ . Since  $|P_t \cap B| \leq (1 - \zeta/2)\mu$ , it follows that all  $\gamma\lambda < (\zeta/2)\mu$  individuals of  $A'_{\geq(j,\ell)}$  are among the  $\mu$  fittest in the population. Therefore, the probability of selecting an individual from  $A'_{>(j,\ell)}$  indeed is  $\gamma\lambda/\mu = \gamma\alpha_0$ . We assume that the current population has at least  $\gamma_0\lambda$  individuals in levels  $A'_{\geq(j,\ell)}$ . To verify condition (G2), we must estimate the probability of producing an offspring in levels  $A'_{>(j,\ell)}$ , assuming that there are at least  $\gamma\lambda$  individuals in levels  $A'_{>(j,\ell)}$ , for any  $\gamma \in (0, \gamma_0]$ . We distinguish five cases:

- Case 1:  $j \in [0..[m]-1]$  and  $\ell \in [d'_j-1]$ . Assuming that the parent  $(x, \chi/n)$  is in  $A'_{(u,v)} \subseteq A'_{\geq(j,\ell+1)}$ . Since  $\chi/n < \theta'_2 < \theta_1(j) < \eta(j)$  by  $\theta^2$ ,  $\eta$  and Lemma 1, it is “safe” to increase the mutation rate. For a lower bound, we therefore pessimistically only account for offspring where the mutation parameter is increased to  $\min(\chi, \varepsilon n A^{\lceil \log_A(\frac{1}{2\varepsilon}) \rceil})$ . The probability of producing an offspring in levels  $A'_{\geq(j,\ell+1)}$  is at least  $p_{\text{inc}}(1 - A\chi/n)^j > p_{\text{inc}}(1 - A\theta'_2)^j > p_{\text{inc}}(1 - A\eta(j))^j \geq (1 + \delta)/\alpha_0$ .

- Case 2:  $j \in [0..[m] - 1]$  and  $\ell = d'_j$ . We use a stronger assumption that there are at least  $\gamma\lambda$  individuals in  $A_{\geq(j,1)}$  for any  $\gamma \in (0, \gamma_0]$ , which is a subset of  $A'_{>(j,d'_j)}$ . To produce an offspring in levels  $A_{\geq(j,1)}$ , it suffices to first select a parent from  $A_{\geq(j,1)}$ , and secondly create an offspring in levels  $A_{\geq(j,1)}$ . The probability of selecting such a parent is at least  $\gamma\alpha_0$ . By Lemma 7, the probability of producing an offspring in levels  $A_{\geq(j,1)}$  is at least  $(1 + \delta)/\alpha_0$ .
- Case 3:  $j = [m]$  and  $\ell \in [d'_j - 2]$ . Similarly to Case 1, it is “safe” to increase the mutation rate, since  $\chi/n < \eta'$ . For a lower bound, we therefore pessimistically only account for offspring where the mutation parameter is increased to  $\min(\chi, \epsilon n A^{\lfloor \log_A(\frac{1}{2\epsilon}) \rfloor})$ . The probability of producing an offspring in levels  $A'_{\geq([m], \ell+1)}$  is at least  $1 + \delta/\alpha_0$ .

- Case 4:  $j = [m]$  and  $\ell = d'_j - 1$ . By Lemma 7, the probability of producing an offspring in levels  $A'_{\geq([m], d'_{[m]})}$  is at least  $\frac{1+\delta}{\alpha_0}$ .

- Case 5:  $j = [m]$  and  $\ell = d'_{[m]}$ . We use a stronger assumption that there are at least  $\gamma\lambda$  individuals in  $A_{\geq(0,1)}$  for any  $\gamma \in (0, \gamma_0]$ , which is a subset of  $A'_{>([m], d'_{[m]})}$ . The probability of producing an offspring in levels  $A_{\geq(0,1)}$  is at least  $(1 + \delta)/\alpha_0$ .

To produce an offspring in levels  $A'_{>(j,\ell)}$ , it suffices to firstly select a parent  $(x, \chi/n)$  from  $A'_{>(j,\ell)}$ , and then create an offspring  $(x', \chi'/n)$  in levels  $A'_{>(j,\ell)}$ . The probability of selecting such a parent is at least  $\gamma\alpha_0$ . Thus, the probability that the offspring  $(x', \chi'/n)$  in levels  $A'_{>(j,\ell)}$ , is at least  $\gamma\alpha_0 \frac{1+\delta}{\alpha_0} = \gamma(1 + \delta)$ , which (G2) is satisfied.

For condition (G1) of Theorem 1, we assume that there are  $\gamma_0\lambda$  individuals in  $P_t$  in  $A'_{\geq(j,\ell)}$  where  $j \in [0..[m]]$  and  $\ell \in [d'_j]$ . To verify condition (G1), we assume that the parent  $(x, \chi/n)$  is in  $A'_{(j,\ell)}$ , and we distinguish four cases:

- Case 1:  $j \in [0..[m] - 1]$  and  $\ell \in [d'_j - 1]$ . The probability of the offspring in levels  $A'_{\geq(j,\ell+1)}$  is at least  $p_{\text{inc}}(1 - \chi/n)^{[m]-1} = \Omega(1)$ .
- Case 2:  $j \in [0..[m] - 1]$  and  $\ell = d'_j$ . The probability of the offspring in region  $A$ , i.e.,  $A_{\geq(j,1)}$ , is at least  $p_{\text{inc}}(1 - \chi/n)^{[m]-1} = \Omega(1)$ .
- Case 3:  $j = [m]$  and  $\ell \in [d'_j - 1]$ . The probability of the offspring in levels  $A'_{\geq([m], \ell+1)}$  is at least  $p_{\text{inc}}(1 - \chi/n)^{[m]-1} = \Omega(1)$ .
- Case 4:  $j = [m]$  and  $\ell = d'_{[m]}$ . The probability of the offspring in levels  $A_{\geq(0,d_0)}$  is at least  $p_{\text{inc}2}(1 - (1 - 1/2)^{[m]-1}) = \Omega(1/n)$ , where the mutation parameter is changed to  $\min(\chi, \epsilon n A^{\lfloor \log_A(\frac{1}{2\epsilon}) \rfloor})$  and at least one 0-bit of first  $k$  bit-position is flipped.

Thus, a lower bound of the probability of producing an offspring in higher levels, i.e.,  $A'_{>(j,\ell)}$ , is  $\gamma_0\alpha_0\Omega(1/n) = \Omega(1/n \log(n)) =: z'([m], d'_{[m]})$  and  $\gamma_0\alpha_0\Omega(1) = \Omega(1/\log(n)) =: z'(j, \ell)$  except the case of  $j = [m]$  and  $\ell = d'_{[m]}$ .

**Region A:** To verify condition (G2), we distinguish two cases for all  $j \in [0..n - 1]$  and  $\ell \in [d_j]$ :

- Case 1:  $\ell \in [d_j - 1]$ . Firstly, we need to estimate the probability of producing an offspring in levels  $A_{\geq(j,\ell+1)}$ , assuming that there are at least  $\gamma\lambda$  individuals in levels  $A_{\geq(j,\ell+1)}$ , for any  $\gamma \in (0, \gamma_0]$ . To produce an offspring in levels  $A_{\geq(j,\ell+1)}$ , it suffices to first select a parent  $(x, \chi/n)$  from  $A_{\geq(j,\ell+1)}$ , and secondly create an offspring  $(x', \chi'/n)$  in levels  $A_{\geq(j,\ell+1)}$ . The probability of selecting such a parent is at least  $\gamma\alpha_0$ . Assuming that the parent

is in level  $A_{(u,v)} \subseteq A_{\geq(j,\ell+1)}$ , and applying Lemma 7 to level  $A_{(u,v)}$ , the probability that the offspring  $(x', \chi'/n)$  is in levels  $A_{(u,v)} \subseteq A_{\geq(j,\ell+1)}$  is  $(1 + \delta)/\alpha_0$  for some  $\delta \in (0, 1)$ . Thus the probability of selecting a parent in levels  $A_{\geq(j,\ell+1)}$ , then producing an offspring in levels  $A_{\geq(j,\ell+1)}$ , is at least  $\gamma\alpha_0(1 + \delta)/\alpha_0 = \gamma(1 + \delta)$ , so condition (G2) is satisfied.

