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Modeling dynamics of small populations in a simple phenotypic evolutionary algorithm. A space of population states approach

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ABSTRACT

The paper presents a theoretical analysis of a simple phenotypic evolutionary algorithm running with the fitness proportional selection and the Gaussian mutation. The space of population states approach is applied to analyze dynamics of small populations evolving in an unconstrained one-dimensional search space. The approach facilitates a study of a global behavior of evolving populations from a macroscopic point of view. Expected trajectories of population states are regarded in landscapes of various types of fitness functions: unimodal and multimodal, symmetrical and asymmetrical. Phenomena of rapid unification of initially diversified populations and diversification of initially homogeneous populations followed by a movement of a cluster-like population towards the neighborhood of an optimum, observed previously for two-element populations, were confirmed. Studies of a dynamical system generated by the expected states revealed period-doubling bifurcations and chaotic behavior of the system which appear for particular values of a mutation strength parameter and specific fitness functions. A time to convergence to the steady state, as an essential indicator of optimization properties of the process, was also analyzed.

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1. Introduction

Biologically inspired modern heuristics have become highly popular optimization methods mainly due to their versatility and simplicity of use. Although evolutionary algorithms have thousands of real-life applications, the literature devoted to theoretical analysis of these methods is sparse. Because of their complex, non-deterministic nature, populational structure and multitude of versions, theoretical studies of those methods are complicated and existing results are limited to specific cases of evolutionary operators, population sizes or fitness functions. Early successful approaches in theoretical analysis of evolutionary algorithms used Markov chain models [1,2], or dynamical systems theory to study the system generated by infinite populations with a binary coding [3]. In these paradigms, an asymptotic behavior of populations or expected population trajectories (fixed points and their stability) were analyzed. Recently, there have been observed major improvements in the theoretical understanding of evolutionary algorithms and appearance of new techniques such as the population drift

[4], artificial fitness levels [5,6], the family tree [7], branching processes [8] and some others. These techniques allow researchers to determine lower and upper bounds on evolutionary algorithms runtime. The results are obtained mainly for the simple binary coding algorithms (i.e., (1+1)EA) and simple fitness functions such as onemax or linear functions. Some of the results were generalized to populational algorithms [6]. Theoretical analyses of finite small populations with real-coded individuals are particularly scarce and focus mainly on evolution strategies [9,10].

In this paper another approach, based on studying evolution in a space of population states, is presented [11,12]. The state describes a population as a whole. Regarding a population not as a collection of individuals but rather as a unity allows one to consider evolution in terms of macro-evolution models for which probability distributions and expected states can be calculated and their trajectories studied. Unfortunately, an exact (analytic) analysis is possible only in the case of two-element populations and one-dimensional search space, where trajectories of expected states can be accurately calculated. The problem becomes even more complicated when the population size increases and formulas for expected states, calculated using the presented technique, can only be approximated numerically [13,14]. Since two-element populations, as the smallest possible ones, may display very unique behavior, it was compelling to learn whether small but larger than

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two-individual populations behave similarly or not. With the use of the Gaussian function approximation, we study the evolution of population states for three-, four- and five-element populations. The dynamics of transient behavior and convergence to steady states is analyzed for various fitness functions. The research is extended with the examination of a dynamical system generated by the process, keeping trace over its asymptotic behavior (which may be chaotic in some situations) and time to convergence to the steady states. It appears that presented results show behavior qualitatively similar to that of two-element populations.

The paper is organized as follows. In Section 2 preliminaries describing states of a space approach and calculating expected states are presented. The section is supplemented with a description of fitness functions used in the research. In Section 3 trajectories of expected states and analytical calculations of the expected states for initially homogeneous small populations are described. An analysis of dynamics of small populations evolving in different landscapes of fitness functions is presented in Section 4. Results of dynamical system studies (asymptotic behavior and time to convergence to the steady states) are given in Section 5. In Section 6 remarks on possible model extensions are collected. The paper is concluded in Section 7. Exact formulas for expected states of two-element populations and approximated formulas for three-element populations are collected in Appendix A.

2. Preliminaries

2.1. The model of evolution

A simple model of phenotypic evolution is regarded [15]. A population consist of m individuals: $P = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m\}$. Each individual is characterized by its type: n -dimensional real-valued vector of traits $\mathbf{x}_k = (x_{k,1}, x_{k,2}, \dots, x_{k,n})$, $k = 1, \dots, m$, and its quality $q(\mathbf{x})$: a fitness function value for the type. The population evolves in an unconstrained n -dimensional space of types $T = \mathbb{R}^n$, and new generations of individuals are created by only two operators: the fitness proportional selection and the Gaussian mutation. A probability density function of the individual \mathbf{x} in the $(i + 1)$ st generation is given by

$$f_T^{i+1}(\mathbf{x} | P^i) = \sum_{k=1}^m \alpha(\mathbf{x}_k^i | P^i) g(\mathbf{x}, \mathbf{x}_k^i), \tag{1}$$

where $\alpha(\mathbf{x}_k^i | P^i)$ is a probability of selection of individual \mathbf{x}_k^i (for the fitness proportional selection $\alpha(\mathbf{x}_k^i | P^i) = q(\mathbf{x}_k^i) / \sum_{j=1}^m q(\mathbf{x}_j^i)$), $g(\mathbf{x}, \mathbf{x}_k^i)$ denotes a density of mutation of the k th individual (for the Gaussian mutation $g(\mathbf{x}, \mathbf{x}_k^i) = \mathcal{N}(\mathbf{x}; \mathbf{x}_k^i, \sigma) = \exp(-(\mathbf{x} - \mathbf{x}_k^i)^2 / 2\sigma^2) / (\sigma\sqrt{2\pi})$).

