MIXED OPTIMIZATION METHOD BASED ON EVOLUTIONARY COMPUTATION

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1 Introduction

Subject of this contribution is optimization problems for computer simulation of complex dynamical systems. Main goal is to investigate and develop different optimization methods and their modifications for solving parameter-fitting problems in process engineering and systems biology. The general similarities of the investigated models are a complex, nonlinear, multimodal objective function and large set of parameters and constraints. Such objective function's behavior requires a global optimization task solving.

2 Implementation and testing system

The development of a high-efficiency optimization subsystem requires not only implementation of directly optimization numerical methods, but also their testing, integration into simulation environment and preparation for the subsequent parallelizing. In this connection object-oriented model (OOM) of special software system has been developed (fig. 3.1). It includes: interfaces for the tasks definition, interfaces for the classes, which provide optimization, system for the reports forming and experiments statistics gathering, testing system, interface for simulation environment and interface for paralleling subsystem.

For debugging and estimation of the developed optimization algorithms performance a special testing system has been developed. It allows to execute the predetermined sets of tests and to generate the detailed report on testing results. According to these results tester can make an objective choice of the necessary algorithm and its parameters.

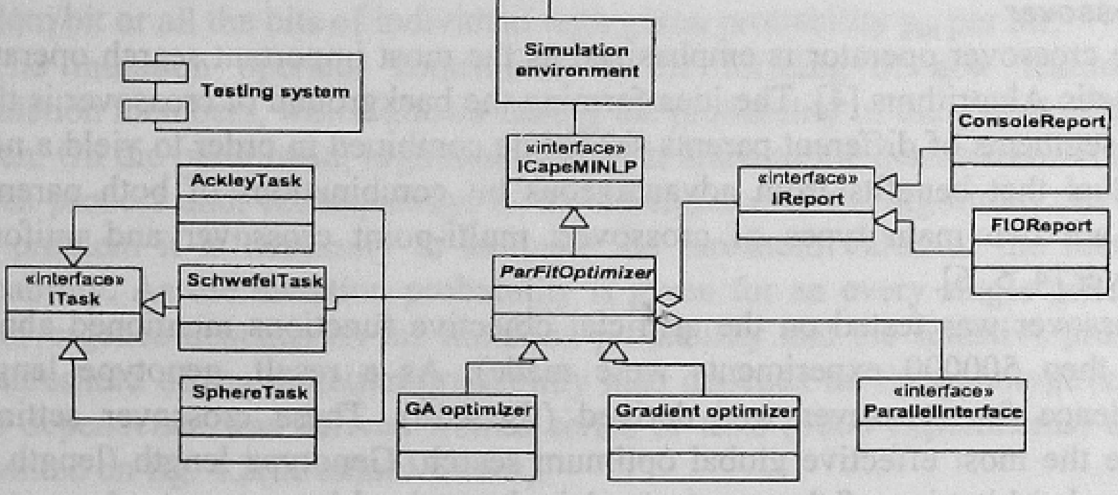


Figure 3.1: OOM of developed software

In a case when the global optimum with the given accuracy is successfully found, the primary assessment criterion of optimization algorithm is a number of objective function evaluations. But if we are testing stochastic methods like genetic algorithms, it is necessary to estimate average values of performance and probability of convergence. Therefore testing system supports multiple running of the same experiments to collect and gather experiments statistics.

For a testing various artificial objective functions were chosen, that commonly accepted as a testing functions for global optimization [4, 6]: sphere, step function, Schwefel function and Ackley function.

3 GA and testing results

Algorithm basics and biological background

The main idea of a Genetic Algorithm [3] is a search strategy in a multidimensional space that simulates the evolution of a population of biological individuals (i.e. the scientific approach based on Darwin's theory).

Basic theory for GA is the schema theory [3]. A schema describes a subset of strings that have similarities at certain string positions. This theory specifies influence of GA operators on solution forming.

For all these genetic operators there is a wide variety of modifications available in the literature [4, 5, 6]. Binary representation of the individuals may be different as well [4]).

Representation

All parameters of the objective function are encoded in GA into a bitstring. On a par with a simple base two representation, it is now common practice to use a Gray code interpretation of the bitstring segments [4]. Bethke was one of the first who indicated the advantages such a code might have on the search [8]. Series of experiments (5400 in all) were made to analyze this. In the majority of tests, Gray code showed a better precision of the found result at the cost of a minor evaluations' increase. Therefore, Gray code was chosen as a default for an algorithm.

