Level-based Analysis of Genetic Algorithms for Combinatorial Optimization

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Abstract

The paper is devoted to upper bounds on run-time of Non-Elitist Genetic Algorithms until some target subset of solutions is visited for the first time. In particular, we consider the sets of optimal solutions and the sets of local optima as the target subsets. Previously known upper bounds are improved by means of drift analysis. Finally, we propose conditions ensuring that a Non-Elitist Genetic Algorithm efficiently finds approximate solutions with constant approximation ratio on the class of combinatorial optimization problems with guaranteed local optima (GLO).

Keywords: Runtime Analysis, Fitness Level, Genetic Algorithm, Local Search, Guaranteed Local Optima

Introduction

The genetic algorithm (GA) proposed by J. Holland [16] is a randomized heuristic search method, based on analogy with the genetic mechanisms observed in nature and employing a population of tentative solutions. Different modifications of GA are widely used in the areas of operations research, pattern recognition, artificial intelligence etc. (see e.g. [23, 27]). Despite of numerous experimental investigations of these algorithms, their theoretical analysis is still at an early stage [7].

Efficiency of a GA in application to a combinatorial optimization problem may be estimated in terms of expected computation time until an optimal
solution or an acceptable approximation solution is visited for the first time. It is very unlikely, however, that there exists a randomized algorithm finding a globally optimal solution for an NP-hard optimization problem on average in polynomially bounded time. This would contradict the well-known hypothesis NP $\neq$ RP which is in use for several decades [18].

The main results of this paper are obtained through comparison of genetic algorithms to local search, which is motivated by the fact that the GAs are often considered to be good at finding local optima (see e.g. [1, 19, 22]).

Here and below we assume that the randomness is generated only by the randomized operators of selection, crossover, mutation and random initialization of population within the GA (the input data is deterministic). A function of input data is called \textit{polynomially bounded}, if there exists a polynomial in the length of the problem input, which bounds the function from above. The terms \textit{efficient algorithm} or \textit{polynomial-time algorithm} are used for an algorithm with polynomially bonded running time.

1 \hspace{1em} \textbf{Combinatorial Optimization Problems and Genetic Algorithms}

\textbf{NP Optimization Problems} \hspace{1em} In this paper, the combinatorial optimization problems are viewed under the technical assumptions of the class of NP optimization problems (see e.g. [2]). Let $\{0, 1\}^*$ denote the set of all strings with symbols from $\{0, 1\}$ and 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 $I \in \{0, 1\}^*$.

\textbf{Definition 1} An NP optimization problem $\Pi$ is a triple $\Pi = (\text{Inst}, \text{Sol}(I), F_I)$, where $\text{Inst} \subseteq \{0, 1\}^*$ is the set of instances of $\Pi$ 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 $X_I := \{0, 1\}^{n(I)}$. 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 $I \in \text{Inst}$, $F_I : \text{Sol}(I) \to \mathbb{N}$ is the objective function (computable in polynomial time) to be maximized if $\Pi$ is an NP maximization problem or to be minimized if $\Pi$ is an NP minimization problem.

Without loss of generality we will consider only the maximization problems. The results will hold for the minimization problems as well. The symbol of problem instance $I$ may often be skipped in the notation, when it is clear what instance $I$ is meant.

**Definition 2** A combinatorial optimization problem $\Pi = (\text{Inst}, \text{Sol}(I), F_I)$ is polynomially bounded, if there exists a polynomial in $|I|$, which bounds the objective values $F_I(x), x \in \text{Sol}(I)$ from above.

**Neighborhoods and local optima** Let a neighborhood $\mathcal{N}_I(y) \subseteq \text{Sol}(I)$ be defined for every $y \in \text{Sol}(I)$. The mapping $\mathcal{N}_I : \text{Sol}(I) \to 2^{\text{Sol}(I)}$ is called the neighborhood mapping. Following [3], we assume this mapping to be efficiently computable, i.e. the set $\mathcal{N}_I(x)$ may be enumerated in polynomial time.

**Definition 3** If the inequality $F_I(y) \leq F_I(x)$ holds for all neighbors $y \in \mathcal{N}_I(x)$ of a solution $x \in \text{Sol}(I)$, then $x$ is called a local optimum w.r.t. the neighborhood mapping $\mathcal{N}_I$.

Suppose $R(\cdot, \cdot)$ is a metric on $\text{Sol}(I)$. The neighborhood mapping

$$\mathcal{N}_I(x) = \{y \mid R(x, y) \leq r\}, \ x \in \text{Sol}(I),$$

is called a neighborhood mapping of radius $r$ defined by metric $R(\cdot, \cdot)$.

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.

**Genetic Algorithms** The Simple GA proposed in [16] has been intensively studied and exploited over four decades. A plenty of variants of GA have been developed since publication of the Simple GA, sharing the basic ideas,
but using different population management strategies, selection, crossover and mutation operators [22].

The GA operates with populations $P^t = (x^{1,t}, \ldots, x^{\lambda,t}), \ t = 0, 1, \ldots$, which consist of $\lambda$ genotypes. In terms of the present paper the genotypes are elements of the search space $\mathcal{X}$.

In a selection operator $\text{Sel} : \mathcal{X}^\lambda \rightarrow \{1, \ldots, \lambda\}$, each parent is independently drawn from the previous population $P^t$ where each individual in $P^t$ 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. Below we assume the following natural form of the fitness function:

- if $x \in \text{Sol}$ then $f(x) = F(x)$;
- if $x \notin \text{Sol}$ then its fitness is defined by some penalty function, such that $f(x) < \min_{y \in \text{Sol}} F(y)$.

In this paper, we consider the tournament selection, $(\mu, \lambda)$-selection and exponential ranking selection (see the details in Section 3 below).

