

HITTING TIMES OF LOCAL AND GLOBAL OPTIMA IN GENETIC ALGORITHMS WITH VERY HIGH SELECTION PRESSURE

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Abstract: The paper is devoted to upper bounds on the expected first hitting times of the sets of local or global optima for non-elitist genetic algorithms with very high selection pressure. The results of this paper extend the range of situations where the upper bounds on the expected runtime are known for genetic algorithms and apply, in particular, to the Canonical Genetic Algorithm. The obtained bounds do not require the probability of fitness-decreasing mutation to be bounded by a constant which is less than one.

Keywords: Combinatorial Optimization, Evolutionary Algorithms, Runtime Analysis, Fitness Level, Local Search.

MSC: 90C59, 90C10.

1. INTRODUCTION

The genetic algorithms (GAs) are randomized heuristic algorithms that employ a population of tentative solutions (individuals), which is iteratively updated by means of selection, mutation and crossover operators, thus simulating an evolutionary type of search for optimal or near-optimal solutions. Different modifications of GAs are widely used in areas of operations research and artificial intelligence. A wider class of *evolutionary algorithms* (EAs), having a more flexible outline, possibly neglecting the crossover operator and admitting a population which consists of a single individual. Two major types of evolutionary algorithm outline are now well-known: the *elitist* EAs keep a certain number of

“most promising” individuals from the previous iteration, while the *non-elitist* EAs compute all individuals of a new population independently using the same randomized procedure.

The theoretical analysis of GAs has been subject of an increasing interest over the last two decades and several different approaches have been developed. A significant progress in understanding of non-elitist GAs was made in [33] by means of dynamical systems. However most of the findings in [33] apply to the infinite population case, so it is not clear how these results can be used to estimate the runtime of GAs, i.e. the expected number of individuals computed and evaluated until the optimum is found for the first time. A theoretical possibility of constructing GAs that provably optimize an objective function with high probability in polynomial time was shown in [32] by rapidly mixing Markov chains. However [32] provides only a very simple artificial example where this approach is applicable. The drift analysis was first adapted to studying elitist EAs in [19] and further extended in [11, 24] to non-elitist EAs without a crossover.

A series of works has attempted to show that the use of crossover operator in GAs and other evolutionary algorithms can reduce their runtime (see e.g. [20, 23, 26, 31]) but most of the positive results apply to families of problem instances with specific structure. At the same time [28] showed that a well-known non-elitist GA with proportional selection operator is inefficient on one of the most simple benchmark functions `ONEMAX`, even when the crossover is used. In [27], a general runtime result is proposed for a class of convex search algorithms, including many non-elitist GAs without mutation, on the so-called concave fitness landscapes (a discrete-space counterpart of a concave maximization problem). As a corollary, for another well-known benchmark function `LEADINGONES`, it is shown that the convex search algorithm has $O(n \log n)$ runtime, which means that it is faster than all EAs using only mutation [27]. Upper bounds obtained for the runtime of GAs with crossover in [10] match (up to a constant factor) the analogous upper bounds known for mutation-only GAs [11]. In [13], sufficient conditions are found under which a non-elitist GA with tournament selection first visits a local optimum of a pseudo-Boolean function in polynomially bounded time on average. The bounds from [13] indicate that if a local optimum is efficiently computable by the local search method, it is also computable in expected polynomial time by a GA with tournament selection.

In the present paper, the genetic algorithms are studied on a wide class of combinatorial optimization problems. The expected number of tentative solutions constructed, until first visiting a desired area for the first time, is considered as the main criterion of GA efficiency. Such an area may consist of locally optimal solutions or of globally optimal solutions or of feasible solutions with sufficiently small relative error. The main result is obtained by combining the approaches from [13, 25] and the result applies to a wider range of selection operators, compared to [13], including the proportional selection of Canonical GA [17] (the term “Canonical GA” was coined in [29]). Considering the selection operators with very high selection pressure, in this paper, we can neglect the probability of downgrading mutations although this probability needs to be taken into account in [10, 11].

By downgrading mutations here we mean mutations that decrease the quality of solutions (a formal definition of downgrading mutation will be given further). In contrast to [10, 11], here we consider explicitly the constrained optimization problems and the expected first hitting time of the set of local optima.

In the most general setting, a combinatorial optimization problem with a maximization criterion is formulated as follows:

$$\max\{F(x) \mid x \in \text{Sol}\}, \quad (1)$$

where $\text{Sol} \subseteq \mathcal{X}$ is the set of feasible solutions, $\mathcal{X} = \{0, 1\}^n$ is the search space, $F(\cdot)$ is the objective function. The optimal value of the criterion is denoted by F^* . The minimization problems are formulated analogously. Without loss of generality, by default we will consider the maximization problems. The results will hold for the minimization problems as well.

Genetic Algorithms. In the process of the GA execution, a sequence of populations $P^t = (x^{1,t}, \dots, x^{\lambda,t})$, $t = 0, 1, \dots$, is computed, where each population consists of λ *genotypes*. In the present paper, by the genotypes we mean the elements of the search space \mathcal{X} , and *genes* x_i , $i \in [n]$ are the components of a genotype $x \in \mathcal{X}$. Here and below, we use the notation $[n] := \{1, 2, \dots, n\}$ for any positive integer n .

An initial population P^0 consists of randomly generated genotypes, and every next population is constructed on the basis of the previous one. For convenience of GA description, in what follows we assume that the population size λ is even.