Crossover

The crossover operator is emphasized as the most important search operator of Genetic Algorithms [4]. The idea forming the background of crossover is that useful segments of different parents should be combined in order to yield a new individual that benefits from advantageous bit combinations of both parents. There are two main types of crossover: multi-point crossover and uniform crossover [4, 5, 6].

Crossover was tested on the artificial objective functions mentioned above (more then 500000 experiments were made). As a result, genotype length dependence for crossover was derived (fig. 4.1a). These crossover settings provide the most effective global optimum search. Genotype length (length of the encoded bitstring of the parameters) is determined by parameters' count of the objective function and their discretization's precision. Results for crossover are presented together with the population size changes (fig. 4.1b), because they are related. According to the results, for the longer genotype higher crossover probability and more crossover points are needed (fig. 4.1a) to solve the global optimization problem successfully. Moreover, a higher population size is needed, but when the crossover probability increases, population size is somewhat lowered, but then keeps increasing until next crossover probability rise (fig. 4.1b).

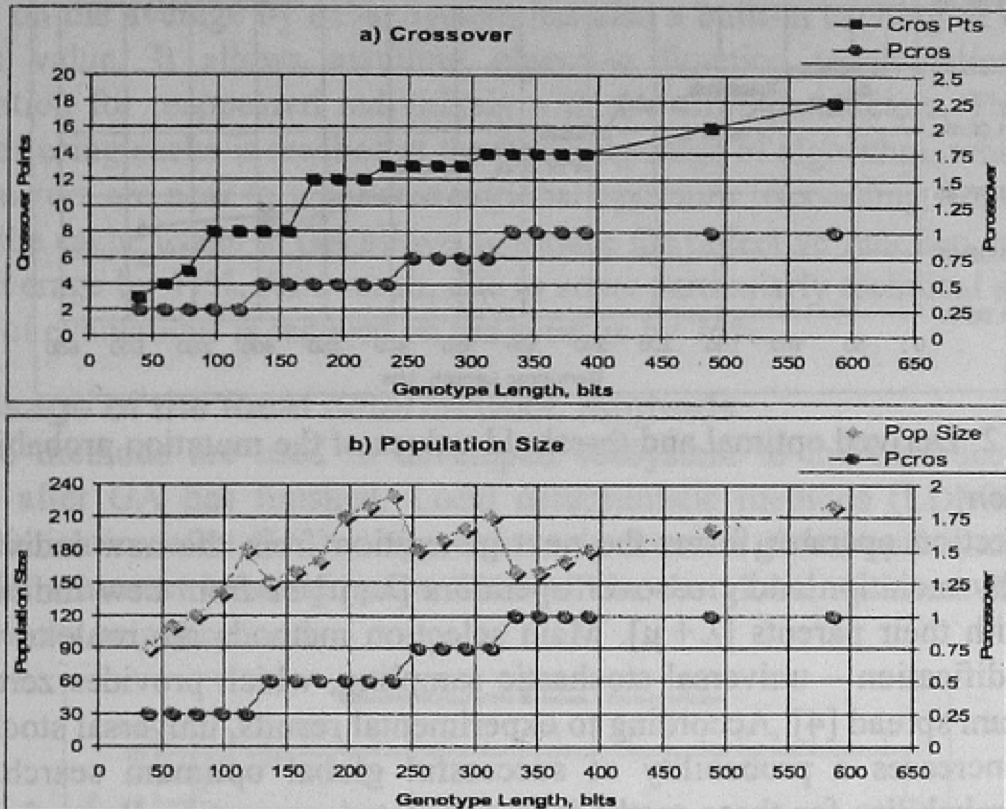


Figure 4.1: Genotype length dependence for crossover (a) and population size (b)

Mutation

The mutation operator is a "background operator" that occasionally changes single bits of individuals by inverting them. Mutation may affect either single random bit or all the bits of individual with given probability p_m per bit.

The mutation operator contributes to the forming of new features of population members, which allows raising the probability of the global optimum search. On the other hand, high mutation level leads to the destabilization of the search process and, consequently, to the divergence of the algorithm. To solve this problem it is necessary to evaluate the threshold value of the mutation probability. As the mutation probability is given for an every single gene, and the divergence depends on the mutation probability and the selective pressure, the threshold of the mutation probability also depends on the genotype length. This dependence was derived from a series of tests (3000 experiments) and is presented on fig. 4.2(threshold values).

