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VERIFICATION OF GLOBAL SEARCH PROCEDURE FOR RESPONSE SURFACE METHOD

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Abstract: *This paper presents a brief overview of the global optimization methods and experimental comparison of appropriate software. By solving of set of the recognized test problems using software based on different search methods, the reliability of obtaining of the global extremums is compared. Based on conducted analysis, it is shown a high effectivity of developed by authors' optimization algorithm in comparison with the modern genetic algorithms. In most cases high reliability is obtained with a noticeably smaller computation labor-intensity.*
Key words: *optimization, stochastic global search, genetic algorithm*

1. INTRODUCTION

The development of competitive technical engineering systems in these days is unimaginable without their optimization. In the development stages of various machines, constructions and complex mechatronic systems, computer modeling on the basis of mathematical models with the purpose of detailed investigation and improvement of their properties is becoming more and more widespread. In the field of mechanical engineering, the so-called virtual prototyping tools – software (Auzins et al., 2003 b; Janushevskis et al., 2000) that allows automatically creating mathematical models of mechanical systems to estimate the dynamical and strength properties of various objects and carry out their parametrical optimization,– are widely used. In practice, one is frequently faced with the so-called global optimization task.
From a mathematical point of view, if the optimization criterion does not satisfy the Lipschitz conditions and the search region is not limited, then factually it is incorrectly formulated in the sense that the criterion function's global optimum cannot be located with given accuracy after a specific limited number of calculations of the criterion function. In the case of the general "black box" model, the global optimization is carried out without a priori knowledge of the surface of the criterion function, which is defined by the criterion and the constraints. The domain of attraction is defined as a surface region where there is a local minimum and the constraints are satisfied. The method of global optimization must have a mechanism that allows to leave local minimums, while local optimization methods do not have such a mechanism and therefore attraction regions "catch" the local search methods. For this reason global search algorithms employ heuristic methods to search for new attraction regions.
The minimums of found promising regions often are located using such local improving procedures as gradient descent, Newton and quasi-Newton and other methods. It must be noted that in many practical tasks the finding of the global optimum is incommensurably costly, and sub-optimal solutions must suffice. Therefore various possibilities of obtaining the global optimum are sought for. One of the approaches is building and optimization of so-called metamodels.

2. THE RESPONSE SURFACE METHOD OF SYSTEM OPTIMIZATION

Optimal design is based on a mathematical model of the object. The level of complexity of practical systems is frequently very high, and their models are complicated non-linear high order equation (differential, integral, algebraic and others) systems, the parameters of which are not precisely known. Their parametric and structural identification and solution demands very large computing time resources. In such cases, to carry out optimization, the response surface method (RSM) (Myers & Montgomery, 2002; Auzins & Janushevskis, 2002; Rikards &Auzins, 2003) or the neural network approach (Waszcyszyn & Ziemianski, 2003) is usually used. The development of metamodels (surrogate models) from a small number of very time-consuming calculations, namely, mathematical experiments (in this case one must speak of a model of a model) or natural experiments, is a applied method of obtaining an empirical model that would allow to relatively easily find the global optimum.
In the construction of metamodels, polynomial functions, stochastic Kriging (Simpson et al., 2001) models, rational base functions (Dyn et al., 1986) or adaptive regression splines (Friedman, 1998) are most often employed. Polynomial functions stand out with the simplicity of their construction and calculation speed, which is very important for the carrying out of global optimization. Using RSM, the acceptable number of criterion and constraint calculations may be significant, and reach hundreds of thousands and even millions of tries, since its calculation requires a significantly smaller amount of time than the criterion calculation of the initial model.