One or two offspring genotypes is created from two parents using the randomized operators of crossover $\text{Cross} : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{X} \times \mathcal{X}$ (two-offspring version) or $\text{Cross} : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{X}$ (single-offspring version) and mutation $\text{Mut} : \mathcal{X} \rightarrow \mathcal{X}$. In general, we assume that $\text{Cross}(x, y)$ and $\text{Mut}(x)$ are efficiently computable randomized routines.

When a population $P^t$ of $\lambda$ offspring is constructed, the GA proceeds to the next iteration $t + 1$. An initial population $P^0$ is generated randomly. One of the ways of initialization consists, e.g. in independent choice of all bits in genotypes.

To simplify the notation below, $GA$ will always denote the non-elitist genetic algorithm with single-offspring crossover based on the following outline.
Algorithm $\mathcal{GA}$

Generate the initial population $P^0$, assign $t := 1$.

While termination condition is not met do:
  
  Iteration $t$.
  
  For $j$ from 1 to $\lambda$ do:
    
    Selection: $i := \text{Sel}(P^{t-1})$, $i' := \text{Sel}(P^{t-1})$.
    
    Crossover: $x := \text{Cross}(x^{i,t-1}, x^{i',t-1})$.
    
    Mutation: $x_{j,t} := \text{Mut}(x)$.
  
  End for.
  
  $t := t + 1$.

End while.

In theoretical analysis of the $\mathcal{GA}$ we will assume that the termination condition is never met. The termination condition, however, may be required to stop a genetic algorithm when a solution of sufficient quality is obtained or the computing time is limited, or because the population is "trapped" in some unpromising area and it is preferable to restart the search (see e.g. [4, 26]).

In what follows, the operators of selection, mutation and single-offspring crossover are associated with the corresponding transition matrices:

- $p_{\text{sel}} : [\lambda] \rightarrow [0, 1]$ represents a selection operator, where $p_{\text{sel}}(i|P_t)$ is the probability of selecting the $i$-th individual from population $P_t$.

- $p_{\text{mut}} : X \times X \rightarrow [0, 1]$, where $p_{\text{mut}}(y|x)$ is the probability of mutating $x \in X$ into $y \in X$.

- $p_{\text{xor}} : X \times X^2 \rightarrow [0, 1]$, where $p_{\text{xor}}(x'|x,y)$ is the probability of obtaining $x'$ as a result of crossover between $x,y \in X$.

The single-offspring crossover may be obtained from two-offspring crossover by first computing $(u,v) := \text{Cross}(x,y)$, and then defining $x' := \text{Cross}(x,y)$ as $x' \sim \text{Unif}\{\{u,v\}\}$.

Crossover and Mutation Operators Let us consider the well-known operators of bitwise mutation $\text{Mut}^*$ and the single-point crossover $\text{Cross}^*$ from Simple GA [15] as examples.

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

$$x' = (x_1, ..., x_Z, y_{Z+1}, ..., y_n), \quad y' = (y_1, ..., y_Z, x_{Z+1}, ..., x_n),$$
where the random number $Z$ 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 operator $\text{Mut}^*$ computes a genotype $y = \text{Mut}^*(x)$, where independently of other bits, each bit $y_i$, $i \in [n]$, is assigned a value $1 - x_i$ with probability $p_m$ and with probability $1 - p_m$ it keeps the value $x_i$. Here and below we use the notation $[n] := \{1, 2, ..., n\}$ for any positive integer $n$. The tunable parameter $p_m$ is also called mutation rate.

The following condition holds for many well-known crossover operators: there exists a positive constant $\varepsilon_1$ which does not depend on $I$, such that given a pair of bitstrings $x, y$, the crossover result $x' = \text{Cross}(x, y)$ satisfies

$$
\varepsilon_1 \leq \begin{cases} 
Pr(f(x') = f(x)), & \text{if } f(x) = f(y), \\
Pr(f(x') > \min\{f(x), f(y)\}), & \text{otherwise}.
\end{cases}
$$

This condition is fulfilled for the single-point crossover with $\varepsilon_1 = 1 - p_c$, if $p_c < 1$ is a constant. Sometimes stronger statements can be deduced, e.g. for the well-known OneMax and LeadingOnes fitness functions the offspring has a fitness $(f(x) + f(y))/2$ with probability at least $1/2$ (see [8]).

Another condition analogous to (1) requires that the fitness of the resulting genotype $x'$ is not less than the fitness of the parents with probability at least $\varepsilon_0$, for some constant $\varepsilon_0 > 0$, i.e.

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

for any $x, y \in X$. This condition is also fulfilled for the single-point crossover with $\varepsilon_0 = 1 - p_c$, if $p_c < 1$ is a constant. Besides that, Condition (2) is satisfied with $\varepsilon_0 = 1$ for the optimized crossover operators, where the offspring is computed as a solution to the optimal recombination problem. Polynomial-time optimized crossover routines are known for Maximum Clique [4], Set Packing, Set Partition and some other NPO problems [9, 10].

### Bitwise Mutation and $K$-Bounded Neighborhood Mappings

Let $D(x, y)$ denote the Hamming distance between $x$ and $y$.

**Definition 4** [3] Suppose $\Pi$ is an NP optimization problem. A neighborhood mapping $N$ is called $K$-bounded, if for any $x \in \text{Sol}$ and $y \in N(x)$ holds $D(x, y) \leq K$, where $K$ is a constant.
The bitwise mutation operator \( \text{Mut}^* \) outputs a string \( y \), given a string \( x \), with probability \( p_m \cdot (1 - p_m)^{n-D(x,y)} \). Note that probability \( p_m \cdot (1 - p_m)^{n-j} \), as a function of \( p_m \), \( p_m \in [0, 1] \), attains its minimum at \( p_m = j/n \). The following proposition gives a lower bound for the probability \( \Pr(\text{Mut}^*(x) = y) \), which is valid for any \( y \in \mathcal{N}(x) \), assuming that \( p_m = K/n \).