In the foregoing series of experiments (see section 4.3) also an optimal genotype length dependency for mutation probability was derived (fig. 4.3, optimal values). Mutation with derived probabilities helps in global optimum search and at the same time does not lead to divergence of GA. This probabilities are smaller then threshold values, because the crossover influence is also considered.

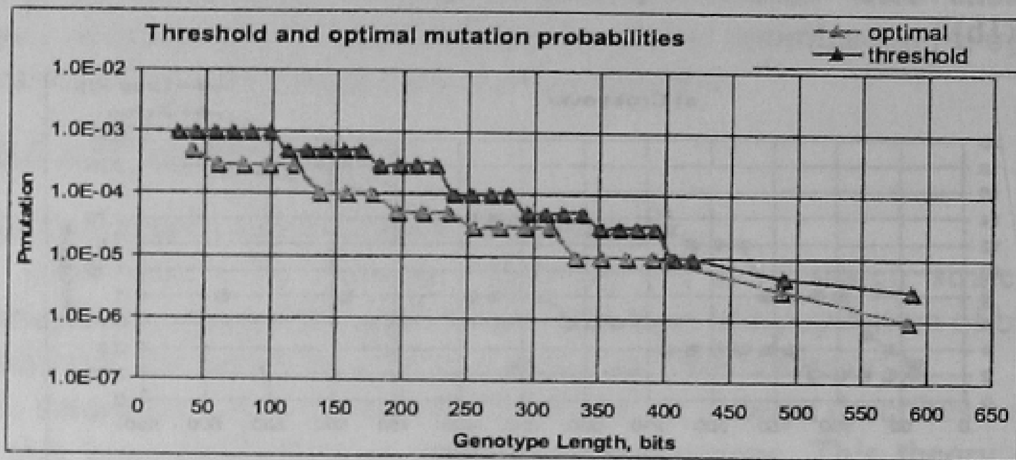


Figure 4.2: Derived optimal and threshold values of the mutation probability

Selection

The selection operator forms the next generation from the new individuals generated by mutation and crossover operators [λ , μ] or from new individuals together with their parents [$\lambda + \mu$]. Main selection methods are roulette wheel and its modification – universal stochastic sampling, which provides zero bias and minimum spread [4]. According to experimental results, universal stochastic sampling increases a probability of successful global optimum search. The selection probability for these methods is calculated proportionally to function fitness or according to the individual's rank, completely ignoring absolute fitness value (ranking selection). The ranking selection allows avoiding scaling approaches necessary for proportional selection, and selective pressure can be controlled more directly then by scaling parameters. Alternative method of selection is the tournament selection [7]. This method selects a single individual by randomly choosing some individuals from the current population and puts the best into the next generation. This process is repeated until the new generation will be completed.

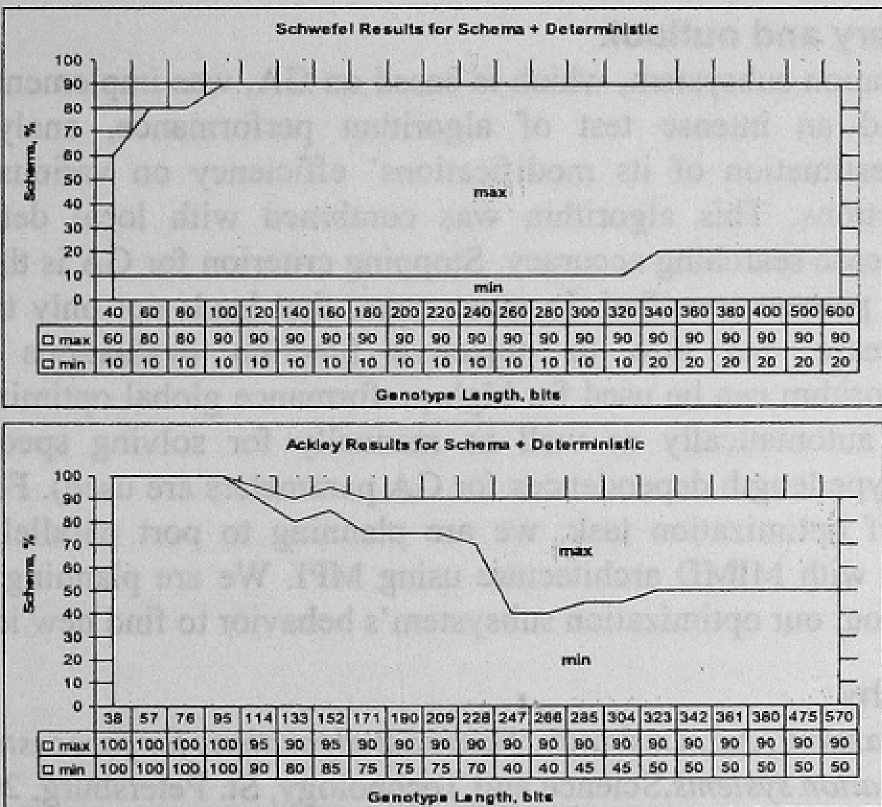
Analyzing results of various selection operators testing, best performance of algorithm is reached in a case of using tournament or linear ranking selection with large population size. Tournament selection has shown the best results in optimization of low complexity functions (sphere, step function), but at testing complex multimodal functions (Schwefel, Ackley) the best was ranking selection with the selective pressure value of 1.7. Tournament and linear ranking with the high selective pressure value provide high intensity of selection. Comparing takeover time values [7] of these two selection mechanisms, the interesting conclusion is that they are close. Therefore, using linear ranking selection for the simple functions' optimization does not lead to significant reduction of optimization productivity and can also be used as the method of selection chosen by default.