3. A SHORT REVIEW OF THE GLOBAL OPTIMIZATION METHODS

In the solution of technical engineering problems, one is frequently faced with mixed non-linear programming problems with constraints, where the role of optimization parameters is taken up both by discrete and continuous variables. In many cases, it is possible to interpret the discrete variables as continuous ones. The constraints are most often taken into account by the transformation of the original problem into a problem without constraints, using penalty functions, barrier methods and Lagrange multipliers. Here we will discuss in more detail the methods used specifically in the case of continuous variables. The global search methods (Horst & Pardalos, 1995) can be divided into deterministic methods and stochastic methods. Deterministic methods employ such heuristic as the modification of search trajectories into trace based methods, as well as the introduction of penalties to avoid regions where there are no optimal solutions. Covering methods (Horst & Tuy, 1993)] isolates a region that does not contain a global optimum, and discards it, not searching there any further. This guarantees quality of the solution, iteratively reducing the search region. The obtaining of the solution requires a very thorough search of the space, that is, these methods are very time-consuming if the size of the problem is large. Branch and bound methods and interval methods recursively divide the search region into smaller sub-regions and separate the regions that do not contain an optimal solution. They are covering methods that estimate the criterion function's lower boundaries in the search sub-regions, allowing to estimate the quality of the local minimum. Combining this with numerically verifiable optimality sufficiency conditions, they allow to confirm the global optimality of the best obtained solution. However, in order to guarantee the quality of the solution, the problem must satisfy the Lipschitz conditions. In the worst case, they demand an exponentially increasing computational burden, and therefore are very time-consuming. In general, this "branch and bound" principle may be successfully employed in other heuristic-based methods. However, if the search region is large, these methods work badly.

Generalized descent methods (Vincent et al., 1992) continue the search trajectory every time that a local minimum is found. In the first approach, the trajectory methods modify the differential equation that describes the local descent trajectory in such a way that they may evacuate themselves from the local minimum. Their weakness is the large number of function calculations that must be carried out in regions that aren't promising. In the second approach, the criterion function is modified by imposing a penalty so that the algorithm would not return to an already found local minimum. The weakness consists in the fact that the more local minimums are found, the more difficult it becomes to minimize the modified criterion function.

So the determined methods may be divided into: 1) point-based methods that calculate the function in discrete points, for example, the generalized descent methods; and 2) region-based methods that calculate the function constraints in compact sets, for example, the covering methods. The point-based methods are unreliable but require less calculation, and vice versa.

The stochastic global optimization methods rely on probabilities to make decisions in searching for extremes. Random search methods include pure random search with single or multiple starts, random search along a line, adaptive random search, partitioning into subsets, substitution of the worst point, evolutionary algorithms and simulated annealing (Horst & Pardalos, 1995). The simplest way of getting out of a local minimum is to restart. The cluster or grouping methods (Torn & Viitanen, 1992) employ cluster analysis to avoid the already found local minimums. There are two strategies for grouping points around local minimums: 1) retaining only points with relatively small function values; 2) transferring every point to the local minimum, making only few local search steps. They work badly if the surface of the function is very rough, or if the search is captured in a deep ravine surface of local optimums. Methods that are based on stochastic models employ random variables to simulate the unknown values of the criterion function. The Bayesian method (Mockus, 1994) is based on a random function and minimizes the expected deviations from the global minimum estimation. Its effectiveness is not high.

Simulated annealing (Aarts & Korst, 1989) uses an analogy for the physical phenomenon that, heating and then slowly cooling metallic wares, a more homogenous crystalline state is obtained, in which the free energy of the base substance has a global minimum. The role of temperature has an important significance, since it allows the system to reach its lowest energy states with probability according to Boltzmann's exponential law, in such a way that it is possible to step over the energy sub-barriers, which would've otherwise forced the system to remain in the local minimum. Similarly as in physical annealing, convergence in simulated annealing may be slow. Therefore many improvements are used to speed up the process.