**Proposition 5** Suppose the neighborhood mapping \( \mathcal{N} \) is \( K \)-bounded, \( K \leq n/2 \) and \( p_m = K/n \). Then for any \( x \in \text{Sol} \) and any \( y \in \mathcal{N}(x) \) holds

\[
\Pr(\text{Mut}^*(x) = y) \geq \frac{K^K}{(en)^K}.
\]

The proof may be found in the appendix.

## 2 Expected First Hitting Time of Target Subset

This section is based on the drift analysis of GAs from [8]. Suppose that for some \( m \) there is an ordered partition of \( \mathcal{X} \) into subsets \( (A_1, \ldots, A_{m+1}) \) called *levels*. Level \( A_{m+1} \) will be the target level in the 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 \( \rho \)-approximation solutions for some approximation factor \( \rho > 1 \). A well-known example of partition is the *canonical* partition, where each level regroups solutions having the same fitness value (see e.g. [20]). For \( j \in [m + 1] \) we denote by \( H_j := \bigcup_{i=j+1}^{m+1} A_i \), the union of all levels starting from level \( j \).

Given a levels partition, there always exists a total order “\( \succ \)” on \( \mathcal{X} \), which is aligned with \( (A_1, \ldots, A_{m+1}) \) in the sense that \( x \succ y \) for any \( x \in A_j \), \( y \in A_{j-1} \), \( j \in [m + 1] \). W.l.o.g. in what follows the elements of a population vector \( P \in \mathcal{X}^\lambda \) will be assumed to form a non-increasing sequence \( x^1, x^2, \ldots, x^\lambda \) in terms of “\( \succ \)” order: \( x^1 \geq x^2 \geq \cdots \geq x^\lambda \). For any constant \( \gamma \in (0, 1) \), the individual \( x^{[\gamma \lambda]} \) will be referred to as the \( \gamma \)-ranked individual of the population.

The *selective pressure* of a selection mechanism \( \text{Sel} \) is defined as follows. For any \( \gamma \in (0, 1) \) and population \( P \) of size \( \lambda \), let \( \beta(\gamma, P) \) be the probability of selecting an individual from \( P \) that belongs to the same or higher level as the individual with rank \( \lceil \gamma \lambda \rceil \), i.e.

\[
\beta(\gamma, P) := \sum_{i : x^i \in H_{j(\gamma)}} p_{\text{sel}}(i \mid P),
\]
where \( j(\gamma) \) is such that \( x[^{\gamma\lambda}] \in A_{j(\gamma)} \).

**Theorem 6** Given a partition \((A_1, \ldots, A_{m+1})\) of \( X \), let \( T := \min \{ t\lambda \mid |P_t \cap A_{m+1}| > 0 \} \) be the runtime of \( GA \). If there exist parameters \( s_1, \ldots, s_m, s_*, p_0, \varepsilon_1 \in (0, 1), \delta > 0, \) and a constant \( \gamma_0 \in (0, 1) \) such that

\((C1)\) \( p_{\text{mut}}(y \in H_{j+1} \mid x \in H_j) \geq s_j \geq s_* \),
\((C2)\) \( p_{\text{mut}}(y \in H_{j+1} \mid x \in H_{j+1}) \geq p_0 \),
\((C3)\) \( p_{\text{xor}}(x \in H_{j+1} \mid u \in H_j, v \in H_{j+1}) \geq \varepsilon \),
\((C4)\) \( \beta(\gamma, P) \geq \gamma \sqrt{\frac{1 + \delta}{\varepsilon_0\gamma_0}} \) for any \( P \in \mathcal{X}^{\lambda} \),
\((C5)\) \( \lambda \geq \frac{2}{a} \ln \left( \frac{32mp_0}{(\delta\gamma_0)^2cs_*\psi} \right) \) with \( a := \frac{\delta^2\gamma_0}{2(1 + \delta)} \), \( \psi := \min\{\frac{\delta}{2}, \frac{1}{2}\} \) and \( c := \frac{a^4}{24} \).

then \( E[T] \leq \frac{2}{cp_0} \left( m\lambda(1 + \ln(1 + c\lambda)) + \frac{p_0}{(1 + \delta)\gamma_0} \sum_{j=1}^{m} \frac{1}{s_j} \right) \).

Informally, condition \((C1)\) requires that for each element of subset \( H_j \), there is a lower limit \( s_j \) on probability to mutate it into level \( j + 1 \) or higher. Condition \((C2)\) requires that there exists a lower limit \( p_0 \) on the probability that the mutation will not ”downgrade” an individual to a lower level. Condition \((C3)\) follows from lower bound \((2)\) assuming \( \varepsilon := \varepsilon_0 \) or from lower bound \((1)\) with \( \varepsilon := \varepsilon_1 \) in the case of the canonical partition. Condition \((C4)\) requires that the selective pressure induced by the selection mechanism is sufficiently strong. Condition \((C5)\) requires that the population size \( \lambda \) is sufficiently large.

Unfortunately, Conditions \((C3)\) and \((C4)\) are unlikely to be satisfied when the target subset \( A_{m+1} \) contains some less fit solutions than the solutions from level \( A_m \), e.g. when \( A_{m+1} \) is the set of all local optima. In order to adapt Theorem \(6\) to analysis of such situations we first prove the following corollary with relaxed version of conditions \((C3),(C4)\) and a slightly strengthened version of \((C2)\).