In each iteration of a GA, $\lambda/2$ pairs of parent genotypes are chosen from the current population P^t using the randomized *selection* procedure $\text{Sel} : \mathcal{X}^\lambda \rightarrow [\lambda]$. In this procedure, a parent genotype is independently drawn from the previous population P^t where each individual is assigned a selection probability depending on its *fitness* $f(x)$. Usually a higher fitness value of an individual implies higher (or equal) selection probability. We assume that the fitness function is defined on the basis of objective function. If $x \in \text{Sol}$ then $f(x) = \phi(F(x))$, where $\phi : \mathbb{R} \rightarrow \mathbb{R}_+$ is a monotone increasing function in the case of maximization problem or a monotone decreasing function in the case of minimization problem. Otherwise (i.e. if $x \notin \text{Sol}$), the fitness incorporates some penalty, which ensures that $f(x) < \min_{y \in \text{Sol}} F(y)$.

Given the current population, each pair of offspring genotypes is created independently from other pairs by the randomized operators of *crossover* and *mutation*. Some authors consider crossover operators that output a single genotype (see e.g. [10, 7, 28, 21, 33]), while others consider crossovers with two output genotypes (see e.g. [5, 17, 29, 32]). For the sake of uniform treatment of both versions of crossover, let us denote the number of output genotypes by r , $r \in \{1, 2\}$. In what follows, we assume that $\text{Cross} : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{X}^r$ and $\text{Mut} : \mathcal{X} \rightarrow \mathcal{X}$ are efficiently computable by randomized routines. When a new population P^{t+1} is constructed, the non-elitist GA proceeds to the next iteration.

Algorithm 1. Non-Elitist Genetic Algorithm in the case of $r = 2$

Generate the initial population P^0 , assign $t := 1$.
While a termination condition is not met **do**:
 Iteration t .
 For j **from** 1 **to** $\lambda/2$ **do**:
 Selection: $i := \text{Sel}(P^t), i' := \text{Sel}(P^t)$.
 Crossover: $(x, y) := \text{Cross}(x^{it}, x^{i't})$.
 Mutation: $x^{2j-1, t+1} := \text{Mut}(x), x^{2j, t+1} := \text{Mut}(y)$.
 End for.
 $t := t + 1$.
End while.

Algorithm 2. Non-Elitist Genetic Algorithm in the case of $r = 1$

Generate the initial population P^0 , assign $t := 1$.
While a termination condition is not met **do**:
 Iteration t .
 For j **from** 1 **to** λ **do**:
 Selection: $i := \text{Sel}(P^t), i' := \text{Sel}(P^t)$.
 Crossover: $x := \text{Cross}(x^{it}, x^{i't})$.
 Mutation: $x^{j, t+1} := \text{Mut}(x)$.
 End for.
 $t := t + 1$.
End while.

The output of a GA is an individual with the maximum fitness value in all populations constructed until the termination condition was met.

In the theoretical analysis of GAs it is often assumed that the algorithm constructs an infinite sequence of populations and that the termination condition is never met. In practice, the termination condition is required not only to stop the search and output the result, but also to perform multiple restarts of the GA with random initialization [5, 8]. Multiple independent runs of randomized algorithms or local search (multistart) are widely used to prevent localization of the search in the “unpromising” areas of the search space (see e.g. [9]) and applicability of multistart to the evolutionary algorithms has some theoretical basis [12, 32].

In this paper, together with the standard version of Non-Elitist GA (Algorithms 1 and 2), we study the *GA with multistart*, where a GA outlined as Algorithm 1 or 2 is ran independently from the previous executions for an unlimited number of times. The stopping criterion in Algorithm 1 or 2 in this case is the iterations limit $t \leq t_{\max}$, where t_{\max} is a tunable parameter.

In what follows, we consider three options for selection operator: the tournament selection [18], the (μ, λ) -selection [25], and the proportional selection [17]. In *k-tournament selection*, k individuals are sampled uniformly at random (with replacement) from the population, and the fittest of these individuals is returned. The tunable parameter k is called the *tournament size*. In (μ, λ) -selection, parents are sampled uniformly at random among the fittest μ individuals in the population P^t .

In the case of proportional selection,

$$\Pr(\text{Sel}(P^t) = i) := \frac{f(x^{it})}{\sum_{j=1}^{\lambda} f(x^{jt})}, \quad (2)$$

if $\sum_{j=1}^{\lambda} f(x^{jt}) > 0$; otherwise the index of the parent individual is chosen uniformly at random.

Canonical Genetic Algorithm proposed in [17] corresponds to the GA outline with $r = 2$, where all individuals of the initial population are chosen independently and uniformly from \mathcal{X} . This GA uses the proportional selection, a *single-point crossover* Cross^* and a *bitwise mutation* Mut^* . The last two operators work as follows.

The single-point crossover computes $(x', y') = \text{Cross}^*(x, y)$ for two input genotypes $x = (x_1, \dots, x_n)$, $y = (y_1, \dots, y_n)$, so that with a given probability p_c ,

$$x' = (x_1, \dots, x_{\chi}, y_{\chi+1}, \dots, y_n), \quad y' = (y_1, \dots, y_{\chi}, x_{\chi+1}, \dots, x_n),$$

where the random position χ is chosen uniformly from 1 to $n-1$. With probability $1 - p_c$ both parent individuals are copied without any changes, i.e. $x' = x$, $y' = y$.

The bitwise mutation Mut^* computes a genotype $x' = \text{Mut}^*(x)$, where independently of other bits, each bit x'_i , $i \in [n]$, is assigned a value $1 - x_i$ with probability p_m and with probability $1 - p_m$ it keeps the value x_i . The tunable parameter p_m is also called the *mutation rate*. Choosing the mutation rate, many authors assume $p_m = 1/n$.

Another well-known operator of *point mutation* with a given probability p_m modifies one randomly chosen bit, otherwise (with probability $1 - p_m$), the given genotype remains unchanged.