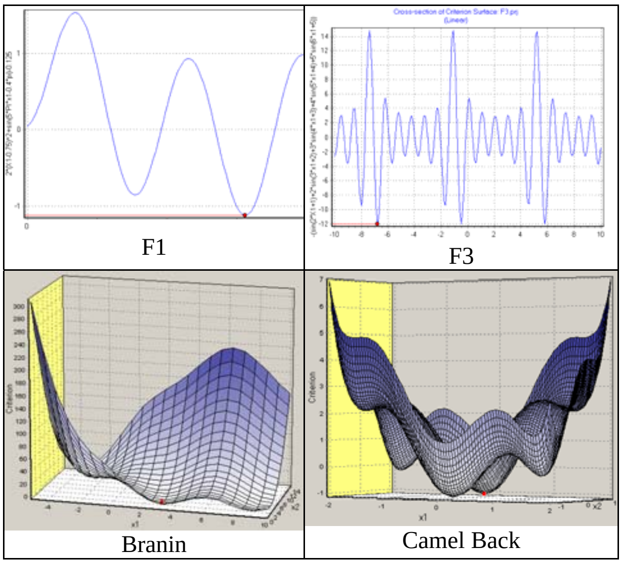
Genetic algorithms (GA) (Andre et al., 2001; Renders & Flasse, 1996; Koza, 1993) use biological evolution analogies, allowing mutations and crossovers between good local optimum candidates in the hope that ever better optimums will be found. In each search stage a configuration of all populations is maintained. Mutations are carried out in local searches, while crossovers operators ensure a possibility of leaving the local minimum attraction regions. The crossovers laws have a large probability of creating offspring of similar or better fitness. The effectiveness of GA depends on the correct conditions of selection and crossovers. The coordinates interchanging are sufficiently good if these coordinates have a nearly independent influence on fitness, but if the influence is strongly correlated, as it is with functions with deep narrow ravine surfaces that are not parallel to coordinate axes, then GA has great difficulties. A successful configuration of GA demands a thorough investigation of the concrete problem.

Taboo search (Battiti, 1994) introduces a taboo list that contains information on the search history. In each iteration a local improvement is made. However, thanks to the taboo list, movement towards already located solutions is forbidden, that is, a taboo has been placed. The taboo list protects from returning to the local optimum from which the search has recently evacuated. Taboo searches give good results in the solution of large discrete optimization problems.

Stochastic methods are classified as unreliable. However, these methods are often the only ones that allow the solution of large-scale problems with an acceptable workload. Currently in engineering practice exactly the stochastic methods are the most frequently applied. Therefore the developed Edaopt (Auzins et al., 1999 and 2003 a) optimization algorithm is compared only with these most effective methods.

4. ANALYSIS OF OBTAINED RESULTS

To evaluate the search effectiveness of the developed random search two-phase multistart optimization algorithm (below Edaopt), it was tested by solving set of test problems (Andre et al., 2001). Figure 1 shows the test functions or their characteristic sections with the global minimums found by Edaopt. They were found with a practically 100% success in all search series. In solving some of the problems (for example, Griewank10, which contains several thousands of local minimums in a 10 parameter space), the algorithm occasionally converged to extremes close to the global optimum rather than to the global optimum itself. In this way in all cases the most promising optimum region was found. This has a great significance, since in practical tasks it is very important not to miss these regions.