**Corollary 7** Given a partition \((A_1, \ldots, A_{m+1})\) of \( X \), let \( T := \min \{ t\lambda \mid |P_t \cap A_{m+1}| > 0 \} \) be the runtime of \( GA \). If there exist parameters \( s_1, \ldots, s_m, s_*, p_0, \varepsilon \in (0, 1), \delta > 0, \) and a constant \( \gamma_0 \in (0, 1) \) such that for all \( \gamma \in (0, \gamma_0) \)
\( (C1) \) \( p_{\text{mut}}(y \in H_{j+1} | x \in H_j) \geq s_j \geq s^*, j \in [m], \)
\( (C2') \) \( p_{\text{mut}}(x | x) \geq p_0, x \in \mathcal{X}, \)
\( (C3') \) \( p_{\text{xor}}(x \in H_{j+1} | u \in H_j, v \in H_{j+1}) \geq \varepsilon, j \in [m-1], \)
\( (C4') \) \( \beta(\gamma, P) \geq \gamma \sqrt{\frac{1+\delta}{p_0 \gamma_0}} \) for any \( P \in (\mathcal{X} \setminus A_{m+1})^\lambda, \)
\( (C5) \) \( \lambda \geq \frac{2}{a} \ln \left( \frac{32mp_0}{(\delta \gamma_0)^2c_\lambda \psi} \right) \) with \( a := \frac{\delta^2 \gamma_0}{2(1+\delta)}, \psi := \min\{\delta, \frac{1}{2}\} \) and \( c := \frac{\psi^4}{2a} \)

then \( \mathbb{E}[T] \leq \frac{2}{c_\psi} \left( m\lambda(1 + \ln(1 + c\lambda)) + \frac{p_0}{(1+\delta)\gamma_0} \sum_{j=1}^{m} \frac{1}{s_j} \right). \)

**Proof.** Given a genetic algorithm \( GA \) with certain initialization procedure for \( P_0 \), selection operator \( Sel \), crossover and mutation \( Cross \) and \( Mut \) and population size \( \lambda \), consider a genetic algorithm \( GA' \) defined as the following modification of \( GA \).

- Let the initialization procedure for population \( P_0 \) in \( GA' \) coincide with that of \( GA \).
- Operator of selection \( Sel'(P) \) performs identically to operator \( Sel(P) \), except for the cases when the input population \( P \) contains an element from \( A_{m+1} \). In the latter cases \( Sel'(P) \) returns the index of the first representative of \( A_{m+1} \) in \( P \).
- Operator of crossover \( Cross' \) performs identically to \( Cross \) except for the cases when the input contains an element from \( A_{m+1} \). In the latter cases an element of \( A_{m+1} \) is just copied to the output of the operator.
- Operator of mutation \( Mut' \) is the same as \( Mut \).
- The population size in \( GA' \) is \( \lambda \).

Note that \( GA' \) meets Conditions (C1)-(C5) of Theorem \( \Box \). Indeed, Condition (C2) follows from (C2’). Condition (C3) is satisfied for \( j \in [m-1] \) by (C3’), and for \( j = m \) it holds with \( \varepsilon = 1 \) by definition of operator \( Cross' \). Condition (C4) is satisfied for any \( P \in (\mathcal{X} \setminus A_{m+1})^\lambda \) by (C4’), and in the cases when population \( P \) contains at least one element from \( A_{m+1} \), holds \( \beta(\gamma, P) = 1 \) by definition of operator \( Sel' \). Thus, by Theorem \( \Box \)

\[
\mathbb{E}[T'] \leq \frac{2}{c_\psi} \left( m\lambda(1 + \ln(1 + c\lambda)) + \frac{p_0}{(1+\delta)\gamma_0} \sum_{j=1}^{m} \frac{1}{s_j} \right),
\]
where $T' := \min\{t\lambda \mid |P'_t \cap A_{m+1}| > 0\}$ is defined for the sequence of populations $P'_0, P'_1, \ldots$ of $GA'$.

Executions of $GA$ and $GA'$ before iteration $T'/\lambda$ are identical. On iteration $T'/\lambda$ both algorithms place elements of $A_{m+1}$ into the population for the first time. Thus, realizations of random variables $T'$ and $T$ coincide and $E[T] = E[T']$.

3 Lower Bounds on Cumulative Selection Probability

Let us see how to parameterise three standard selection mechanisms in order to ensure that the selective pressure is sufficiently high. We consider three selection operators with the following mechanisms.

By definition, in $k$-tournament selection, $k$ individuals are sampled uniformly at random with replacement from the population, and a fittest of these individuals is returned. In $(\mu, \lambda)$-selection, parents are sampled uniformly at random among the fittest $\mu$ individuals in the population. The ties in terms of fitness function are resolved arbitrarily.

A function $\alpha: \mathbb{R} \to \mathbb{R}$ is a ranking function \[14\] if $\alpha(x) \geq 0$ for all $x \in [0, 1]$, and $\int_0^1 \alpha(x)dx = 1$. In ranking selection with ranking function $\alpha$, the probability of selecting individuals ranked $\gamma$ or better is $\int_0^\gamma \alpha(x)dx$. We define exponential ranking parameterised by $\eta > 0$ as $\alpha(\gamma) := \eta e^{\eta(1-\gamma)}/(e^\eta - 1)$.

The following lemma is analogous to Lemma 1 from \[8\].

Lemma 8 \[8\] Let the levels $A_1, \ldots, A_m$ satisfy

$$f(x) < f(y) \text{ for any } x \in A_{j-1}, \ y \in A_j, \ j = 2, \ldots, m.$$ (3)

for all $x, y$ from $A_2, \ldots, A_m$.

Then for any constants $\delta' > 0$, $p_0 \in (0, 1)$ and $\varepsilon \in (0, 1)$, there exist two constants $\gamma_0 > 0$ and $\delta > 0$ such that

1. $k$-tournament selection with $k \geq 4(1 + \delta')/(\varepsilon p_0)$,

2. $(\mu, \lambda)$-selection with $\lambda/\mu \geq (1 + \delta')/(\varepsilon p_0)$ and

3. exponential ranking selection with $\eta \geq 4(1 + \delta')/(\varepsilon p_0)$.
satisfy (C4'), i.e. \( \beta(\gamma', P) \geq \gamma' \sqrt{\frac{1 + \delta}{\rho_{0 \gamma'}}} \) for any \( \gamma' \in (0, \gamma_0] \) and any \( P \in (\mathcal{X} \setminus \mathcal{A}_{\lambda+1})^\lambda \).