The following condition holds for many well-known crossover operators: there exists a positive constant ε_0 which does not depend on the problem instance, such that the output of crossover $(x', y') = \text{Cross}(x, y)$ satisfies the inequality

$$\varepsilon_0 \leq \Pr\left(\max\{f(x'), f(y')\} \geq \max\{f(x), f(y)\}\right). \quad (3)$$

for any $x, y \in \mathcal{X}$. Condition (3) suggests that the fitness of at least one of the genotypes resulting from crossover $(x', y') = \text{Cross}(x, y)$ is not lower than the fitness of the parents $x, y \in \mathcal{X}$ with probability at least ε_0 . This condition is fulfilled for the single-point crossover with $\varepsilon_0 = 1 - p_c$, if $p_c < 1$ is a constant. In the case of crossover operator with a single output genotype $x' = \text{Cross}(x, y)$, the analogous condition is as follows

$$\varepsilon_0 \leq \Pr\left(f(x') \geq \max\{f(x), f(y)\}\right). \quad (4)$$

Condition (4) is also satisfied with $\varepsilon_0 = 1$ for the optimized crossover operators, where at least one of the two offspring is computed as a solution to optimal recombination problem (see e.g., [1, 5, 15]). It was shown in [10] that for some well-known crossover operators and simple fitness functions condition (4) holds with $\varepsilon_0 = 1/2$.

2. THE MAIN RESULT

In this section, we give a generalization of Non-Elitist Genetic Algorithm analysis, carried out in [13], adapting it to different selection operators and making it applicable to the GAs with multistart, which allows us to deal with both feasible and infeasible solutions.

Suppose that for some m there is an ordered partition of \mathcal{X} into subsets A_0, \dots, A_{m+1} , called *levels* [10]. Level A_0 may be an empty set. Level A_{m+1} will be the target level in subsequent analysis. The target level may be chosen as the set of solutions with maximal fitness or the set of local optima, or the set of ρ -approximation solutions for some approximation factor $\rho > 1$ (a feasible solution y to a maximization problem is called ρ -approximation solution if it satisfies the inequality $F^*/F(y) \leq \rho$). A well-known example of partition is the *canonical* partition, where $A_0 = \emptyset$ and each level A_j , $j \in [m+1]$ regroups solutions having the same fitness value (see e.g. [11, 30]). In what follows, level A_0 may be used to encompass the set of infeasible solutions.

In this paper, we will often use values which are independent of an instance of problem (1) and of a levels partition, but completely determined by the GA outline and its operators. Such values will be called constants. The same applies to the constants in $O(\cdot)$ notation. It will be convenient to use the symbol $H_j := \cup_{i=j}^{m+1} A_i$ for the union of all levels starting from level j , $j \in [m+1]$. The symbol e in what follows denotes the base of the natural logarithm.

Extending the notation from [10, 25], we will define the *selective pressure* $\beta(0, P)$ of a selection operator $\text{Sel}(P)$ as the probability of selecting an individual that belongs to the highest level occupied by the individuals of P .

Theorem 2.1. *Given a partition A_0, \dots, A_{m+1} of \mathcal{X} , let there exist parameters s_*, p_1, ε and β_0 from $(0, 1]$, such that for any $j \in [m]$:*

$$(C1) \quad \Pr(\text{Mut}(x) \in H_{j+1}) \geq s_*, \text{ for any } x \in A_j,$$

$$(C2) \quad \Pr(x^{i,0} \in H_1 \text{ for some } i \in [\lambda]) \geq p_1,$$

$$(C3) \quad \beta(0, P) \geq \beta_0 \text{ for any } P \in (\mathcal{X} \setminus A_{m+1})^\lambda,$$

$$(C4) \quad \lambda \geq \frac{2(1+\ln m)}{s_* \varepsilon \beta_0 (2-\beta_0)},$$

$$(C5) \quad \text{for any } (x, y) \in (H_j \times \mathcal{X}) \cup (\mathcal{X} \times H_j)$$

$$\varepsilon \leq \begin{cases} \Pr(\text{Cross}(x, y) \in H_j), & \text{in case of } r = 1, \\ \Pr(\text{Cross}(x, y) \in (H_j \times \mathcal{X}) \cup (\mathcal{X} \times H_j)), & \text{in case of } r = 2. \end{cases}$$

Then with probability not less than p_1/e at least one of the populations P^0, P^1, \dots, P^m contains an individual from A_{m+1} .

Let us informally describe the conditions of the theorem. Condition (C1) requires that for each level j , there is a lower bound s_* on the “upgrade” probability from level j . Condition (C2) ensures that at least one individual of the initial population is above level 0 with probability not less than p_1 . Condition (C3) requires that the selective pressure induced by the selection mechanism is sufficiently high. Condition (C4) requires that the population size λ is sufficiently large. Condition (C5) is a level-based analog of inequalities (3) and (4). This condition follows from (3) or (4) with $\varepsilon = \varepsilon_0$ in the case of the canonical partition.

Proof of Theorem 2.1. For any $t = 0, 1, \dots$ let the event E_i^{t+1} , $i \in [\lambda/2]$, consist in fulfilling of the following three conditions when the i -th pair of offspring is computed:

1. At least one of the two parents is chosen from the highest level A_j to which the individuals of population P^t belong.
2. When the crossover operator is applied, at least one of its outputs belongs to H_j . W.l.o.g. we assume that this output is x .
3. The mutation operator applied to x produces a genotype in H_{j+1} .