- Case 2:  $\ell = d_j$ . We assume that there are at least  $\gamma\lambda$  individuals in levels  $A_{\geq(j+1,1)}$ , for  $\gamma \in (0, \gamma_0]$ . We again apply Lemma 7 to show the probability of selecting an individual from  $A_{\geq(j+1,1)}$  and producing a new individual also in  $A_{\geq(j+1,1)}$  is at least  $\gamma(1 + \delta)$ , showing condition (G2) is satisfied.

To verify condition (G1), we assume that there are  $\gamma_0\lambda$  individuals in  $P_t$  in  $A_{\geq(j,\ell)}$  where  $j \in [0..n - 1]$  and  $\ell \in [d_j]$ . If the parent  $(x, \chi/n)$  is in  $A_{\geq(j,\ell)}$ , then

- Case 1:  $\ell \in [d'_j - 1]$ . The probability of the offspring in levels  $A_{\geq(j,\ell+1)}$  is at least  $(1 + \delta)/\alpha_0 = \Omega(1)$ .
- Case 2:  $\ell = d'_j$ . By Lemma 8, the probability of the offspring in  $A_{\geq(j+1,1)}$  is at least  $\Omega(1/j)$ .

Thus, a lower bound of the probability of producing an offspring in higher levels, i.e.,  $A_{(j,d_j)}$  is  $\gamma_0\alpha_0\Omega(1) = \Omega(1/\log(n)) =: z(j, d_j)$  for  $j \in [0..[m]]$ , and  $\gamma_0\alpha_0\Omega(1/j) = \Omega(1/j \log(n)) =: z(j, \ell)$  for  $j \in [0..[m]]$  and  $\ell \in [d_j - 1]$ .

To verify that  $\lambda \geq c \log^2(n)$  is large enough to satisfy condition (G3), we first must calculate the number of total sub-levels  $m'$ . The depth of each level  $j$  is no more than  $d'_j < \lceil \log_A(\frac{n}{2\epsilon}) \rceil = O(\log(n))$  for all  $j \in [0..[m]]$  and  $d_j < \lceil \log_A(\frac{n}{2\epsilon}) \rceil = O(\log(n))$  for all  $j \in [0..n - 1]$ . Therefore, by  $\gamma_0 = \Omega(1/\log(n))$ ,  $m' = O(n \log(n))$  and  $z_{\min} = \Omega(1/n \log(n))$ , we know that  $\lambda \geq c \log^2(n)$  satisfies condition (G3) for a large enough  $c > 1$ .

Overall, assuming no failure, the expected time to reach the last level can be calculated by considering regions  $A'$  and  $A$  separately, which is no more than

$$\begin{aligned}
 t_0(n) &\leq \frac{8}{\delta^2} \left( \sum_{j=0}^{[m]-1} \sum_{\ell=1}^{d'_j} \left( \lambda \log \left( \frac{6\delta\lambda}{4 + z'_{(j,\ell)}\delta\lambda} \right) + \frac{1}{z'_{(j,\ell)}} \right) \right. \\
 &\quad + \sum_{\ell=1}^{d'_j-1} \left( \lambda \log \left( \frac{6\delta\lambda}{4 + z'_{([m],\ell)}\delta\lambda} \right) + \frac{1}{z'_{([m],\ell)}} \right) \\
 &\quad + \lambda \log \left( \frac{6\delta\lambda}{4 + z'_{([m],d'_j)}\delta\lambda} \right) + \frac{1}{z'_{([m],d'_j)}} \\
 &\quad + \sum_{j=0}^{n-1} \sum_{\ell=1}^{d_j-1} O \left( \lambda \log \left( \frac{1}{z_{(j,\ell)}} \right) + \frac{1}{z_{(j,\ell)}} \right) \\
 &\quad \left. + \sum_{j=0}^{n-1} O \left( \lambda \log(\lambda) + \frac{1}{z_{(j,d_j)}} \right) \right) \\
 &= O(n\lambda \log(n) \log(\log(n)) + n^2 \log(n)).
 \end{aligned}$$

Finally, we account for “failed” generations where our assumption that there are less than  $(1 - \zeta/2)\mu$  individuals in region  $B$  does not hold. We refer to a sequence of  $2t_0(n)/\lambda$  generations as a *phase*, and call a phase *good* if for  $2t_0(n)/\lambda$  consecutive generations there are fewer than  $(1 - \zeta/2)\mu$  individuals in region  $B$ . By Lemma 9 and a union bound, a phase is good with probability  $1 - 2t_0(n)/\lambda e^{-\Omega(\mu)} = \Omega(1)$ , for  $\mu = \Omega(\log(n))$ . By Markov’s inequality, the probability of reaching a global optimum in a good phase is

at least  $1/2$ . Hence, the expected number of phases required, each costing  $2t_0(n)$  function evaluations, is  $O(1)$ .  $\square$

## 6 EXPERIMENTS

The theoretical analysis considers an idealised scenario, and it is interesting to evaluate its performance on problems with more complex structure. In this section, we empirically analyse the performance of the MOSA-EA on two well-known combinatorial optimisation problems, random NK-LANDSCAPE and  $k$ -SAT instances. We also compare the performances of the MOSA-EA with other popular randomised search heuristics.

### 6.1 Problems

The NK-LANDSCAPE problem [20] can be described as: given  $n, k \in \mathbb{N}$  satisfying  $k \leq n$ , and a set of sub-functions  $f_i : \{0, 1\}^k \rightarrow \mathbb{R}$  for every  $i \in [n]$ , to maximise  $\text{NK-LANDSCAPE}(x) := \sum_{i=1}^n f_i(\Pi(x, i))$ , where the function  $\Pi : \{0, 1\}^n, [n] \rightarrow \{0, 1\}^k$  returns a bit-string containing  $k$  right-side neighbours of the  $i$ -th bit of  $x$ , i.e.,  $x_i, \dots, x_{(i+k-1) \bmod n}$ . Typically, each sub-function is defined as a lookup table with  $2^{k+1}$  values between  $(0, 1)$ . We generate 100 random NK-LANDSCAPE instances with  $n = 100$  for each  $k \in \{5, 10, 15, 20, 25\}$  by uniformly sampling values in the lookup table. We run each algorithm once on each instance, and record the highest fitness value achieved in the evaluation budget.

The  $k$ -SAT problem is an optimisation problem that aims to find an assignment  $\{0, 1\}^n$  which maximises the number of satisfied clauses of a given Boolean formula in the conjunctive normal form [1, 6, 18]. For each random  $k$ -SAT instance, all  $m$  clauses have the same size  $k \in [n]$  and are sampled  $k$  elements from  $[n]$  without replacement. For  $k \geq 3$ , Coja-Oghlan [4] gives a *threshold for satisfiability*  $r_{k\text{-SAT}} = 2^k \ln 2 - \frac{1}{2}(1 + \ln 2) + o_k(1)$ , where the probability to sample a satisfiable instance is nearly 0 if  $\frac{m}{n}$  is close to this threshold. The notation  $o_k(1)$  signifies a term that tends to 0 in the limit of large  $k$ . We firstly generate 100 random  $k$ -SAT instances with  $k = 5$  and  $m = \lceil (2^k \ln 2 - (1 + \ln 2)/2)n \rceil \approx nr_{k\text{-SAT}}$  and for each  $n \in \{100, 200, 300\}$ . Similarly to experiments on NK-LANDSCAPE, we then run each algorithm among these random instances, and record the minimal numbers of unsatisfied clauses during the algorithm running in the fitness evaluation budget.

### 6.2 Algorithms

We compare the MOSA-EA with other EAs on the NK-LANDSCAPE and  $k$ -SAT problems. For the MOSA-EA used in experiments, we use the  $(\mu, \lambda)$  selection described in Algorithm 8 and the self-adapting mutation rate strategy shown in Algorithm 4. For the parameter setting, we use  $\mu = \lambda/8$ , the minimal mutation rate  $\varepsilon = 1.0/n$ , the self-adapting mutation rate parameters  $A = 1.01$  and  $p_{\text{inc}} = 0.4$ . The initial mutation rates of each individual is set as  $\varepsilon A^\ell$  where  $\ell \sim \text{Unif}([0, \lceil \log_A(1/2\varepsilon) \rceil])$ .