4 Caching system

An implemented to the system genetic method provides preservation of the objective function value for all individuals which are copied without changes from the previous generations. Due to this, objective function evaluations are reduced on the average by 61%. System has also a built-in caching of objective function value. It allows avoiding objective function recalculation during optimization for reappeared individuals with the same parameters. The largest benefit of using cache is reached at the finishing stage of algorithm, when values of parameters are near to a point of a global optimum. According to the testing results, the cache usage in GA allows to reduce the objective function evaluation on the average by 41%. As a result, due to some particularly technical solutions, amount of evaluations is reduced on the average by 76%.

5 Usage of the local deterministic methods

These methods are used in developed subsystem to increase accuracy of solution after GA has finished. Local deterministic methods (LDM) proceed with optimization after GA has approximately found a global optimum and just search for a nearest local optimum. This will be the global optimum if GA has stopped in its neighborhood.



	40	60	80	100	120	140	160	180	200	220	240	260	280	300	320	340	360	380	400	500	600
□ max	60	80	80	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90
□ min	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	20	20	20	20	20	20

	38	57	76	95	114	133	152	171	190	209	228	247	266	285	304	323	342	361	380	475	570
□ max	100	100	100	100	95	90	95	90	90	90	90	90	90	90	90	90	90	90	90	90	90
□ min	100	100	100	100	90	80	85	75	75	75	70	40	40	45	45	50	50	50	50	50	50

Figure 6.1: Effective formed schema percents for LDM start

Thus, LDM not only increase the accuracy of the solution, but also might decrease the number of objective function evaluations, when GA stops earlier. Stopping criterion for GA is the forming of the schema percent specified. Schema percent is percent of fixed schema positions among all individuals (ratio of schema order [Bäck96] to the genotype length). A series of experiments (about 100000) for different complex functions (Schwefel and Ackley) were made to determine the schema percent when the GA can be stopped (i.e. the neighborhood of the global optimum has been found). The results are presented on fig. 6.1 and they show minimal schema percent, when a global optimum already can be found, and a maximal schema percent, when an evaluations decrease is still present. According to these diagrams, smooth enough functions (e.g. Schwefel) can be effectively solved with low schema percent formed (about 10-20%). It is already possible for a small genotype length (for a small number of parameters). Whereas for the functions with strong beating (e.g. Ackley) good efficiency can be acquired only for a large genotype length (for a large number of parameters) when at least 50% of the schema have been formed.

Usage effectiveness of a combination GA + LDM compared to pure GA was derived. Although for small genotype length, effectiveness is not so big (particularly for functions with strong beating), but for a large genotype length decrease of objective function evaluations comes to 75% for Schwefel function and 45% for Ackley function on the average.

6 Summary and outlook

An optimization subsystem, which is based on GA, was implemented. There was performed an intense test of algorithm performance, analytical and experimental estimation of its modifications' efficiency on various artificial objective functions. This algorithm was combined with local deterministic method to increase searching accuracy. Stopping criterion for GA is the forming of the schema percent specified. In most cases, that leads not only to solution accuracy increase, but also to objective function evaluations decrease. Developed algorithm can be used for high-performance global optimization and can be setup automatically as well as manually for solving specific tasks (derived genotype length dependences for GA parameters are used). For parallel computation of optimization task, we are planning to port parallel GA's to supercomputer with MIMD architecture using MPI. We are planning to gather information about our optimization subsystem's behavior to find new ideas.

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