Let p denote the probability of the union of events E_i^{t+1} , $i \in [\lambda/2]$. In what follows, we will construct a lower bound $\ell \leq p$, which holds for any population P^t . According to the outline of GA, $\Pr(E_1^{t+1}) = \dots = \Pr(E_{\lambda/2}^{t+1})$. Let us denote this probability by q . Note that q is bounded from below by $s_*\varepsilon(1 - (1 - \beta_0)^2) = s_*\varepsilon\beta_0(2 - \beta_0)$. Given a population P^t , the events E_j^{t+1} , $j = 1, \dots, \lambda/2$, are independent, so $p \geq 1 - (1 - q)^{\lambda/2} \geq 1 - e^{-q\lambda/2}$. In what follows we shall use the fact that condition (C4) implies

$$\lambda \geq \frac{2}{s_*\varepsilon\beta_0(2 - \beta_0)} \geq 2/q. \tag{5}$$

To bound probability p from below, let us first note that for any $z \in [0, 1]$ holds

$$1 - \frac{z}{e} \geq e^{-z}. \tag{6}$$

Assume $z = e^{-q\lambda/2+1}$. Then in view of inequality (5), $z \leq 1$, and consequently, we get

$$p \geq \exp\{-e^{-q\lambda/2}\} \geq \exp\{-e^{1-s_*\varepsilon\beta_0(2-\beta_0)\lambda/2}\}. \tag{7}$$

We will use the right-hand side expression of (7) as the lower bound ℓ for p .

For any $t = 1, 2, \dots$ let us define the event $\mathcal{E}_t := E_1^t + \dots + E_{\lambda/2}^t$. Note that event \mathcal{E}_t captures some of the possible scenarios of “upgrading” the best individuals of the current population to the next level. Besides that, let \mathcal{E}_0 denote the event that $x^{i,0} \in H_1$ for some $i \in [\lambda]$. Then the probability to reach the target level A_{m+1} in a series of at most m iterations is lower bounded by $\Pr(\mathcal{E}_0 \& \dots \& \mathcal{E}_m)$ and

$$\Pr(\mathcal{E}_0 \& \dots \& \mathcal{E}_m) = \Pr(\mathcal{E}_0) \prod_{t=0}^{m-1} \Pr(\mathcal{E}_{t+1} | \mathcal{E}_0 \& \dots \& \mathcal{E}_t) \geq p_1 \ell^m. \tag{8}$$

in view of condition (C2). Now using condition (C4), we get:

$$\ell^m = \exp\left\{-me^{1-s, \varepsilon \beta_0(2-\beta_0)\lambda/2}\right\} \geq \exp\left\{-me^{-\ln m}\right\} = 1/e.$$

Q.E.D.

An event of *downgrading mutation* of a genotype x may be defined in terms of levels partition as $\text{Mut}(x) \notin H_j$, where j is the level the individual x belongs to. Unlike the results from [10, 11], Theorem 2.1 is applicable to the GAs where the probability of non-downgrading mutation may tend to zero as the problem size grows. Examples of such operators may be found in highly competitive GAs for Maximum Independent Set Problem and Set Covering Problem [1, 7] and many other GAs in the literature on operations research. Note that in case $|A_{m+1}| = 1$, given an optimal genotype $x \in A_{m+1}$, the bitwise mutation with a constant mutation rate (as used in [1]) causes non-downgrading mutations only with probability $(1 - p_m)^n = o(1)$ and the mutation operator that inverts m_f bits, where $m_f > 0$ is a given parameter [7], has zero probability of non-downgrading mutations.

3. LOWER BOUNDS FOR SELECTION PRESSURE

The following two propositions may be applied to check condition (C3) in Theorem 2.1.

Proposition 3.1. *Let levels A_1, \dots, A_m satisfy the monotonicity condition*

$$f(x) < f(y) \text{ for any } x \in A_{j-1}, y \in A_j, j = 2, \dots, m. \quad (9)$$

Then

(i) *k -tournament selection with $k \geq \alpha\lambda$, where the constant $\alpha > 0$, satisfies condition (C3) with $\beta_0 = 1 - e^{-\alpha}$.*

(ii) *(μ, λ) -selection with a constant parameter $\mu \leq \lambda$ satisfies condition (C3) where $\beta_0 = 1/\mu$.*

Proof. In the case of k -tournament selection $\beta(0, P) \geq 1 - (1 - 1/\lambda)^k$ and $(1 - 1/\lambda)^k \leq (1 - 1/\lambda)^{\alpha\lambda} \leq e^{-\alpha}$, so part (i) follows. Part (ii) follows from the definition of (μ, λ) -selection immediately. *Q.E.D.*

The operator of proportionate selection does not have a tunable parameter that allows to set its selection pressure. However such a parameter (let it be ν) may be introduced into the fitness function by assuming that $f(x) = F(x)^\nu$ for any $x \in \text{Sol}$. The proof of the following proposition is similar to that of Lemma 8 in [25]. Here and below \mathbb{Z}_+ denotes the set of non-negative integers.

Proposition 3.2. *Let the levels A_1, \dots, A_m satisfy the monotonicity condition (9), $F : \text{Sol} \rightarrow \mathbb{Z}_+$ and the fitness function is of the form $f(x) = F(x)^\nu$, where $\nu > \max(0, \ln(\alpha\lambda)F^\alpha)$ for some $\alpha > 0$. Then the proportional selection satisfies condition (C3) with $\beta_0 = 1/(1 + \alpha^{-1})$.*

Proof. Let F_0^v be the maximal fitness value in population P and let k denote the number of individuals in P with fitness F_0^v . The probability to choose one of the fittest individuals is lower bounded as follows

$$\beta(0, P) \geq \frac{kF_0^v}{(\lambda - k)(F_0 - 1)^v + kF_0^v} \geq \frac{k}{\lambda(1 - 1/F_0)^v + k} \geq \frac{k}{1/\alpha + k} \geq \frac{1}{1/\alpha + 1},$$

since $(1 - 1/F_0)^v \leq (1 - 1/F^*)^v \leq e^{-v/F^*} \leq 1/(\alpha\lambda)$. *Q.E.D.*

Proposition 3.2 requires the fitness function to scale very fast as the objective function grows. Scaling of objective function might be unavoidable in the case of proportional selection. Even for the simple benchmark fitness function $\text{ONEMAX} := \sum_{i=1}^n x_i$, P. Oliveto and C. Witt show [28] that in the case of proportional selection, GA with high probability makes exponential number of iterations until the optimum is visited. The need for scaling the fitness function is also acknowledged in practical use of Canonical GA (see e.g. [17], where a dynamical mechanism for fitness scaling was proposed).