The baseline algorithm  $(1+1)$  EA can be implemented by the  $(\mu + \lambda)$  EA with  $\lambda = \mu = 1$ . We use the standard mutation rate  $\chi/n = 1/n$ . For the  $(\mu, \lambda)$  EA, we set the population parameter  $\mu = \lambda/8$  and the mutation rate a little bit below the error threshold, i.e.,  $\chi/n = 2.07/n < \ln(\lambda/\mu)$ . The UMDA [24] has only two parameters, population parameters  $\lambda$  and  $\mu$ . Consistently, we set  $\mu = \lambda/8$  in experiments. We configure the mutation rate of the 3-tournament

EA as  $\chi/n = 1.09812/n$  following [8, 9]. For fair comparisons, we use the same population size  $\lambda = 20000$  for all population-based algorithms and the same budget of fitness evaluations  $10^8$ .

### 6.3 Results

Figures 4 and 5 illustrate the experimental results on random NK-LANDSCAPE and  $k$ -SAT instances, respectively. Each box shows the distribution of one algorithm among 100 random instances on one problem setting. Tables 2 and 3 (shown in Appendix E) show statistics for results on NK-LANDSCAPE and  $k$ -SAT, respectively. Figure 4 and Table 2 indicate that the highest fitness values achieved by the MOSA-EA are statistically significantly higher than all other algorithms with significance level  $\alpha = 0.05$  for all NK-LANDSCAPE with  $k \in \{10, 15, 20, 25\}$ . Figure 5 and Table 3 indicate that the number of unsatisfied clauses achieved by the MOSA-EA are statistically significantly less than all other algorithms with significance level  $\alpha = 0.05$  for all tested  $k$ -SAT problems.

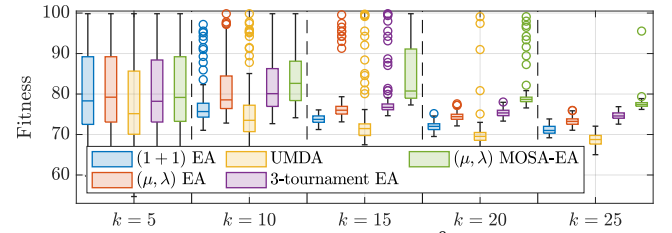


Figure 4: The highest fitness value in  $10^8$  fitness evaluations on random NK-LANDSCAPE instances ( $n = 100$ )

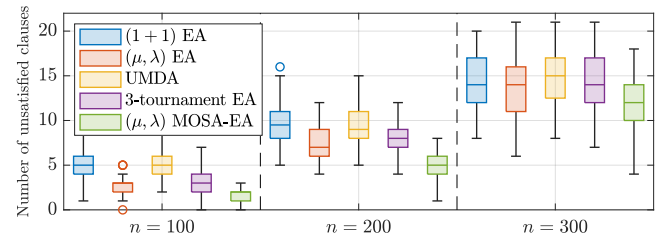


Figure 5: The number of unsatisfied clauses in  $10^8$  fitness evaluations on random  $k$ -SAT instances ( $k = 5$ )

## 7 CONCLUSION

In this paper, we first introduce the MOSA-EA for single-objective optimisation, which treats parameter control from the perspective of multi-objective optimisation: The algorithm simultaneously maximises the fitness and the mutation rates. To achieve this, we propose the multi-objective sorting mechanism, which sorts the population based on the strict non-dominated fronts. Theoretically, we demonstrate that the MOSA-EA can escape from sparse local optima of  $\text{PEAKEDLO}_{m,k}$  for any  $k \in \Omega(n)$ , where fixed mutation rate EAs may be trapped. Empirically, we show that the MOSA-EA can outperform some popular random search heuristics on complex combinatorial optimisation problems, i.e., random NK-LANDSCAPE and  $k$ -SAT problems.

## ACKNOWLEDGMENTS

This work was supported by a Turing AI Fellowship (EPSRC grant ref EP/V025562/1). The computations were performed using University of Birmingham's BlueBEAR and Baskerville HPC service.



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## A NEGATIVE DRIFT FOR POPULATION

We define the *reproductive rate* [21] of the individual  $P_t(j)$  in Algorithm 6 as the expected number of times the individual is sampled from  $P_{sel}(P_t)$ , i.e.,  $E[R_t(j) \mid P_t]$  where  $R_t(j) := \sum_{i=1}^{\lambda} [I_t(i) = j]$  for  $t \in \mathbb{N}$  and  $j \in [\lambda]$ . Informally, the negative drift theorem for populations [21] (Theorem 6 in Appendix B) states that if all individuals close to a given search point  $x^* \in \mathcal{X}$  have reproductive rate below a certain threshold  $\alpha_0$ , then the algorithm needs exponential time to reach  $x^*$ . This threshold  $\alpha_0$  is maximal reproductive rate within the population. Without uncertainties, it is well-known that  $\alpha_0 = 2(1 - 1/\lambda)$  and  $\alpha_0 = \lambda/\mu$  for 2-tournament selection and  $(\mu, \lambda)$ , respectively [23]. By Theorem 6, the runtime of optimising any single-modal function, e.g., ONEMAX and LEADINGONES, of non-elitist EAs is exponential with  $1 - e^{-\Omega(n)}$  probability, if the mutation rate is greater than  $(\ln(\alpha_0) + \delta)/n$  for a constant  $\delta > 0$ . We say  $\ln(\alpha_0)$  is the *error threshold* of a non-elitist EA.

**THEOREM 6 ([21]).** *The probability that a non-elitist EA shown in Algorithm 6 with population size  $\lambda = \text{poly}(n)$ , mutation rate  $\chi/n$  and maximal reproductive rate bounded by  $\alpha_0 < e^\chi - \delta$ , for a constant  $\delta > 0$ , optimises any function with a polynomial number of optima within  $e^{cn}$  generations is  $e^{-\Omega(n)}$ , for some constant  $c > 0$ .*

## B USEFUL INEQUALITIES AND LEMMAS

**LEMMA 2 ([25]).**  $(1 + \frac{x}{n})^n \geq e^x \left(1 - \frac{x^2}{n}\right)$  for  $n \in \mathbb{N}^*$ ,  $|x| \leq n$ .

**LEMMA 3 ([5]).** For all  $c \in (0, 1)$  and  $j \geq 1$ ,  $1 - c^{1/j} \geq (1 - c)/j$ .

**LEMMA 4.** For all  $-1 < x < 0$ ,  $1 + \frac{1}{x} < \frac{1}{\ln(1+x)}$ .

**PROOF.** It is immediately from a well-known inequality  $\frac{x}{x+1} < \ln(1+x)$  for all  $-1 < x < 0$ .  $\square$

**LEMMA 5.** For all  $b \in (0, 1)$  and  $x > 0$ ,  $1 - b^{\frac{1}{x}} \leq -\frac{\ln(b)}{x}$ .

**PROOF.** Let  $f(x) := 1 - b^{\frac{1}{x}} + \frac{\ln(b)}{x}$ . For all  $b \in (0, 1)$  and  $x > 0$ , we know that  $f(x)$  is a monotone increasing function by its derivative  $f'(x) = \left(b^{\frac{1}{x}} - 1\right) \frac{\ln(b)}{x^2} > 0$ . Thus,  $f(x) \leq \lim_{x \rightarrow \infty} f(x) = \lim_{x \rightarrow \infty} \left(1 - b^{\frac{1}{x}} + \frac{\ln(b)}{x}\right) = 0$ .  $\square$

## C ALGORITHMS MISSING FROM THE PAPER

### Algorithm 6 Non-elitist EA

**Require:** Fitness function  $f$ . Population size  $\lambda \in \mathbb{N}$  where  $\lambda \geq 2$ . Mutation parameter  $\chi > 0$ . Initial population  $P_0 \in \mathcal{X}^\lambda$ .

- 1: **for**  $t = 0, 1, 2, \dots$  until termination condition met **do**
- 2:   Sort  $P_t$  such that  $f(P_t(1)) \geq \dots \geq f(P_t(\lambda))$
- 3:   **for**  $i = 1$  to  $\lambda$  **do**
- 4:     Sample  $I_t(i) \sim P_{sel}([\lambda])$ ; set  $z := P_t(I_t(i))$ .
- 5:     Create  $x'$  by independently flipping each bit of  $x$  with probability  $\chi/n$ .
- 6:     Set  $P_{t+1}(i) := x'$ .