The presented model has only two parameters: population size m and the standard deviation of mutation σ , and introduces a simple generational evolutionary algorithm called *evolutionary search with soft selection* [16]. Populations evolving according to the model can effectively cross wide and deep saddles separating adaptive peaks of multimodal fitness functions, which is crucial for global optimization [16–18].

Due to the simplicity of the model, it was possible to examine its theoretical properties for two extreme cases: infinite [19] and two-element [12] populations. This paper presents an advancement of the latter case on still small but larger than two-element populations.

2.2. The space of population states

Evolving populations can be modeled in two different ways: in the space of types T where every individual can be considered separately, or in the space of population states S where each point

indicates not a single individual but a whole population. The space of population states has a more complicated structure than the space T : (i) dimensionality of S depends on the population size and is m times higher than dimensionality of T : $\dim(S) = n \cdot m$; (ii) $m!$ points in S represent exactly the same population with different permutation of individuals. As the dynamics of evolution does not depend on ordering of individuals in a population, an *equivalence relation* U has to be introduced to avoid this ambiguity. The equivalence relation identifies all points corresponding to permutations of individuals in a population. The space S with defined U becomes a *quotient space* $S_U = S/U = \mathbb{R}^{m \cdot n} / U$. Despite the described complications, the space of states approach allows one to analyze theoretically the evolution of small populations in one-dimensional search space, and therefore we restrict our studies to such cases of $n = 1$ ($\dim(S) = m$).

To carry out further analysis, a rule to determine one among all population elements indistinguishable w.r.t. U must be determined. In the paper, for one-dimensional search space, it is assumed that the relation U ranks individuals within a population in a decreasing order. A population is therefore represented as a state (point) $\mathbf{s} = (x_1, x_2, \dots, x_m)$ in the quotient space, such that $x_1 \geq x_2 \geq \dots \geq x_m$. The space is limited by a line $x_1 = x_2 = \dots = x_m$ indicating homogeneous populations (for which the types of all individuals in a population are equal), and called the *identity line* later on. A joint probability density function of m -element population in S is given by a product of m densities (1). In the quotient space S_U , a “reflection” of the density relative to the identity line takes place. The joint density becomes asymmetrical and is located in the right semi-plane bounded by the line. The joint probability density function of the population state in the $(i + 1)$ st generation is given by

$$f_{S_U}^{i+1}(\mathbf{s} | \mathbf{s}^i) = m! \prod_{j=1}^m f_T^{i+1}(\mathbf{x}_j | \mathbf{s}^i) = m! \prod_{j=1}^m \prod_{k=1}^m \alpha(\mathbf{x}_k^i | \mathbf{s}^i) g(\mathbf{x}_j, \mathbf{x}_k^i). \tag{2}$$

The calculation of the probability of selection $\alpha(\mathbf{x}_k^i | \mathbf{s}^i)$ is usually based on a fitness function, which is naturally defined in the space of types T . In the space of population states, fitness of the whole population is defined as the average fitness of all its individuals (as it is often used in biological models). Thus, evolution in the space of population states is defined by a sequence of states \mathbf{s}^j , $j = 0, 1, \dots$ describing a trajectory of the population in the landscape of average fitness $\bar{q}(\mathbf{x})$.

2.3. Expected values of population state

Given an initial population state, the expected value of the next population state can be calculated using a joint probability density function (2) as

$$E[\mathbf{x}_\bullet | \mathbf{s}^i] = \int_{-\infty}^{\infty} \int_{-\infty}^{x_1} \dots \int_{-\infty}^{x_{m-1}} \mathbf{x}_\bullet f_{S_U}^{i+1}(\mathbf{s} | \mathbf{s}^i) dx_m \dots dx_1. \tag{3}$$

Note that the limits of integration of inner integrals do not range from $-\infty$ to $+\infty$ but the upper limits are constrained since the density is defined in the quotient space S_U . It causes some difficulties in calculating integrals and exact formulas for the expectations can be derived only for two-element populations [11,12]. For three-element populations, formulas for expected coordinates are given but they require numerical evaluation of singular integrals (cf. Appendix A) [13,14].

Besides that, we developed an efficient and numerically stable procedure to calculate expected states of small populations. The basic idea of the procedure is to replace one-dimensional Gaussian distribution of mutation $\mathcal{N}(\mathbf{x}_j; \mathbf{x}_k^i, \sigma)$ by its polynomial approximation, such that distributions for given σ and \mathbf{x}_k^i are derived from the standard normal distribution approximated by piecewise-

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