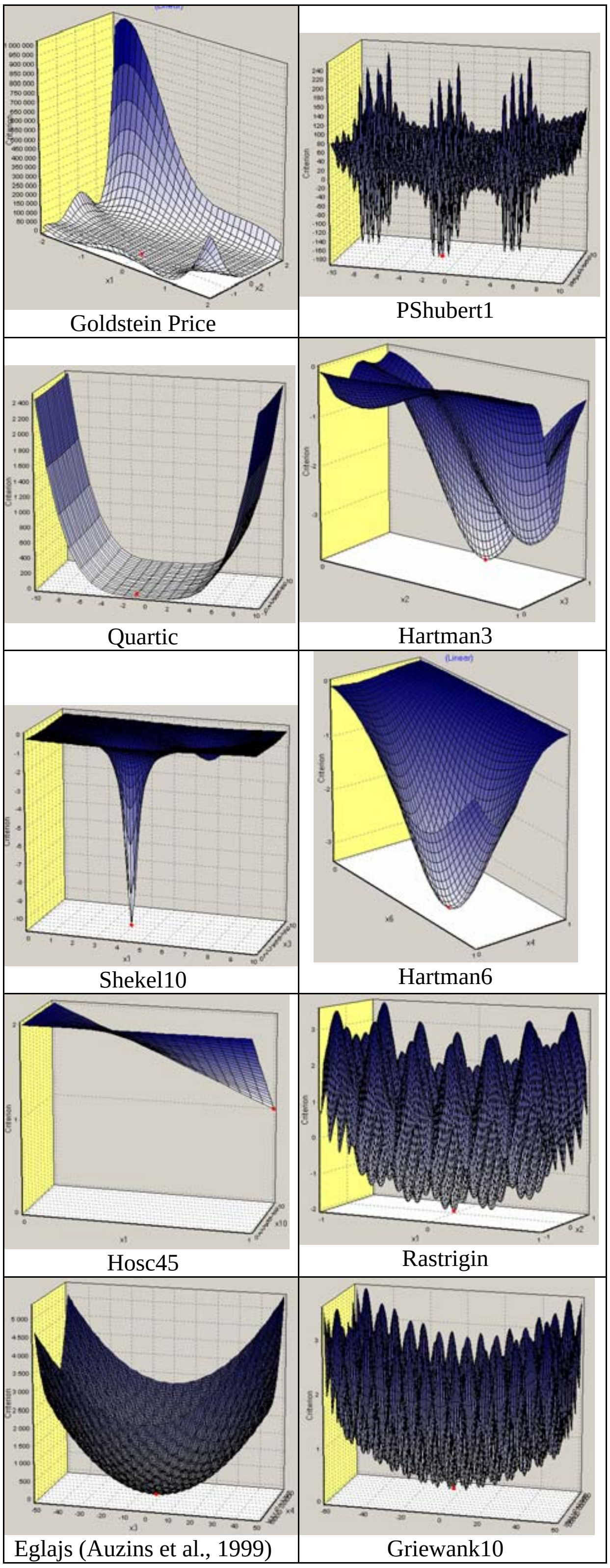


Fig. 1. Test function minimums found by Edaopt

Table 1 shows comparative results between Edaopt and standard GA and improved genetic algorithm (GA+) software. To make objective comparison possible, it was necessary to adhere to the calculation conditions given in literature (Andre et al., 2001). Since stochastic methods were evaluated, then the search for each function's minimum was attempted 100 times. The search was considered successful if the function's global minimum was found with the given accuracy. As can be seen, standard GA guarantees a 100% success (global minimum

Function (Number of para-meters)	Number of calculations			Absolute error			Success %	
	GA	GA+	Edaopt	GA	GA+	Edaopt	GA	GA+
F1 (1)	5566	784	156	0.000	0.000	0.0000	100	100
F3 (1)	5347	744	131	0.001	0.014	0.0002	100	100
Branin (2)	8125	2040	593	0.003	0.002	0.0018	81	100
Camel Back (2)	1316	1316	346	0.005	0.005	0.0048	98	100
Goldstein Price (2)	8185	4632	816	0.229	0.013	0.0127	59	100
PShubert 1 (2)	7192	8853	32849	4.563	0.983	0.4467	63	100
PShubert 2 (2)	7303	4116	1430	4.772	0.986	0.8593	59	100
Quartic (2)	8181	3168	1134	0.003	0.002	0.0018	83	100
Hartman 3 (3)	1993	1680	1150	0.025	0.020	0.0197	94	100
Shekel5 (4)	7495	36388	500187	6.067	0.072	0.0521	1	97
Shekel7 (15)	8452	36774	390185	4.856	0.165	0.0939	0	98
Shekel10 (4)	8521	36772	390175	5.126	0.074	0.0950	0	100
Hartman 6 (6)	19452	53792	650475	0.144	0.033	0.0118	23	92
Hosc45 (10)	11140	126139	14020	1.000	0.392	0.0000	0	2

Table 1. Characteristics of optimization algorithm effectiveness (GA and GA+ results taken from (Andre et al., 2001), success of Edaopt for all cases equal 100%)

found in all 100 attempts) only with one-dimensional F8 and F9 functions, while with other functions the success is more modest and in some cases GA is entirely unable to find global minimums.