### Algorithm 7 Population-based Algorithm

**Require:** Finite state space  $\mathcal{Z}$  and population size  $\lambda \in \mathbb{N}$ . Map  $D$  from  $\mathcal{Z}^\lambda$  to the space of probability distributions over  $\mathcal{Z}$ . Initial population  $P_0 \in \mathcal{Z}^\lambda$ .

- 1: **for**  $t = 0, 1, 2, \dots$  until termination condition met **do**
- 2:   **for**  $i = 1$  to  $\lambda$  **do**
- 3:     Sample  $P_{t+1}(i) \sim D(P_t)$

### Algorithm 8 $(\mu, \lambda)$ selection

**Require:** Population size  $\lambda \in \mathbb{N}$ . Parameter  $\mu \in [\lambda]$ .

- 1:  $I_t \sim \text{Unif}([\mu])$ .
- 2: **return**  $I_t$ .

### Algorithm 9 2-tournament selection

**Require:** Population size  $\lambda \in \mathbb{N}$ .

- 1:  $i_1 \sim \text{Unif}([\lambda])$
- 2:  $i_2 \sim \text{Unif}([\lambda])$
- 3: **if**  $i_2 \geq i_1$  **then**  $I_t \leftarrow x_1$  **else**  $I_t \leftarrow x_2$ .
- 4: **return**  $I_t$ .

### Algorithm 10 $(\mu + \lambda)$ EA

**Require:** Population sizes  $\lambda \in \mathbb{N}$ . Parameter  $\mu \in \mathbb{N}$ . Mutation parameter  $\chi > 0$ . Initial population  $P_0 \in \mathcal{X}^\mu$ .

- 1: **for**  $t = 0, 1, 2, \dots$  until termination condition met **do**
- 2:   **for**  $i = 1, \dots, \lambda$  **do**
- 3:     Sample  $I_t(i) \sim \text{Unif}([\mu])$ , and set  $x := P_t(I_t(i))$ .
- 4:      $P(i) \leftarrow y$  where  $y$  created by mutating  $x$  with mutation rate  $\chi/n$ .
- 5:   Set  $P_{t+1}$  as the  $\mu$  best individuals of  $P_t \cup P$ .

## D LEMMAS AND PROOFS MISSING FROM THE PAPER

### D.1 Proof of Theorem 2

**PROOF.** For the  $(\mu + \lambda)$  EA (Algorithm 10), from initial population  $P_0 = \{0^k * n^{-k}\}^\mu$ , if there is no individual with fitness greater than  $m$ , then the initial population will be always the  $\mu$  best individuals. We now prove that with probability  $1 - e^{-\Omega(n)}$  during the first  $e^{cn^d}$  function evaluations, none of search point  $1^{\min\{n, \lceil m \rceil\}} * n^{-\min\{n, \lceil m \rceil\}}$  is created. To create a search point  $1^{\min\{n, \lceil m \rceil\}} * n^{-\min\{n, \lceil m \rceil\}}$ , it is necessary to mutate from one of individuals in the initial population  $P_0 = \{0^k * n^{-k}\}^\mu$ , where at least  $\min\{k, \min\{n, \lceil m \rceil\}\}$  0-bits must be flipped. The probability of such an event is  $n^{-\Omega(n)}$  for the mutation rate  $\frac{\chi}{n} = O\left(\frac{1}{n}\right)$ . Thus by a union bound, the probability of no search point  $1^{\min\{n, \lceil m \rceil\}} * n^{-\min\{n, \lceil m \rceil\}}$  is created within  $e^{cn^d}$  fitness evaluations is  $1 - e^{cn^d} n^{-\Omega(n)} = 1 - e^{-\Omega(n)}$ .  $\square$

### D.2 Proof of Theorem 3

**PROOF.** The result for  $\chi \geq \ln(\lambda/\mu) + \delta$  follows directly from Theorem 6 by that  $P_0$  is still at distance  $\Omega(n)$  away from  $1^n$ .

When  $\chi \leq \ln(\lambda/\mu) - \delta$ , it suffices to prove by induction that with high probability, the  $\mu$  best individuals are still  $0^k *^{n-k}$  during the first  $e^{c\lambda}$  generations for some constant  $c$  sufficiently small. Since the  $\mu$  best individuals of  $P_0$  are  $0^k *^{n-k}$ , it is certain that the selected parents to produce offspring in the next generation are  $0^k *^{n-k}$ . Then, to create an offspring which is  $0^k *^{n-k}$ , it is suffices to not modify any bit from the parent, the corresponding probability is  $\left(1 - \frac{\chi}{n}\right)^k \geq \left(1 - \frac{\chi}{n}\right)^n \geq (1 - \sigma)e^{-\chi} \geq \frac{\mu(1-\sigma)e^\delta}{\lambda}$  for any constant  $\sigma > 0$  by Lemma 2. Choosing  $\sigma$  so that  $\frac{1+\sigma}{1-\sigma} = e^\delta$  then this probability is at least  $\frac{\mu}{\lambda}(1 + \delta)$ . By a Chernoff bound, the probability that the population has less than  $\mu$  individuals are  $0^k *^{n-k}$  in the next generation is  $e^{-\Omega(\lambda)} = e^{-\Omega(n)}$ . In order for those individuals to be the best of the population, no individual  $1^{\min\{n, \lceil m \rceil\}} *^{n-\min\{n, \lceil m \rceil\}}$  must be created, but the probability of such creation by mutation  $0^k *^{n-k}$  is  $n^{\min(k, \lceil m \rceil)} = n^{\Omega(n)}$  and still  $n^{\Omega(n)}$  for the  $\lambda$  sampling. By induction and an union bound, with probability  $1 - e^{-\Omega(n)}$ , the  $\mu$  best individuals are those from  $0^k *^{n-k}$  during the next  $e^{cn}$  generations for some sufficiently small constant  $c$ .

□

### D.3 Proof of Theorem 4

PROOF. By the negative drift theorem for population (Theorem 6), we know that for any mutation rate  $\chi \geq \ln(2) + \delta$  where  $\delta \in (0, 1)$  is some constant, the probability that the algorithm optimises  $\text{PEAKEDLO}_{m,k}$  within  $e^{cn}$  generations is  $e^{-\Omega(n)}$  for some constant  $c > 0$ .

We then prove that for any  $k \leq an$ , the runtime of the 2-tournament EA on  $\text{PEAKEDLO}_{m,k}$  problems any mutation rate  $\chi \leq \ln(2) + \delta - \varepsilon$  satisfied  $\Pr(T \leq e^{cn}) = e^{-\Omega(\lambda)}$  for a constant  $c > 0$ .

We will prove a stronger statement that with probability  $1 - e^{-\Omega(\lambda)}$ , all individuals during the first  $e^{cn}$  generations have less than  $\min\{n, \lceil m \rceil\}$  leading 1-bits, where  $c > 0$  is a constant.