Note that the assumption of monotonicity of mutation w.r.t. all fitness levels (see [8]) is substituted here by Inequality (3).

**Proof.** Denote \( \varepsilon' := \varepsilon_0 p' \).

1. Consider \( k \)-tournament selection. In order to select an individual from the same level as the \( \gamma \)-ranked individual or higher, by Inequality (3) it is sufficient that the randomly sampled tournament contains at least one individual with rank \( \gamma \) or higher. Hence, one obtains for \( 0 < \gamma < 1 \),

\[
\beta(\gamma) > 1 - (1 - \gamma)^k.
\]

Note that

\[
(1 - \gamma)^k < e^{-\gamma k} < \frac{1}{1 + \gamma k}.
\]

So for \( k \geq 4(1 + \delta')/\varepsilon' \), we have

\[
\beta(\gamma) \geq 1 - \frac{1}{1 + \gamma k} \geq 1 - \frac{1}{1 + 4\gamma(1 + \delta')/\varepsilon'} = \frac{4\gamma(1 + \delta')/\varepsilon'}{1 + 4\gamma(1 + \delta')/\varepsilon'}
\]

If \( \gamma_0 := \varepsilon'/(4(1 + \delta')) \), then for all \( \gamma' \in (0, \gamma_0] \) it holds that \( 4(1 + \delta')/\varepsilon' \leq 1/\gamma' \) and

\[
\beta(\gamma') \geq \frac{\gamma' 4(1 + \delta')/\varepsilon'}{\gamma'(1/\gamma') + 1} = \frac{2(1 + \delta') \gamma'}{\varepsilon'}
\]

\[
= \sqrt{\left(\frac{1 + \delta'}{\varepsilon'(\varepsilon'/4(1 + \delta'))}\right) \gamma'} = \sqrt{\frac{1 + \delta'}{\varepsilon' \gamma_0} \gamma'}
\]

2. In \( (\mu, \lambda) \)-selection, for all \( \gamma \in (0, \mu/\lambda] \) we have \( \beta(\gamma) = \lambda \gamma / \mu \) if \( \gamma \lambda \leq \mu \), and \( \beta(\gamma) = 1 \) otherwise (see by Inequality (3)). It suffices to pick \( \gamma_0 := \mu/\lambda \) so that with \( \lambda/\mu \geq (1 + \delta')/\varepsilon' \), for all \( \gamma' \in (0, \gamma_0] \). Then

\[
\beta(\gamma') \geq \frac{\lambda \gamma'}{\mu} = \sqrt{\lambda^2 \gamma'} = \sqrt{\frac{\lambda}{\mu \gamma_0} \gamma'} \geq \sqrt{\frac{1 + \delta'}{\varepsilon' \gamma_0} \gamma'}.
\]
3. In exponential ranking selection, we have
\[
\beta(\gamma) \geq \int_0^\gamma \eta e^\eta (1-x) dx = \left( \frac{e^\eta}{e^\eta - 1} \right) \left( 1 - \frac{1}{e^\eta} \right) \geq 1 - \frac{1}{1 + \eta \gamma}
\]

The rest of the proof is similar to tournament selection with \( \eta \) in place of \( k \), e.g. based on the input condition on \( \eta \), it suffices to pick \( \gamma_0 := \varepsilon'/(4(1 + \delta')) \).

\[\blacksquare\]

4. **Expected First Hitting Time of the Set of Local Optima**

Suppose an NP maximization problem \( \Pi = (\text{Inst}, \text{Sol}, F_I) \) is given and a neighborhood mapping \( N_I \) is defined. Given \( I \in \text{Inst} \), let \( s(I) \) be a lower bound on the probability that a mutation operator transforms a given feasible solution \( x \) into a specific neighbor \( y \in N_I(x) \), i.e.

\[
s(I) \leq \min_{x \in \text{Sol}(I), \ y \in N_I(x)} \Pr(\text{Mut}(x) = y). \quad (4)
\]

The greater the value \( s(I) \), the more consistent is the mutation with the neighborhood mapping \( N_I \).

In Subsections 4.1 and 4.2, the symbol \( I \) is suppressed in the notation for brevity. The size of population \( \lambda \) and the selection parameters \( k, \mu \) and \( \eta \), the number of levels \( m \) and the fitness function \( f \) are supposed to depend on the input data \( I \) implicitly.

The set of all local optima is denoted by \( \mathcal{LO} \) (note that global optima also belong to \( \mathcal{LO} \)).

4.1. **No Infeasible Solutions**

In many well-known NP optimization problems, such as the Maximum Satisfiability Problem [13], the Maximum Cut Problem [13] and the Ising Spin Glass Model [5], the set of feasible solutions is the whole search space, i.e. \( \text{Sol} = \{0, 1\}^n = \mathcal{X} \). Let us consider the GAs applied to problems with such a property.

We choose \( m \) to be the number of fitness values \( f_1 < \cdots < f_m \) attained by the solutions from \( \mathcal{X}\setminus\mathcal{LO} \). Then starting from any point, the local search
method finds a local optimum within at most $m$ steps. Let us use a modification of canonical $f$-based partition where all local optima are merged together:

$$A_j := \{ x \in \mathcal{X} | f(x) = f_j \} \setminus \mathcal{L}_\mathcal{O}, \ j \in [m],$$

$$A_{m+1} := \mathcal{L}_\mathcal{O}.$$  

Application of Corollary 7 and Lemma 8 w.r.t. this partition yields the following theorem.