4. UPPER BOUNDS ON EXPECTED HITTING TIME OF TARGET SUBSET

Let T denote the random variable, equal to the number of tentative solutions evaluated until some element of the current population is sampled from A_{m+1} for the first time. In the case when A_{m+1} is the set of optimal solutions, T is usually called the *runtime* of an evolutionary algorithm.

Corollary 4.1. *Suppose that conditions (C1)-(C5) of Theorem 2.1 hold and $A_0 = \emptyset$. Then, for the GA we have $E[T] \leq em\lambda$.*

Proof. Consider a sequence of series of the GA iterations, where the length of each series is m iterations. Suppose, D_i , $i = 1, 2, \dots$, denotes an event of absence of solutions from A_{m+1} in the population throughout the i -th series. The probability of each event D_i , $i = 1, 2, \dots$, is at most $1 - 1/e$ according to Theorem 2.1. Analogously to bound (8), we obtain the inequality $\Pr(D_1 \& \dots \& D_i) \leq (1 - 1/e)^i$.

Let Y denote the random variable equal to the number of the first run when a solution from A_{m+1} was obtained. By the properties of expectation (see e.g. [16]),

$$E[Y] = \sum_{i=0}^{\infty} \Pr(Y > i) = 1 + \sum_{i=1}^{\infty} \Pr(D_1 \& \dots \& D_i) \leq 1 + \sum_{i=1}^{\infty} (1 - 1/e)^i = e.$$

Consequently, the average number of iterations until an element of the target subset is first obtained is at most em . *Q.E.D.*

Assuming $\lambda = \left\lceil \frac{2(1+\ln(m))}{s_* \varepsilon \beta_0 (2-\beta_0)} \right\rceil$ and constant β_0 and ε , Corollary 4.1 implies $E[T] \leq cm \ln(m)/s_*$, where $c > 0$ is a constant. In the special case where $r = 1$ and the probability of non-downgrading mutation $\Pr(\text{Mut}(x) \in H_j \mid x \in A_j)$, $j \in [m]$ is lower bounded by a positive constant, the result from [10] gives an upper bound

$E[T] \leq c'm (\ln(m/s_*) \ln \ln(m/s_*) + 1/s_*)$ with some positive constant c' . The latter bound is less demanding to selection pressure and it is asymptotically tighter than the bound $E[T] \leq cm \ln(m)/s_*$ e.g. when $s_* \leq 1/m$.

Note that the assumption $A_0 = \emptyset$ in Corollary 4.1 can not be dismissed. Indeed, suppose that $A_0 \neq \emptyset$, and consider a GA where the mutation operator has the following properties. On the one hand, it never outputs an offspring in H_1 , given an input from A_0 . On the other hand, given a genotype $x \in H_1$, the result of mutation is in A_0 with a probability at least c , where $c > 0$. Finally, assume that the initialization procedure produces no genotypes from A_{m+1} in population P^0 and the crossover makes no changes to the parent genotypes. Now all conditions of Corollary 4.1 can be satisfied but with a positive probability of at least c^λ the whole population P^1 consists of solutions from A_0 , and subject to this event all populations P^1, P^2, \dots contain no solutions from H_1 . Therefore, $E[T]$ is unbounded.

As an example of the usage of Corollary 4.1 we consider the GA with tournament selection applied to the family of unconstrained optimization problems with objective function `LEADINGONES`, which is frequently used in the analysis of evolutionary algorithms. The objective function `LEADINGONES` : $\{0, 1\}^n \rightarrow \mathbb{Z}_+$ is defined as

$$\text{LEADINGONES}(x) = \sum_{i=1}^n \prod_{j=1}^i x_j$$

i.e. the optimal solution is $x^* = (1, \dots, 1)$.

Let us use the canonical levels partition: $A_j = \{x \mid F(x) = j - 1\}$, $j \in [n + 1]$, $m = n$. Assume that the bitwise mutation operator has the mutation rate $p_m = 1/n$. To move from level A_j to level A_{j+1} under mutation, it suffices to modify the first zero bit and not to modify the rest of the bits. So we can use $s_* = (1/n)(1 - 1/n)^{n-1} = \Omega(1/n)$. Suppose that in the single-point crossover $p_c = 1$. Then in the case of `LEADINGONES`, as it was shown in [10], the constant $\epsilon = 1/2$ satisfies condition (C5). Assuming the tournament size $k = \Theta(\lambda)$, Proposition 3.1 ensures satisfaction of condition (C3) with a positive constant β_0 . Application of Corollary 4.1 to the GA with $r = 1$ or $r = 2$ and $\lambda = \Theta(n \ln(n))$, satisfying (C4), gives the upper bound $E[T] = O(n^2 \ln(n))$.

The GA runtime analysis from [10] with $r = 1$ implies that $E[T] = O(n^2 + n\lambda \log \lambda)$, provided that $\lambda \geq C_1 \log n$ and $k \geq C_2$ for some specific constants $C_1, C_2 > 0$. This yields the runtime bound $E[T] = O(n^2)$ in the case of $\lambda = \Theta(\log n)$, but in the case of $\lambda = \Theta(n \log n)$ the analysis from [10] yields a greater runtime bound $E[T] = O(n^2 \ln(n)^2)$. Thus for relatively small population sizes the runtime bound from [10] is preferable, while the new bound is preferable for sufficiently large population sizes.