Choose the parameter  $\delta' \in (0, 1)$  such that  $\ln\left(\frac{1+\delta'}{1-\delta'}\right)/a = \varepsilon \in (0, 1)$ . We call an individual is a peak individual if it is  $0^k *^{n-k}$ . We first show by induction that with probability  $1 - e^{-\Omega(\lambda)}$ , there are at least  $\frac{\lambda}{2}\left(1 + \frac{\delta'}{2}\right)$  peak individuals in each of the first  $e^{c\lambda}$  generations, and we call the run of the algorithm failure otherwise. Then, by Lemma 2, the probability of not mutating any first  $k$  bits is

$$\begin{aligned} \left(1 - \frac{\chi}{n}\right)^k &\geq e^{-a\chi(1-\delta')} \\ &\geq \left(\frac{1}{2}\right)^a \left(\frac{1}{e^\delta}\right)^a e^{a\varepsilon(1-\delta')} \geq \left(\frac{1}{2}\right)^a \frac{1}{e^\delta} (1 + \delta') \end{aligned}$$

let  $\xi := 1 - 1/e^\delta$ , then for all  $\delta \in (0, 1)$  we have  $\xi \in (0, 2/3)$ , such that

$$\begin{aligned} &= \left(\frac{1}{2}\right)^a (1 - \xi)(1 + \delta') > \left(\frac{1}{e}\right)^a (1 - \xi)(1 + \delta') \\ &\geq \frac{2}{3} (1 + \delta'). \end{aligned}$$

Assume that there are  $\gamma\lambda \geq \frac{\lambda}{2}$  peak individuals in the current population. A peak individual is produced if a peak individual is

selected and non of its first  $k$  0-bits flipped. The probability of this event is

$$\begin{aligned} \left(\gamma^2 + 2(1-\gamma)\gamma\right) \left(1 - \frac{\chi}{n}\right)^k &\geq \gamma(2-\gamma) \left(1 - \frac{\chi}{n}\right)^{an} \\ &\geq \frac{3}{4} \left(1 - \frac{\chi}{n}\right)^{an} \geq \frac{1}{2} (1 + \delta'). \end{aligned}$$

Hence, by a Chernoff bound, the probability that the next generation contains less than  $\frac{\lambda}{2}\left(1 + \frac{\delta'}{2}\right)$  peak individuals is  $e^{-\Omega(\lambda)}$ . By induction and a union bound, the probability that the next  $e^{c\lambda}$  generations contain less than  $\frac{\lambda}{2}\left(1 + \frac{\delta'}{2}\right)$  peak individuals is still  $e^{-\Omega(\lambda)}$ , if  $c > 0$  is a sufficiently small constant.

We now assume that the run is not a failure. Furthermore, we assume that the algorithm is optimising the function  $g(x) := \min(\lceil m \rceil, \text{PEAKEDLO}_{m,k}(x))$  instead of  $\text{PEAKEDLO}_{m,k}$ . Clearly, the time to reach at least  $\lceil m \rceil$  leading 1-bits is the same, whether the algorithm optimises  $g$  or  $\text{PEAKEDLO}_{m,k}$ . Assume that there are more than  $\frac{\lambda}{2}\left(1 + \frac{\delta'}{2}\right)$  peak individuals, the reproductive rate of any non-peak individual is always less than

$$\lambda \left( \left(\frac{1}{\lambda}\right)^2 + \frac{2}{\lambda} \left(1 - \frac{1}{\lambda} - \frac{1 + \delta'/2}{2}\right) \right) < 1 - \frac{\delta'}{2} =: \alpha_0$$

For non-peak individuals, the last  $n - \min(n, \lceil m \rceil)$  bit-positions are irrelevant when the algorithm optimises  $g$ . We can therefore apply the negative drift theorem for population (Theorem 6) with respect to the algorithm limited to the first  $\min(n, \lceil m \rceil)$  bit-positions only. The mutation operator flips each of the  $\min(n, \lceil m \rceil)$  bits independently with probability  $\frac{\chi'}{\min(n, \lceil m \rceil)}$ , where  $\chi' = \frac{\chi m}{n}$ . Hence, we have  $e^{-\chi'} < 1 = \frac{1 - \delta'/2}{\alpha_0}$ , and the conditions of the theorem are satisfied.

□

### D.4 Proof of Lemma 1

PROOF. By the assumption,

$$\begin{aligned} \lceil m \rceil &< \frac{\ln\left(\frac{\alpha_0 p_{\text{inc}}}{1+\delta}\right)}{2A \ln\left(\frac{\alpha_0}{1-\delta}\right)} k - \ln\left(\frac{\alpha_0 p_{\text{inc}}}{1+\delta}\right) + 1 \\ \lceil m \rceil - 1 &< \ln\left(\frac{\alpha_0 p_{\text{inc}}}{1+\delta}\right) \left( \frac{an}{2A \ln\left(\frac{\alpha_0}{1-\delta}\right)} - 1 \right) \\ \lceil m \rceil - 1 &< \ln\left(\frac{1+\delta}{\alpha_0 p_{\text{inc}}}\right) \left( 1 + \frac{1}{-\ln\left(\frac{\alpha_0}{1-\delta}\right) \frac{2A}{an}} \right) \end{aligned}$$

by Lemma 4,

$$< \ln\left(\frac{1+\delta}{\alpha_0 p_{\text{inc}}}\right) / \ln\left(1 - \ln\left(\frac{\alpha_0}{1-\delta}\right) \frac{2A}{an}\right)$$

we know  $\frac{1+\delta}{\alpha_0 p_{\text{inc}}} < 1$  by condition  $p_{\text{inc}} > (1+\delta)/\alpha_0$ , then

$$\begin{aligned} \left( \frac{1+\delta}{\alpha_0 p_{\text{inc}}} \right)^{\frac{1}{\lceil m \rceil - 1}} &< \left( \frac{1+\delta}{\alpha_0 p_{\text{inc}}} \right)^{-\frac{\ln(1 - \ln(\frac{\alpha_0}{1-\delta}) \frac{2A}{an})}{\ln(\frac{1+\delta}{\alpha_0 p_{\text{inc}}})}} \\ &= e^{-\ln(1 - \ln(\frac{\alpha_0}{1-\delta}) \frac{2A}{an})} = 1 - \ln\left(\frac{\alpha_0}{1-\delta}\right) \frac{2A}{an}. \end{aligned}$$

By the definition,  $\theta_1(j)$  is a monotone decreasing function, then for all  $j \in [0.. \lceil m \rceil - 1]$ ,

$$\theta_1(j) \geq \theta_1(\lceil m \rceil - 1) = 1 - \left( \frac{1+\delta}{\alpha_0 p_{\text{inc}}} \right)^{\frac{1}{\lceil m \rceil - 1}} > \ln\left(\frac{\alpha_0}{1-\delta}\right) \frac{2A}{an}$$

by Lemma 5,

$$\geq 2A \left( 1 - \left( \frac{1-\delta}{\alpha_0} \right)^{\frac{1}{k}} \right) = \theta'_2. \quad \square$$

## D.5 Lemma of useful inequalities to Theorem 5

LEMMA 6. Assume that the parameters  $A$ ,  $\alpha_0$ ,  $p_{\text{inc}}$ ,  $p_{\text{inc}2}$  and  $k$  satisfy the constraints in Theorem 5. Then there exists a constant  $\delta \in (0, 1/10)$  such that for all  $j \in [0..n-1]$  and  $\chi \in [\varepsilon n, n/2]$ ,

- (i)  $\theta_1(0) < \eta(0) < \varepsilon A^{\lceil \log_A(\frac{1}{2\varepsilon}) \rceil} \leq 1/2 < \theta_2(0)$ ,
- (ii)  $\theta_2(j) = \Omega(1/j)$ , (v)  $\eta(j)/A = \theta_1(j)$ ,
- (iii)  $\theta_1(j) = O(1/j)$ , (vi)  $\theta_2(j)/A < \theta_2(j+1)$ ,
- (iv)  $A\eta(j) \leq \theta_2(j)$ , (vii)  $A\theta_1(j) \leq \theta_2(j+1)$ ,
- (viii) if  $\frac{\chi}{n} \leq \eta(j)$ , then  $r(j, A\chi) \geq \frac{1+\delta}{\alpha_0 p_{\text{inc}}}$ ,
- (ix) if  $\frac{\chi}{n} \leq \theta_2(j)$ , then  $r(j, \chi/A) \geq \frac{1+\delta}{\alpha_0(1-p_{\text{inc}}-o(1))}$ .

Furthermore,

- (x) if  $\frac{\chi}{n} \leq \eta'$ , then  $r'(\lceil m \rceil, A\chi) \geq \frac{1+\delta}{\alpha_0 p_{\text{inc}}}$ , and
- (xi) if  $\frac{\chi}{n} \leq \theta'_2$ , then  $r'(\lceil m \rceil, \chi/A) \geq \frac{1+\delta}{\alpha_0(1-p_{\text{inc}}-o(1))}$ .