Significantly better results are provided by GA+, the "heuristic coefficients" of which have been improved. From practice we know that with specific test problems these coefficients may be fitted in such a way that the global extremes for these functions can be found with only a few iterations, while for the optimization of other functions the algorithm becomes practically useless. Regardless, we will compare the developed algorithm exactly with GA+. The table shows data only on the functions with a number of parameters up to 10, on which the work (Andre et al., 2001) gives GA+ effectiveness data. In optimizing F1, F3, Branin, Camel Back, Goldstein Price, PShubert2 and Quartic functions, the global minimum finding accuracy is higher and simultaneously the number of function calculations is 3 to 5.5 times smaller with Edaopt than with GA+, that is, the effectiveness of Edaopt is definitely higher. This is especially obvious in optimization of the Hosc45 function, where the location of the global minimum with Edaopt requires 9 times less points (function calculations), and the percentage of success is 100% for Edaopt compared to 2% for GA+, which shows the high reliability of our algorithm, at the same time signifying a rather unsuccessful fit of coefficients for the GA+ method.

The obtained results do not, however, show that GA is not suitable for global search procedures, quite the contrary, GA, simulated annealing and taboo search are among the most effective methods, since the finding of a practical solution never confines itself to a few search series, but is always connected with a thorough and detailed investigation, namely, building of sensitivity curves and evaluation of functioning stability in optimality regions, etc.

It should be noted that it is hard to achieve a 100% success rate with stochastic search methods, since there is always a probability of carrying out an ineffective search with a limited number of points. For example, when attempting to find global minimums for the Hartman6 function and Shekel function with 5 and 7 local minimums in a 4 parameter space with 100% success, it turned out that the number of points necessary for Edaopt is about ten times greater than for the GA+ method with a corresponding 92%, 97% and 98% success. This fact does not indicate the superiority of one or the other method, but it shows that in order to achieve reliability close to 100%, the minimal point number must be of the given order. To achieve a more or less objective comparison, it would be necessary to ensure a precise coincidence of absolute errors and successes. Since the aim was to obtain not a formal numeral evaluation, but a qualitative evaluation of the algorithms, such a comparison was not carried out. More so since with the Edaopt standard interface the search is not terminated on a given precision, but on the computer precision (10-byte float point calculation), and the only parameter necessary to provide is the maximal number of algorithm iterations and no other parameters ("heuristic coefficients") are required. It must be noted that with some test problems we had to carry out the comparison with, in our opinion, high relative error level, namely, 1%, when the deviation of the parameters from their optimal values may be very significant. Manipulation with precision may bring a great amount of subjectivity into the evaluation.

In the end it should be noted that the global minimums for the Rastrigin and Eglajs functions were located with Edaopt without much difficulty. Searching for minimums for the Branin function, each of the 3 global minimums was found with a 1/3 probability, while for the Camel Back function both global minimums were found with a 1/2 probability.

5. CONCLUSIONS

The solution of a wide scope of test problems has shown that the developed Edaopt algorithm gives a significantly higher reliability in searching for global optimums, in comparison with traditional standard stochastic search algorithms, and must be considered as an effective alternative. In most cases high reliability is obtained with a noticeably smaller computation labor-intensity. However this is less important in cases where the metamodel approach is applied. In cases where the RSM is used, the reliability of the optimum finding arises as the most important characteristic of the optimization algorithm. Additionally, the Edaopt software allows the user to visually orientate himself in the seemingly endless optimization jungle.

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