**Theorem 9** Suppose that

- $p_{\text{mut}}(y \mid x) \geq s$ for any $x \in \text{Sol}$, $y \in \mathcal{N}(x)$,
- Conditions (C2') and (C3') are satisfied for some constants $p_0 > 0$ and $\varepsilon > 0$,
- $\text{Sol} = \mathcal{X}$,
- $\mathcal{G}A$ is using either $k$-tournament selection with $k \geq \frac{4(1+\delta')}{\varepsilon_0 p_0}$, or $(\mu, \lambda)$-selection with $\frac{\lambda}{\mu} \geq \frac{(1+\delta')}{\varepsilon p_0}$ or exponential ranking selection with $\eta \geq \frac{4(1+\delta')}{\varepsilon p_0}$ for some constant $\delta' > 0$.

Then there exist two constants $b$ and $b'$, such that for population size $\lambda \geq b \ln \left( \frac{m s}{4} \right)$, a local optimum is reached for the first time after at most $b\left( m \lambda \ln \lambda + \frac{m s}{4} \right)$ fitness evaluations on average.

A similar result for the $\mathcal{G}A$ with tournament selection and two-offspring crossover was obtained in [12, 11] without a drift analysis. In particular, Lemma 1 and Proposition 1 in [11] imply that with appropriate settings of parameters, a non-elitist genetic algorithm reaches a local optimum for the first time within $O \left( \frac{m \ln m}{s} \right)$ fitness evaluations on average. The upper bound from Theorem 9 in the present paper has advantage in to the bound from [11] if $1/s$ is at least linear in $m$. (Note that the size of many well-known neighborhoods grows as some polynomial of $m$.)

### 4.2 Illustrative Examples

**Royal Road Functions** Let us consider a family of *Royal Road Functions* $RR_{n,r}$ defined on the basis of the principles proposed by M. Mitchell,
S. Forrest, and J. Holland in [21]. The function $RR_{n,r}$ is defined on the search space $\mathcal{X} = \{0, 1\}^n$, where $n$ is a multiple of $r$, and the set of indices $[n]$ is partitioned into consecutive blocks of $r$ elements each. By definition $RR_{n,r}(x)$ is the number of blocks where all bits are equal to 1.

We consider a crossover operator, denoted by $\text{Cross}^p$, which returns one of the parents unchanged with probability $1 - p_c$. In particular, $\text{Cross}^p$ may be built up from any standard crossover operator so that with probability $p_c$ the standard operator is applied and the offspring is returned, otherwise with probability $1 - p_c$ one of the two parents is returned with equal probabilities.

The following corollary for royal road functions $RR_{n,r}(x)$ results from Theorem 9 with the neighborhood defined by the Hamming distance with radius $r$.

Corollary 10 Suppose that the GA uses a $\text{Cross}^p$ crossover operator with $p_c$ being any constant in $[0, 1)$, the bitwise mutation with mutation rate $p_m = \chi/n$ for a constant $\chi > 0$, $k$-tournament selection with $k \geq 8(1+\delta) e^{\chi}/(1-p_c)$, or $(\mu, \lambda)$-selection with $\lambda/\mu \geq 2(1+\delta) e^{\chi}/(1-p_c)$, or exponential ranking selection with $\eta \geq 8(1+\delta) e^{\chi}/(1-p_c)$, where $\delta > 0$ is a constant. Then there exists a constant $b > 0$ such that the GA with population size $\lambda = \lceil b \ln n \rceil$, has expected runtime $O(n r^2 + 1)$ on $RR_{n,r}(x)$.

Proof.
Note that fitness function $RR_{n,r}(x)$ of any solution $x$ with some non-optimal bits (i.e. bits equal to zero) can be increased by an improving move within Hamming neighborhood of radius $r$. So there is just one local optimum and it is the global optimum $x = (1, \ldots, 1)$. We now apply Theorem 9 with the canonical partition $A_j := \{x \mid RR_{n,r}(x) = j - 1\}$ for $j \in [m+1]$ where $m := n/r$.

The probability of not flipping any bit position by mutation is $$(1 - \chi/n)^n = (1 - \chi/n)^{n/\chi-1} \chi (1 - \chi/n)^\chi \geq e^{-\chi}(1 - \chi/n)^\chi.$$ In the rest of the proof we assume that $n$ is sufficiently large to ensure that $(1 - \chi/n)^n \geq \frac{e^{-\chi}}{1+\delta/2}$ for the constant $\delta > 0$. Let $p_0 := \frac{e^{-\chi}}{1+\delta/2}$.

The lower bound to upgrade probability may be found if we consider the worst-case scenario where only one block contains some incorrect bits and the number of such bits is $r$. Then $s := (\chi/n)^r (1 - \chi/n)^{n-r} = \Omega(1/n^r)$.

We can put $\varepsilon_0 := (1 - p_c)/2$ because the crossover operator returns one of the parents unchanged with probability $1 - p_c$, and with probability at
least 1/2, this parent is not less fit than the other one. Then conditions of Theorem \( \text{9} \) regarding \( k, \mu, \lambda, \) and \( \eta \) are satisfied for the constant \( \delta' := \frac{1 + \delta}{1 + \delta/2} - 1 > 0. \)

It therefore follows by Theorem \( \text{9} \) that there exists a constant \( b > 0 \) such that if the population size is \( \lambda = \lceil b \ln n \rceil \), the expected runtime of \( GA \) on \( RR_{n,r}(x) \) is upper bounded by \( b' (n (\lambda \ln \lambda + n^r)) \) for some constant \( b' \).

The corollary implies that the \( GA \) with proper population size has a polynomial runtime on the royal road functions if \( r \) is a constant.