PROOF. Before proving statements (i)–(ix), we derive bounds on the three constants  $q$ ,  $\zeta$ , and  $r_0$ . By the assumptions  $p_{\text{inc}} < 2/5$  and  $\alpha_0 \geq 4$  from Theorem 5 and  $\delta < 1/10$ ,

$$r_0 < \frac{11}{6\alpha_0} < 1. \quad (3)$$

Furthermore, since  $r_0 = \frac{1+\delta}{\alpha_0(1-p_{\text{inc}}-o(1))} < 1$  and  $\alpha_0 \geq 4$ , we have

$$\zeta > 1 - \alpha_0(r_0)^2 > 1 - \frac{1}{\alpha_0} \left( \frac{11}{6} \right)^2 \geq \frac{23}{144}. \quad (4)$$

Finally, since  $\delta, \zeta, p_{\text{inc}} \in (0, 1)$ , we have from the definitions of  $r_0$  and  $q$  that

$$0 < q < r_0. \quad (5)$$

From the definition of the functions  $\theta_1$ ,  $\eta$ , and the constant  $\delta \in (0, 1/10)$ , it follows that

$$\begin{aligned} \theta_1(0) < \eta(0) < \eta(1) < \frac{1}{2A} \left( 1 - \frac{1}{\alpha_0 p_{\text{inc}}} \right) < \frac{1}{2A} \\ &\leq \varepsilon A^{\lceil \log_A(\frac{1}{2\varepsilon}) - 1 \rceil} \leq \varepsilon A^{\lceil \log_A(\frac{1}{2\varepsilon}) \rceil} \leq \frac{1}{2}. \end{aligned}$$

Also, we have from the definition of  $q$ , the constraint  $\alpha_0 \geq 4$  from Theorem 5, and the bound  $\zeta > 23/144$  from Eq. (4) that

$$\theta_2(0) > \theta_2(1) > 1 - q = 1 - \frac{1 - \zeta}{\alpha_0} > 1 - \frac{1 - \frac{23}{144}}{4} = \frac{455}{576}.$$

Thus, we have proven statement (i).

Statement (ii) follows directly from Lemma 3, the definition of  $\theta_2$  and the constant  $q$ ,

$$\theta_2(j) = 1 - q^{1/j} \geq (1 - q)/j = \Omega(1/j).$$

For statement (iii), we define  $c := \frac{1+\delta}{\alpha_0 p_{\text{inc}}} < 1$ , and observe that the inequality  $e^x \geq 1 + x$  implies

$$\theta_1(j) < 1 - c^{1/j} = 1 - e^{(1/j)\ln(c)} \leq -(1/j)\ln(c) = O(1/j).$$

For statement (iv), first note that Eq. (5) and the assumption  $p_{\text{inc}} < 2/5$  imply

$$0 < q < r_0 < \frac{1+\delta}{\alpha_0 p_{\text{inc}}}.$$

For  $j \geq 1$ , we therefore have  $1/j > 0$  and

$$\theta_2(j) = 1 - q^{1/j} \geq 1 - \left( \frac{1+\delta}{\alpha_0 p_{\text{inc}}} \right)^{1/j} \geq A\eta(j).$$

For  $j = 0$ , the definition of  $\eta(0)$ , statement (iv) for the case  $j = 1$  shown above, and the definition of  $\theta_2(0)$  gives

$$A\eta(0) < \eta(1) \leq \frac{\theta_2(1)}{A} = \theta_2(0).$$

Statement (v) follows from the definition of  $\theta_1(j)$ .

We now show statement (vi). The statement is true by definition for  $j = 0$ , so assume that  $j \geq 1$ . We first derive an upper bound on the parameter  $b$  in terms of the constant  $q$ . In particular, the constraint on  $A$  from Theorem 5 and the relationship  $0 < q < r_0$  from Eq. (5) gives

$$\frac{1}{A} \leq \frac{1}{1 + \sqrt{r_0}} < \frac{1}{1 + \sqrt{q}} = \frac{1 - \sqrt{q}}{1 - q}. \quad (6)$$

The right hand side of Eq. (6) can be further bounded by observing that the function  $g(j) := \frac{1 - q^{1/(j+1)}}{1 - q^{1/j}}$  with  $q > 0$  increases monotonically with respect to  $j$ . Thus, for all  $j \in \mathbb{N}$ , we have

$$\frac{1}{A} < \frac{1 - \sqrt{q}}{1 - q} \leq \frac{1 - q^{1/(j+1)}}{1 - q^{1/j}}. \quad (7)$$

This upper bound on parameter  $1/A$  now immediately leads to the desired result

$$\frac{\theta_2(j)}{A} = \frac{(1 - q^{1/j})}{A} \leq 1 - q^{1/(j+1)} = \theta_2(j+1). \quad (8)$$

Statement (vii) follows by applying the previous three statements in the order (v), (iv), and (vi)

$$A\theta_1(j) = \eta(j) \leq \theta_2(j)/A \leq \theta_2(j+1).$$

Next we prove statement (viii). The statement is trivially true for  $j = 0$ , because  $r(0, A\chi) = 1$ , so assume that  $j \geq 1$ . By the assumption  $\chi/n \leq \eta(j)$  and the definition of  $\eta(j)$ ,

$$\begin{aligned} r(j, A\chi) &= \left( 1 - \frac{A\chi}{n} \right)^j \geq (1 - A\eta(j))^j \\ &\geq \left( 1 - \left( 1 - \left( \frac{1+\delta}{\alpha_0 p_{\text{inc}}} \right)^{1/j} \right) \right)^j = \frac{1+\delta}{\alpha_0 p_{\text{inc}}}. \end{aligned} \quad (9)$$

Finally, we prove statement (ix). Again, the statement is trivially true for  $j = 0$ , because  $r(0, \chi/A) = 1$ , so assume that  $j \geq 1$ . We

derive an alternative upper bound on parameter  $1/A$  in terms of  $r_0$  and  $q$ . By the constraint on  $A$  in Lemma 6,

$$\begin{aligned} \frac{1}{A} &\leq \frac{1}{1 + \sqrt{r_0}} = \frac{\ln(r_0)}{\ln(r_0) + \sqrt{r_0} \ln(r_0)} \\ &= \frac{\ln(r_0)}{\ln(r_0 r_0^{\sqrt{r_0}})} = \frac{\ln r_0}{\ln q}. \end{aligned} \quad (10)$$

Furthermore, note that the function  $h(j) := \frac{1-r_0^{1/j}}{1-q^{1/j}}$  decreases monotonically with respect to  $j$  when  $r_0 > q > 0$ , and has the limit  $\lim_{j \rightarrow \infty} h(j) = \ln(r_0)/\ln(q)$ . Using Eq. (10), it therefore holds for all  $j \in \mathbb{N}$  that

$$\frac{1}{A} \leq \frac{\ln r_0}{\ln q} \leq \frac{1 - r_0^{1/j}}{1 - q^{1/j}}. \quad (11)$$

The assumption  $\chi/n \leq \theta_2(j)$ , the definition of  $\theta_2(j)$ , and (11) now give

$$\begin{aligned} r(j, \chi/A) &= \left(1 - \frac{\chi}{An}\right)^j \geq \left(1 - \frac{\theta_2(j)}{A}\right)^j \\ &= \left(1 - \frac{(1 - q^{1/j})}{A}\right)^j \geq \left(1 - (1 - r_0^{1/j})\right)^j = r_0, \end{aligned}$$

which completes the proof of statement (ix).

For statements (x)-(xi), if the first  $k$  0-bits are not flipped, then the individual survives, by the assumption  $\chi/n \leq \eta'$  and the definition of  $\eta'$ ,

$$\begin{aligned} r'(\lceil m \rceil, A\chi) &= \left(1 - \frac{A\chi}{n}\right)^k \geq (1 - A\eta')^k = (1 - A\eta(k))^k \\ &\geq \left(1 - \left(1 - \left(\frac{1 + \delta}{\alpha_0 p_{\text{inc}}}\right)^{1/k}\right)\right)^k = \frac{1 + \delta}{\alpha_0 p_{\text{inc}}}, \end{aligned}$$

and by the assumption  $\chi/n \leq \theta'_2$  and the definition of  $\theta'_2$ ,

$$\begin{aligned} r'(\lceil m \rceil, \chi/A) &= \left(1 - \frac{\chi}{An}\right)^k \geq \left(1 - \frac{\theta'_2}{A}\right)^k = \left(1 - \frac{\theta_2(k)}{A}\right)^k \\ &= \left(1 - \frac{(1 - q^{1/k})}{A}\right)^k \geq \left(1 - (1 - r_0^{1/k})\right)^k = r_0. \end{aligned}$$

□

## D.6 Lemma to support the proof of (G2)

LEMMA 7. Assume that the parameters  $A, p_{\text{inc}}, p_{\text{inc}2}, k$  and  $m$  satisfy the constraints in Theorem 5. Then there exists a constant  $\delta \in (0, 1/10)$  such that for all  $j \in [0..n-1]$  and  $\ell \in [d_j]$ , if Line 4 of Algorithm 1 selects a parent  $(x, \chi/n) \in A_{(j, \ell)}$ , then the offspring  $(x', \chi'/n)$  created in Lines 5 (using Algorithm 5) and 6 of Algorithm 1 satisfies  $\Pr((x', \chi'/n) \in A_{\geq(j, \ell)}) \geq \frac{1+\delta}{\alpha_0}$ .