Analogously to Corollary 4.1 we obtain

Corollary 4.2. *Let the GA with multistart use the termination condition with $t_{\max} = m$. Then $E[T] \leq \epsilon m \lambda / p_1$ holds under conditions (C1)-(C5).*

As an illustrative example for Corollary 4.2, we consider Canonical GA on the family of instances of Set Cover Problem proposed by E. Balas in [4]. In general, the set cover problem (SCP) is formulated as follows. Given: $M = \{1, \dots, m\}$ and a set of subsets $M_j \subseteq M, j \in [n]$. A subset $J \subseteq [n]$ is called a *cover* if $\cup_{j \in J} M_j = M$. The goal is to find a cover of minimum cardinality. In what follows we denote by N_i the set of indices of the subsets that cover an element i , i. e. $N_i = \{j : i \in M_j\}$ for any i .

In the family $\mathcal{B}(n, p)$ of SCPs introduced by E. Balas in [4], it is assumed that $m = C_n^{p-1}$ and the set $\{N_1, N_2, \dots, N_m\}$ consists of all $(n - p + 1)$ -element subsets of $[n]$. Thus $J \subseteq [n]$ is an optimal cover iff $|J| = p$.

Family $\mathcal{B}(n, p)$ is known to have a large fractional cover [4], which implies that these SCPs are likely to be hard for integer programming methods. In particular, it was shown in [34] that problems from this class are hard to solve by the L -class enumeration method [22]. When n is even and $p = n/2$, the L -class enumeration method needs an exponential number of iterations in n . In what follows, we analyze GA in this special case.

In the binary encoding of solutions we assume that each bit $x_j \in \{0, 1\}, j \in [n]$, indicates whether j belongs to the encoded set or not, i.e. $J(x) := \{j \in [n] : x_j = 1\}$. If $J(x)$ is a cover, then we assume $F(x) = n - |J(x)| + 1$, otherwise, we put $F(x) = 0$ as a penalty.

Consider Canonical GA with multistart and scaled fitness function $f(x) = F(x)^v$, the termination condition where $t_{\max} = n/2$, a constant parameter $p_c < 1$, and the mutation rate $p_m = 1/n$.

Assume that A_0 is the set of all infeasible solutions and the rest of the levels A_1, \dots, A_{m+1} are defined according to the canonical partition on Sol, where $m = n/2$. In the case of $p = n/2$, with probability $1/2$, a random individual of P^0 is feasible and there exists a constant $p_1 > 0$ satisfying condition (C2). The constant $\epsilon = 1 - p_c$ satisfies condition (C5). The probability that, under mutation, a genotype from level A_j produces an element of $H_{j+1}, j \in [m]$ in the case of problems of family $\mathcal{B}(n, p)$ is lower bounded by $s_* = \Omega(1)$. Choosing $v > \ln(\alpha\lambda)n/2$ with constant $\alpha > 0$ we ensure condition (C3), according to Proposition 3.2. Finally, appropriate $\lambda = \Theta(\ln(n))$, satisfies condition (C4). Therefore, Corollary 4.2 implies that an optimal solution is attained for the first time after $E[T] = O(n \ln(n))$ tentative solutions in expectation.

5. APPLICATIONS TO LOCAL SEARCH PROBLEMS

In this section, GAs are compared to the local search method. In order to keep track of running times w.r.t. the length of problem instance encoding, here the combinatorial optimization problems are viewed under the technical assumptions of the class of NP optimization problems (see e.g. [3]). Let $\{0, 1\}^*$ denote the set of all strings with symbols from $\{0, 1\}$ and the arbitrary string length. For a string $S \in \{0, 1\}^*$, the symbol $|S|$ will denote its length. In what follows, \mathbb{N} denotes the set of positive integers and given a string $S \in \{0, 1\}^*$, the symbol $|S|$ denotes

the length of the string S . To denote the set of polynomially bounded functions we define Poly as the class of functions from $\{0, 1\}^*$ to \mathbb{N} bounded above by a polynomial in $|I|$, where $I \in \{0, 1\}^*$.

Definition 5.1. An NP optimization problem Π is a triple $\Pi = (\text{Inst}, \text{Sol}(I), F_I)$, where $\text{Inst} \subseteq \{0, 1\}^*$ is the set of instances of Π and:

1. The relation $I \in \text{Inst}$ is computable in polynomial time.
2. Given an instance $I \in \text{Inst}$, $\text{Sol}(I) \subseteq \{0, 1\}^{n(I)}$ is the set of feasible solutions of I , where $n(I)$ stands for the dimension of the search space $\mathcal{X}_I := \{0, 1\}^{n(I)}$. Given $I \in \text{Inst}$ and $x \in \{0, 1\}^{n(I)}$, the decision whether $x \in \text{Sol}(I)$ may be done in polynomial time, and $n(\cdot) \in \text{Poly}$.
3. Given an instance $I \in \text{Inst}$, $F_I : \text{Sol}(I) \rightarrow \mathbb{N}$ is the objective function (computable in polynomial time) to be maximized if Π is an NP maximization problem or to be minimized if Π is an NP minimization problem.

The symbol of problem instance I may often be skipped in the notation, when it is clear what instance I is meant. A combinatorial optimization problem $\Pi = (\text{Inst}, \text{Sol}(I), F_I)$ is called polynomially bounded, if there exists a polynomial in $|I|$, which bounds the objective values $F_I(x)$, $x \in \text{Sol}(I)$ from above.