**Vertex Cover Problems with Regular Structure**

In general, given a graph \( G = (V, E) \), the Vertex Cover Problem (VCP) asks for a subset \( C \subseteq V \) (called a vertex cover), such that every edge \( e \in E \) has at least one endpoint in \( C \). The size of \( C \) should be minimized. Let us consider a representation of the problem solutions, where \( n = |E|, \mathcal{X} = \{0, 1\}^n \) and each coordinate \( x_i \in \{0, 1\}, i = 1, \ldots, |E| \) of \( x \) corresponds to an edge \( e_i \in E \), assigning one of its endpoints to be included into the cover \( C(x) \) (one endpoint of \( e_i \) is assigned if \( x_i = 0 \) and the other one is if \( x_i = 1 \)). Thus, \( C(x) \) contains all vertices, assigned by at least one of the coordinates of \( x \), and the feasibility of \( C(x) \) is guaranteed. This representation is a special case of the so-called non-binary representation for a more general set covering problem (see e.g. [6]).

The fitness function is by definition \( f(x) := |V| - |C(x)| \).

Family of vertex covering instances \( G(\kappa), \kappa = 1, 2, \ldots \) consists of VCP problems with \( n = 3\kappa \) where \( G \) is a union of \( \kappa \) disjoined cliques of size 3 (triangles). An optimal solution contains a couple of vertices from each clique and there are \( 3^\kappa \) optimal solutions.

Consider the neighborhood system defined by Hamming distance with radius 1. All local optima for \( G(\kappa) \) are globally optimal in this case. For the bit-wise mutation operator with mutation rate \( p_m = 1/n \) by Proposition \( \text{5} \) we have \( P(\text{Mut}^*(x) = y) \geq 1/(en) \) for any \( y \in \mathcal{N}(x), x \in \mathcal{X} \). Analogously to Corollary \( \text{10} \) we obtain

**Corollary 11** Suppose that the \( GA \) uses a Cross\(^{pc} \) crossover operator with \( p_c \) being any constant in \( [0, 1) \), the bitwise mutation with mutation rate \( p_m = 1/n \), \( k \)-tournament selection with \( k \geq 8e(1 + \delta)/(1 - p_c) \), or \((\mu, \lambda)\)-selection with \( \lambda/\mu \geq 2e(1 + \delta)/(1 - p_c) \), or exponential ranking selection with \( \eta \geq 8e(1 + \delta)/(1 - p_c) \), where \( \delta > 0 \) is a constant. Then there exists a constant \( b > 0 \), such that the \( GA \) with population size \( \lambda = b[\ln n] \), has expected runtime \( O(n \ln n \ln \ln n) \) on the VCP family \( G(\kappa) \).
It is interesting that the VCP instances $G(\kappa)$ in integer linear programming formulation are hard for the Land and Doig branch and bound algorithm (for a description of Land and Doig algorithm see e.g. [25], Chapt. 24). This exact algorithm makes $2^{\kappa+1}$ branchings on the problems from $G(\kappa)$ (see [24]).

4.3 The General Case of NP Optimization Problems

Consider the general case where $\text{Sol}(I)$ may be a proper subset of $\mathcal{X}$. Let us add another modification to the levels partition. Besides merging all local optima we assume that all infeasible solutions constitute level $A_1$. The rest of solutions are stratified by their objective function values. Let $m-1$ be the number of fitness values $f_2 < \cdots < f_m$ attained by the feasible solutions from $\text{Sol}(I) \setminus \mathcal{LO}_I$.

$$A_1 := \mathcal{X} \setminus \text{Sol}(I),$$

$$A_j := \{x \in \text{Sol}(I) | f(x) = f_j\} \setminus \mathcal{LO}_I, \quad j = 2, \ldots, m,$$

$$A_{m+1} := \mathcal{LO}_I.$$

Application of Corollary 7 with this partition yields the following lemma.

**Lemma 12** Suppose that Condition (C2') holds and

(L1) $\sigma(I) \leq \min \{\Pr(\text{Mut}(x) = y) | x \in \text{Sol}(I), \ y \in \mathcal{N}_I(x)\}$.

(L2) $\sigma(I) \leq \Pr(\text{Mut}(x) \in \text{Sol}(I)), \ x \in \mathcal{X} \setminus \text{Sol}(I)$.

(L3) Inequality (4) holds for some positive constant $\varepsilon_0$

and $\mathcal{GA}$ is using either $k$-tournament selection with $k \geq \frac{4(1+\delta')}{\varepsilon_0}$ or $(\mu, \lambda)$-selection with $\frac{\lambda}{\mu} \geq \frac{(1+\delta')}{\varepsilon_0}$ or exponential ranking selection with $\eta \geq \frac{4(1+\delta')}{\varepsilon_0}$ for some constant $\delta' > 0$.

Then there exist two constants $b$, and $b'$ such that for population size $\lambda \geq b \ln \left(\frac{m(I)}{\sigma(I)}\right)$, a local optimum is reached for the first time after at most $b' \left(\frac{m(I) \lambda \ln \lambda + \frac{m(I)}{\sigma(I)}}{\sigma(I)}\right)$ fitness evaluations on average.

**Proof.** Assumption (L1) is equivalent to Inequality (4) with $\sigma(I) \equiv s(I)$. Condition (L2) imposes a lower bound on probability of producing feasible
solutions by mutation of an infeasible bitstring. Thus together (L1) and (L2) give the lower bound for (C1). Condition (L3) implies (C3').

Operators Mut and Cross are supposed to be efficiently computable and the selection procedure requires only a polynomial time. Therefore the time complexity of computing a pair of offspring in the GA is polynomially bounded and the following theorem holds.