Furthermore, there exists a constant  $\delta \in (0, 1/10)$  such that for all  $j \in [0..\lceil m \rceil]$  and  $\ell \in [d'_j]$ , if Line 4 of Algorithm 1 selects a parent  $(x, \chi/n) \in A'_{(j, \ell)}$ , then the offspring  $(x', \chi'/n)$  created in Lines 5 (using Algorithm 5) and 6 satisfies  $\Pr((x', \chi'/n) \in A'_{\geq(j, \ell)}) \geq \frac{1+\delta}{\alpha_0}$ .

PROOF. We will prove the stronger statement for Eq. (7) that with probability  $(1 + \delta)/\alpha_0$ , we have simultaneously

$$x' \in A_{\geq j} \quad \text{and} \quad \min\left\{\frac{\chi'}{n}, \theta_1(j)\right\} \leq \frac{\chi'}{n} \leq \theta_2(j). \quad (12)$$

The event Eq. (12) is a subset of the event  $(x', \chi'/n) \in A_{(j, \ell)}$ , because a lower level  $A_{(j, \ell)}$  may contain search points  $(x', \chi'/n)$  with mutation rates  $\chi'/n < \min(\chi/n, \theta_1(j))$ .

By the definition of levels, the parent satisfies  $x \in A_{\geq j}$  and  $\chi/n \leq \theta_2(j)$ . We distinguish between two cases.

Case 1:  $\chi/n \leq \eta(j)$ . By Lemma 6 (i), and the monotonicity of  $\eta$ , we have  $\eta(j) < 1/2$ . Note that in this case, it is still “safe” to increase the mutation rate. For a lower bound, we therefore pessimistically only account for offspring where the mutation parameter is increased from  $\chi$  to  $\min\left(A\chi, \varepsilon n A^{\lfloor \log_A(\frac{1}{2\varepsilon}) \rfloor}\right)$ .

Note first that since  $A > 1$ , we have

$$\frac{\chi'}{n} = \frac{\min\left(A\chi, \varepsilon n A^{\lfloor \log_A(\frac{1}{2\varepsilon}) \rfloor}\right)}{n} > \frac{\chi}{n}.$$

Also, Lemma 6 (iv) implies the upper bound

$$\frac{\chi'}{n} \leq \frac{A\chi}{n} \leq A\eta(j) \leq \theta_2(j).$$

To lower bound the probability that  $x' \in A_{\geq j}$ , we consider the event where the mutation rate is increased, and the event that none of the first  $j$  bits in the offspring are mutated with the new mutation parameter  $\min\left(A\chi, \varepsilon n A^{\lfloor \log_A(\frac{1}{2\varepsilon}) \rfloor}\right)$ . By definition of Algorithm 5 and using Lemma 6 (viii), these two events occur with probability at least

$$p_{\text{inc}} r(j, A\chi) \geq (1 + \delta)/\alpha_0. \quad (13)$$

Case 2:  $\eta(j) < \chi/n \leq \theta_2(j)$ . Note that in this case, it may be “unsafe” to increase the mutation rate. For a lower bound, we pessimistically only consider mutation events where the mutation parameter is decreased from  $\chi$  to  $\chi/A$ . Analogously to above, since  $1/A < 1$ , we have

$$\frac{\chi'}{n} = \frac{\chi}{An} < \frac{\chi}{n} \leq \theta_2(j).$$

Furthermore, Lemma 6 (v) implies the lower bound

$$\frac{\chi'}{n} = \frac{\chi}{An} > \frac{\eta(j)}{An} \geq \theta_1(j).$$

To lower bound the probability that  $x' \in A_{\geq j}$ , we consider the event where the mutation parameter is decreased from  $\chi$  to  $\chi/A$ , and the offspring  $x'$  is not downgraded to a lower level. By the definition of Algorithm 5,  $p_{\text{inc}2}$ ,  $r(j, \chi/A)$ , and using Lemma 6 (ix), these two events occur with probability

$$(1 - p_{\text{inc}} - p_{\text{inc}2})r(j, \chi/A) \geq (1 + \delta)/\alpha_0.$$

Hence, we have shown that in both cases, the event in Eq. (12) occurs with probability at least  $(1 + \delta)/\alpha_0$ .

Now, we consider Eq. (7). By the definition of levels and Lemma 1, we know that individuals in  $A'_{(j, \ell)}$  have mutation rates  $\chi/n < \theta'_2 < \theta_1(j) < \eta(j)$  for all  $j \in [0..\lceil m \rceil - 1]$  and  $\ell \in [d'_j]$ . Thus, it is “safe” to increase the mutation rate, such that a lower bound of the probability that  $x' \in A_{\geq j}$  is

$$p_{\text{inc}} r'(j, A\chi) \geq (1 + \delta)/\alpha_0.$$



Note that for the individual  $(x, \chi) \in A'_{(j, d'_j)}$ , the offspring  $(x', \chi') \in A_{\geq j} \subset A'_{\geq j}$  if the mutation rate  $\chi$  of the individual is increased from  $\chi$  to  $A\chi$  and non of the first  $j$  bits of  $x$  are flipped.

For the individuals in  $A'_{(\lceil m \rceil, \ell)}$ , where  $\ell \in [d'_j]$ , analogously to the proofs of Eq. (7), we distinguish two cases:  $\chi/n \leq \eta'$  and  $\eta' \leq \chi/n < \theta'_2$ , where lower bounds of such probabilities that  $x' \in A_{\geq j}$  are, by Lemma 6 (x)-(xi),

$$p_{\text{inc}} r'(\lceil m \rceil, A\chi) \geq (1 + \delta)/\alpha_0,$$

and

$$(1 - p_{\text{inc}} - p_{\text{inc}}) r'(\lceil m \rceil, \chi/A) \geq (1 + \delta)/\alpha_0,$$

respectively. Thus, the proof is completed.  $\square$

## D.7 Lemma to support the proof of (G1)

LEMMA 8. Assume that the parameters  $A, p_{\text{inc}}, p_{\text{inc}2}, k$  and  $m$  satisfy the constraints in Theorem 5. Then for any  $j \in [0..n-1]$ , and any search point  $(x, \chi/n) \in A_{(j, d_j)}$  selected in Line 4 of Algorithm 1 applied to PEAKEDLO $_{m,k}$ , the offspring  $(x', \chi'/n)$  created in Line 5 (using Algorithm 5) and Line 6 of Algorithm 1 satisfies  $\Pr((x', \chi'/n) \in A_{\geq(j+1,1)}) = \Omega(1/j)$ .

PROOF. By the definition of level  $A_{(j, d_j)}$ , we have  $\theta_1(j) \leq \chi/n \leq \theta_2(j)$  and so by Lemma 6 (vi), we have  $\chi/(An) \leq \theta_2(j+1)$ . Given the definition of levels  $A_{(j+1,1)}$ , it suffices for a lower bound to only consider the probability of producing an offspring  $(x', \chi'/n)$  with lowered mutation rate  $\chi'/n = \chi/(An) \leq \theta_2(j+1)$  and fitness  $\text{LO}(x') \geq j+1$ .

We claim that if the mutation rate is lowered, the offspring has fitness  $\text{LO}(x') \geq j+1$  with probability  $\Omega(1/j)$ . Since the parent belongs to level  $A_{(j, d_j)}$ , it has fitness  $\text{LO}(x) \geq j$ , so we need to estimate the probability of not flipping the first  $j$  bits, and obtain a 1-bit in position  $j+1$ .