Let a neighborhood $\mathcal{N}(y) \subseteq \text{Sol}$ be defined for every $y \in \text{Sol}$. The mapping $\mathcal{N} : \text{Sol} \rightarrow 2^{\text{Sol}}$ is called the *neighborhood mapping*. The family $\{\mathcal{N}(y) : y \in \text{Sol}\}$ is called the *neighborhoods system*. One of the standard neighborhoods systems on $\text{Sol} = \{0, 1\}^n$ is *Hamming neighborhoods system*: $\mathcal{N}(y) = \{x \mid d(x, y) \leq R\}$, $y \in \text{Sol}$, where the radius R is a constant and $d(\cdot, \cdot)$ denotes the Hamming distance. If the inequality $F(y) \leq F(x)$ holds for all neighbors $y \in \mathcal{N}(x)$ of a solution $x \in \text{Sol}$, then x is called a local optimum w.r.t. \mathcal{N} . In what follows, the set of all local optima is denoted by \mathcal{LO} .

A local search method starts from some feasible solution y_0 . Each iteration of the algorithm consists in moving from the current solution to a new solution in its neighborhood, such that the value of objective function is increased. The way to choose an improving neighbor, if there are several of them, will not matter in this paper. The algorithm continues until a local optimum is reached.

Suppose that some neighborhood system \mathcal{N} is defined for problem (1) and s is the lower bound for probability that the mutation operator transforms a given solution x into a specific neighbor $y \in \mathcal{N}(x)$, i.e.

$$s \leq \Pr(\text{Mut}(x) = y), \quad x \in \text{Sol}, \quad y \in \mathcal{N}(x). \quad (10)$$

Many well-known combinatorial optimization problems, such as Maximum Satisfiability Problem, Maximum Cut Problem, and Ising Spin Glass Model [6] have a set of feasible solutions equal to the whole search space $\text{Sol} \equiv \mathcal{X}$. The following two corollaries apply to the problems with such a property.

Let m be the number of different values of the fitness function $f_1 < \dots < f_m$ on $\mathcal{X} \setminus \mathcal{LO}$, i.e. $m = |\{g : g = f(x), x \in \mathcal{X} \setminus \mathcal{LO}\}|$. Then, starting from any initial solution, the local search method attains a local optimum within at most m iterations. Let us use a modification of the canonical levels partition, grouping all

local optima into the target subset A_{m+1} :

$$A_j := \{x \in \mathcal{X} | f(x) = f_j\} \setminus \mathcal{LO}, \quad j \in [m], \quad (11)$$

$$A_{m+1} := \mathcal{LO}. \quad (12)$$

Application of Corollary 4.1 and Proposition 3.1 with levels partition (11), (12) gives

Corollary 5.2. *Suppose that $\text{Sol} \equiv \mathcal{X}$, a constant $\epsilon_0 > 0$ satisfies inequality (3) or (4), $s > 0$ satisfies inequality (10) and the GA uses a k -tournament selection with $k > \alpha\lambda$ or (μ, λ) -selection, where α and μ are constants. Then, there exists a constant $c > 0$ such that a GA with population size $\lambda \geq c \ln(m) / s$ first visits a local optimum of problem (1) after at most $e\lambda m$ tentative solutions in expectation.*

Therefore, with an appropriate population size, e.g. $\lambda = \lceil c \ln(m) / s \rceil$, under conditions of Corollary 5.2, a local optimum of problem (1) is visited for the first time after evaluation of at most $em \ln(m) / s$ tentative solutions on average. This fact in the special case of the tournament selection and $r = 2$ was proved in [13].

In order to consider bitwise mutation in more detail, we will use the following definition from [2]. A neighborhood mapping \mathcal{N} is called K -bounded, if for any $y \in \text{Sol}$ and $x \in \mathcal{N}(y)$ holds $d(x, y) \leq K$, where K is a constant.

The bitwise mutation operator Mut^* outputs a string x , given a string y , with probability $p_m^{d(x,y)} (1 - p_m)^{n-d(x,y)}$. Note that probability $p_m^j (1 - p_m)^{n-j}$, as a function of p_m , $p_m \in [0, 1]$, attains its minimum at $p_m = j/n$. The following proposition from [13] gives a lower bound for the probability $\Pr\{\text{Mut}^*(y) = x\}$, which is valid for any $x \in \mathcal{N}(y)$, assuming that $p_m = K/n$. We reproduce this proposition here with a proof for the sake of completeness.

Proposition 5.3. *Suppose that the neighborhood mapping \mathcal{N} is K -bounded, $K \leq n/2$ and $p_m = K/n$. Then, for any $y \in \text{Sol}$ and any $x \in \mathcal{N}(y)$ holds $\Pr\{\text{Mut}^*(y) = x\} \geq (K/en)^K$.*

Proof. For any $y \in \text{Sol}$ and $x \in \mathcal{N}(y)$ holds

$$\Pr\{\text{Mut}^*(y) = x\} = \left(\frac{K}{n}\right)^{d(x,y)} \left(1 - \frac{K}{n}\right)^{n-d(x,y)} \geq \left(\frac{K}{n}\right)^K \left(1 - \frac{K}{n}\right)^{n-K},$$

since $p_m = K/n \leq 1/2$. Now $\frac{\partial}{\partial n} (1 - K/n)^{n-K} < 0$ for $n > K$, and $(1 - K/n)^{n-K} \rightarrow 1/e^K$ as $n \rightarrow \infty$. Therefore $(1 - K/n)^{n-K} \geq 1/e^K$. Q.E.D.