**Theorem 13** If problem $\Pi = (\text{Inst}, \text{Sol}(I), F_I)$ is polynomially bounded, Conditions (C2'), (L1), (L2) and (L3) are satisfied for a lower bound $\sigma(I)$, $1/\sigma(I) \in \text{Poly}$, and positive constants $\epsilon_0 > 0$ and $p_0 > 0$, then GA using tournament selection or $(\mu, \lambda)$-selection or exponential ranking selection with a suitable choice of parameters first visits a local optimum on average in polynomially bounded time.

Note that Condition (L2) in formulation of Theorem 13 can not be dismissed. Indeed, suppose that problem $\Pi = (\text{Inst}, \text{Sol}(I), F_I)$ is polynomially bounded, 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 $\pi(x, I)$, $0 < \epsilon(I) < \pi(x, I)$. Finally assume that the initialization procedure produces no local optima in population $P^0$. Now all conditions of Theorem 13 can be satisfied, but with a positive probability of at least $\epsilon(I)^3$ the whole population $P^1$ consists of infeasible solutions, and subject to this event all populations $P^1, P^2, \ldots$ are infeasible. Therefore, expected hitting time of a local optimum is unbounded.

In order to estimate applicability of Theorem 13 it is sufficient to recall that the set $\mathcal{N}(x)$ for $x \in \text{Sol}(I)$ may be enumerated efficiently by definition, so there exists a mutation operator Mut($x$) that generates a uniform distribution over $\mathcal{N}(x)$ if $\mathcal{N}(x) \neq \emptyset$ and every point in $\mathcal{N}(x)$ is selected with probability at least $\sigma(I)$, $1/\sigma(\cdot) \in \text{Poly}$. To deal with the cases where $x \notin \text{Sol}(I)$ or $x \in \text{Sol}(I)$ but $\mathcal{N}(x) = \emptyset$, we can recall that there are large classes of NP-optimization problems, where at least one feasible solution $y_I$ is computable in polynomial time (see e.g. the classes PLS in [17] and GLO in [3]). For such problems in case of $x \notin \text{Sol}(I)$ or $\mathcal{N}(x) = \emptyset$, a mutation operator may output the feasible solution $y_I$ with probability 1.

Alternatively we can consider a repair heuristic (see e.g. [6]) which follows some standard mutation operator and, if the output of mutation is infeasible then the heuristic substitutes this output by a feasible solution, e.g. $y_I$. 
5 Analysis of Guaranteed Local Optima Problems

In this section, Theorem 13 is used to estimate the GA capacity of finding the solutions with approximation guarantee.

An algorithm for an NP maximization problem $\Pi = (\text{Inst}, \text{Sol}(I), F_I)$ has a guaranteed approximation ratio $\rho$, $\rho \geq 1$, if for any instance $I \in \text{Inst}$, $\text{Sol}(I) \neq \emptyset$, it delivers a feasible solution $x'$, such that

$$F_I(x') \geq \max\{F_I(x) | x \in \text{Sol}(I)\}/\rho.$$  

In the case of an NP minimization problem, the guaranteed approximation ratio is defined similarly, except that the latter inequality changes into

$$F_I(x') \leq \rho \min\{F_I(x) | x \in \text{Sol}(I)\}.$$  

**Definition 14** [3] A polynomially bounded NP optimization problem $\Pi$ belongs to the class of Guaranteed Local Optima (GLO) problems, if the following two conditions hold:

1) At least one feasible solution $y_I \in \text{Sol}$ is efficiently computable for every instance $I \in \text{Inst}$;

2) A $K$-bounded neighborhood mapping $N_I$ exists, such that for every instance $I$, any local optimum of $I$ with respect to $N_I$ 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 [3].

If a problem $\Pi$ belongs to GLO and $n$ is sufficiently large, then in view of Proposition 5 for any $x \in \text{Sol}$ and $y \in N(x)$, the bitwise mutation operator with $p_m = K/n$ satisfies the condition $\Pr\{\text{Mut}^*(x) = y\}^{-1} \in \text{Poly}$. Besides that, for a sufficiently large $n$ for any $x \in \text{Sol}$ holds $p_{\text{mut}}(x | x) \geq e^{-K}/2 =: p_0$, which is a constant. Therefore, Theorem 13 implies the following

**Corollary 15** If $\Pi \in \text{GLO}$, then given suitable values of parameters, $\mathcal{G}A$ with tournament selection or $(\mu, \lambda)$-selection, a crossover operator that satisfies Inequality (2) for some positive constant $\varepsilon_0$ and the bitwise mutation followed by repair heuristic, first visits a solution with a constant guaranteed approximation ratio in polynomially bounded time on average.
6 Conclusion

The obtained results indicate that if an NPO problem is polynomially bounded and a feasible solution is easy to find, then a local optimum is computable in expected polynomial time by the non-elitist GA with tournament selection or \((\mu, \lambda)\)-selection or exponential ranking selection. Besides that, given suitable parameters, the non-elitist GA with tournament selection or \((\mu, \lambda)\)-selection approximates any problem from GLO class within a constant ratio in polynomial time on average.

The paper does not take into account the possible improvement of parent solutions in the crossover operator. The further research might address the ways of using this potential. Another open question is whether it is possible to prove an analog of Theorem 13, provided that the initial population contains a sufficient amount of feasible solutions, and the infeasible bitstrings mutate into feasible ones at least with exponentially small probability.

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Appendix

Proof of Proposition 5. For any $x \in \text{Sol}$ and $y \in \mathcal{N}(x)$ holds

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

$$\geq \left(\frac{K}{n}\right)^K \left(1 - \frac{K}{n}\right)^{n-K},$$

since $p_m = K/n \leq 1/2$. Now $\frac{\partial}{\partial n}(1 - K/n)^{n-K} < 0$ for $n > K$, and besides that, $(1 - K/n)^{n-K} \to 1/e^K$ as $n \to \infty$. Therefore $(1 - K/n)^{n-K} \geq 1/e^K$, which implies the required inequality. \hfill \blacksquare