We now estimate the probability of obtaining a 1-bit in position  $j+1$ , assuming that the parent  $x$  already has a 1-bit in this position, for any  $j \in [0..n-1]$ . Using that  $\theta_2(j)$  decreases monotonically in  $j$ , the definition of  $\theta_2(0)$ , and the lower bound on the parameter  $\zeta > 23/144$  from Eq. (4), the probability of not mutating bit-position  $j+1$  with the lowered mutation rate  $\chi/(An)$  is

$$\begin{aligned} 1 - \frac{\chi}{An} &\geq 1 - \theta_2(j)/A \geq 1 - \theta_2(0)/A \\ &= 1 - \theta_2(1) = 1 - \frac{1 - \zeta}{\alpha_0} > 1 - \frac{1 - \frac{23}{144}}{\alpha_0} = \Omega(1). \end{aligned}$$

If the parent  $x$  does not have a 1-bit in position  $j+1$ , we need to flip this bit-position. By the definition of  $\theta_1(j)$ , the probability of this event is in the case  $j \geq 1$

$$\frac{\chi}{An} \geq \theta_1(j)/A = \frac{1}{2A^3} \left( 1 - \left( \frac{1 + \delta}{\alpha_0 p_{\text{inc}}} \right)^{1/j} \right) \quad (14)$$

$$\geq \frac{1}{2A^3 j} \left( 1 - \frac{1 + \delta}{\alpha_0 p_{\text{inc}}} \right) = \Omega(1/j), \quad (15)$$

where the last inequality follows from Lemma 3. If  $j = 0$ , we use that  $\theta_1(j)$  decreases monotonically in  $j$  and Eqs. (14)–(15) to show

that the probability of flipping bit  $j+1 = 1$  is

$$\frac{\chi}{An} \geq \frac{\theta_1(0)}{A} > \frac{\theta_1(1)}{A} = \Omega(1).$$

The claim that we obtain a 1-bit in position  $j+1$  with probability  $\Omega(1/j)$  is therefore true.

Thus, the probability of lowering the mutation rate to  $b\chi/n$ , obtaining a 1-bit in position  $j+1$ , and not flipping the first  $j$  positions is, using the definition of  $\theta_2(j)$ ,

$$\begin{aligned} (1 - p_{\text{inc}}) \Omega\left(\frac{1}{j}\right) \left(1 - \frac{\chi}{An}\right)^j \\ > \Omega\left(\frac{1}{j}\right) (1 - \theta_2(j))^j = \Omega\left(\frac{1}{j}\right) \left(\frac{1 - \zeta}{\alpha_0}\right)^j = \Omega\left(\frac{1}{j}\right), \end{aligned}$$

which completes the proof.  $\square$

## D.8 Lemma to show not too many individuals in B region

LEMMA 9. Let  $B \subset \mathcal{Y}$  be as defined in Eq. (1) for a constant  $\zeta \in (0, 1)$ . Then for any generation  $t \in \mathbb{N}$  of the algorithm used in Theorem 5 on PEAKEDLO $_{m,k}$  with  $k$  and  $m$  described in Theorem 5,  $\Pr(|B \cap P_t| \geq \mu(1 - \zeta/2)) \leq e^{-\Omega(\mu)}$ .

PROOF. Consider some parent  $(x, \chi/n)$  selected in generation  $t-1 \geq 0$  and the  $(\mu, \lambda)$  selection (Algorithm 8). First a new mutation parameter  $\chi'$  is chosen, a new bit-string  $x'$  is obtained from  $x$  using bitwise mutation with mutation rate  $\chi'/n$ . To obtain an upper bound on the probability that  $(x', \chi'/n)$  is in  $B$ , we proceed in cases based on the outcome of sampling  $\chi'$ , namely, whether  $(x', \chi'/n)$  is in  $B$ .

Case 1:  $(x, \chi'/n) \in B$ . It follows immediately from the definition of  $B$  that independently of the chosen parent  $x$ , it holds

$$\Pr((x', \chi'/n) \in B) < \frac{1 - \zeta}{\alpha_0}.$$

Case 2:  $(x, \chi'/n) \notin B$ .

- If  $x \neq 0^k *^{n-k}$  then for  $(x', \chi'/n) \in B$  to end up in  $B$ , by Eq. (2), it is necessary that  $x' \in A_{\geq u}$  for some  $u > j$ , where  $x \in A_j$  and  $r(u, \chi') < (1 - \zeta)/\alpha_0$ . Since  $\chi'/n < 1/2$ , the probability of obtaining  $x' \in A_{\geq u}$  or  $x' = 0^k *^{n-k}$  is no more than

$$\left(1 - \frac{\chi'}{n}\right)^{u-1} \left(\frac{\chi'}{n}\right) < \left(1 - \frac{\chi'}{n}\right)^u < \frac{1 - \zeta}{\alpha_0}.$$

- If  $x = 0^k *^{n-k}$  then for  $(x', \chi'/n) \in B$  to end up in  $B$ , it is necessary that  $x' = 0^k *^{n-k}$ , where  $r'(\lceil m \rceil, \chi') < (1 - \zeta)/\alpha_0$ . Then the probability of obtaining  $x' \in A_{\geq u}$  or  $x' = 0^k *^{n-k}$  is no more than

$$\left(1 - \frac{\chi'}{n}\right)^k < \left(1 - \frac{\theta'_2}{n}\right)^k < \frac{1 - \zeta}{\alpha_0}.$$

Since each of the  $\lambda$  individuals in population  $P_t$  are sampled independently and identically,  $|B \cap P_t|$  is stochastically dominated by a binomially distributed random variable  $Z \sim \text{Bin}\left(\lambda, \frac{1 - \zeta}{\alpha_0}\right)$ ,

which has expectation  $\mu(1 - \zeta)$ . By a Chernoff bound,

$$\begin{aligned} \Pr\left(|B \cap P_t| \geq \mu\left(1 - \frac{\zeta}{2}\right)\right) &\leq \Pr\left(Z \geq \mu\left(1 - \frac{\zeta}{2}\right)\right) \\ &= \Pr\left(Z \geq E[Z]\left(1 + \frac{1}{2(1 - \zeta)}\right)\right) = e^{-\Omega(\mu)}. \end{aligned}$$

□

## E EXPERIMENTS RESULTS

**Table 2: Statistical results of experiments on NK-LANDSCAPE instances ( $p$ -values of each algorithm come from Wilcoxon rank-sum tests between the algorithm and MOSA-EA.)**

$k$	Stat.	(1+1) EA	$(\mu, \lambda)$ EA	UMDA	3-tour. EA	MOSA-EA
5	Median	78.3071	79.2195	75.1502	78.2089	<b>79.1638</b>
	$p$ -value	0.6985	0.8498	0.0236	0.8661	-
10	Median	75.6720	78.5569	73.5105	80.0956	<b>82.6345</b>
	$p$ -value	3.2e-15	7.0e-04	1.6e-15	0.0387	-
15	Median	73.7398	76.0001	71.4659	76.7120	<b>80.7450</b>
	$p$ -value	2.6e-34	6.4e-24	1.3e-22	6.1e-21	-
20	Median	72.0112	74.4063	69.5371	75.3354	<b>78.6688</b>
	$p$ -value	2.6e-34	3.3e-34	1.5e-29	2.4e-33	-
25	Median	70.9949	73.2404	68.7581	74.5825	<b>77.3945</b>
	$p$ -value	2.6e-34	2.6e-34	2.6e-34	6.7e-34	-

**Table 3: Statistical results of experiments on random  $k$ -SAT instances ( $p$ -values of each algorithm come from Wilcoxon rank-sum tests between the algorithm and MOSA-EA.)**

$n$	Stat.	(1+1) EA	$(\mu, \lambda)$ EA	UMDA	3-tour. EA	MOSA-EA
100	Median	5	3	5	3	<b>2</b>
	$p$ -value	3.7e-33	1.4e-16	9.5e-34	1.4e-16	-
200	Median	9.5	7	9	8	<b>5</b>
	$p$ -value	9.7e-30	1.7e-22	1.7e-30	1.9e-25	-
300	Median	14	14	15	14	<b>12</b>
	$p$ -value	1.6e-07	7.8e-04	2.9e-09	1.1e-07	-