Application of Corollary 4.1 and Propositions 3.2 and 5.3 to Canonical GA yields

Corollary 5.4. *Suppose that $\text{Sol} \equiv \mathcal{X}$, $F : \text{Sol} \rightarrow \mathbb{Z}_+$, a neighborhood mapping \mathcal{N} is K -bounded, $p_c < 1$ is a constant, $p_m = K/n$ and the fitness function has a form $f(x) = F(x)^v$, where $v > \ln(\alpha\lambda)F^*$. Then, there exists such constant $c > 0$ that Canonical GA with $\lambda \geq c \ln(F^*) / n^K$ visits a local optimum to problem (1) for the first time after at most $eF^*\lambda$ tentative solutions in expectation.*

Corollary 5.4 implies that in the case of polynomially bounded unconstrained NP optimization problem, Canonical GA given appropriate choice of parameters finds a local optimum in Hamming neighborhoods system within expected polynomial time.

Let us consider a GA with multistart applied to an NP optimization problem, i.e. in general Sol may be a proper subset of X . Corollary 4.2 and Proposition 3.1 yield

Corollary 5.5. *Suppose that inequality (3) or (4) holds for some constant $\epsilon_0 > 0$, bound s satisfies inequality (10) and condition (C2) is satisfied for some constant $p_1 > 0$. Besides, assume that GA with multistart uses a termination condition $t_{\max} = m$ and one of the following selection operators:*

- *k-tournament selection with $k > \alpha\lambda$ where $\alpha > 0$ is a constant or*
- *(μ, λ) -selection with a constant μ or*
- *proportional selection in the case of $F : \text{Sol} \rightarrow \mathbb{Z}_+$ and the fitness function is of the form $f(x) = F(x)^\nu$ where $\nu > \ln(\alpha\lambda)F^*$ and $\alpha > 0$ is a constant.*

Then, there exists such positive constant c that with population size $\lambda \geq c \ln(m)/s$ a local optimum is first reached by the GA with multistart after evaluation of at most $em\lambda$ tentative solutions in expectation.

Corollary 5.5 is formulated for the GA with multistart rather than single-run GA because, in general, this result does not hold for the single-run GA. Indeed, suppose $\text{Sol} \neq X$ and consider a GA where the mutation operator has the following properties. On one hand Mut never outputs a feasible offspring, given an infeasible input. On the other hand, given a feasible genotype x , Mut(x) is infeasible with a *positive* probability, lower bounded by a constant $\epsilon \in (0, 1]$. Finally, assume that the initialization procedure for population P^0 produces only feasible solutions, but none of them is locally optimal. Now all conditions of Corollary 5.5 are satisfied, but with a positive probability of at least ϵ^λ the whole population P^1 consists of infeasible solutions, and subject to this event all populations P^1, P^2, \dots are infeasible. Therefore, if the GA is run without restarts, the expected number of iterations until the first improvement of the best found solution is unbounded, and the expected hitting time of a local optimum is unbounded as well. The need for restarting the GA was overlooked in the first publication of a result analogous to Corollary 5.5 in [13]. The GA considered in [13] should be replaced by the GA with multistart using the termination condition $t_{\max} = m$ to make the results in [13] correct in the case of $\text{Sol} \neq X$. This correction is implemented in [14].

Corollary 5.5 may be used to estimate the capacities of GAs to find efficiently the solutions with guaranteed approximation ratio if all local optima of a problem have a known approximation ratio.

Definition 5.6. [2] *A polynomially bounded NP optimization problem Π belongs to the class of Guaranteed Local Optima (GLO) problems, if the following two conditions hold:*

- 1) At least one feasible solution $y_1 \in \text{Sol}$ is efficiently computable for every instance $I \in \text{Inst}$;
- 2) A K -bounded neighborhood mapping \mathcal{N}_1 exists, such that for every instance I , any local optimum of I with respect to \mathcal{N}_1 has a constant guaranteed approximation ratio.

The class GLO contains such well-known NP optimization problems as the Maximum Satisfiability and the Maximum Cut problems, besides that, on graphs with bounded vertex degree, the Independent Set problem, the Dominating Set problem, and the Vertex Cover problem also belong to GLO [2].

If a problem Π belongs to GLO and n is sufficiently large, then in view of Proposition 5.3, for any $x \in \text{Sol}$ and $y \in \mathcal{N}(x)$, the bitwise mutation operator with $p_m = K/n$ satisfies the condition $\Pr\{\text{Mut}^*(x) = y\}^{-1} \in \text{Poly}$. Therefore, Corollary 5.5 implies the following

Corollary 5.7. *If $\Pi \in \text{GLO}$ and GA with multistart uses*

1. a polynomial-time initialization procedure that produces a population with at least one feasible solution with probability p_1 such that $1/p_1 \in \text{Poly}$,
2. the tournament selection or the (μ, λ) -selection,
3. a crossover operator satisfying (3) or (4) for some positive constant ε_0 and
4. the bitwise mutation,

then given suitable values of parameters λ, p_m and k or μ , GA with multistart visits a solution with a constant guaranteed approximation ratio within expected polynomially bounded time.

6. CONCLUSIONS

The obtained bounds on the first hitting times for sets of global or local optima are extending some previously known bounds of such kind for genetic algorithms and may be applied to standard benchmarks and genetic algorithms as, well to some state-of-the-art genetic algorithms for combinatorial optimization problems. Considering the selection operators with very high selection pressure, we obtain the bounds that apply even in the cases where the probability of non-downgrading is not lower-bounded by a positive constant.

The obtained results imply that if a problem is polynomially bounded and the feasible solutions are present in the initial population, then a local optimum in a Hamming neighborhood system is computable in expected polynomial time by standard GAs with multistart. Besides, given suitable parameters and initialization procedure, a non-elitist GA with tournament selection or (μ, λ) -selection approximates any problem from GLO class within a constant ratio in polynomial time in expectation.

If an NP optimization problem is polynomially bounded, then Canonical Genetic Algorithm with appropriate parameters tuning and fitness scaling finds a local optimum within expected polynomial time for many standard neighborhood systems.

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