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ON DESIGNING A COMPUTATIONAL EXPERIMENT SYSTEM FOR VARIOUS ENGINEERING INTERPRETATIONS OF A GLOBAL OPTIMIZATION PROBLEM

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ABSTRACT

This article proposes a software system design to achieve a numerical solution of a global optimization problem. A key part of it is the classification of global search algorithms by a methodological criterion, which enables a systematic comparative analysis of specific implementations of each method within the scope of engineering interpretations of a global optimization problem. The proposed architecture accommodates modular extensions of the system, which allows designing algorithmic modifications of global search methods of various classes, taking into account the impact of parameter numerical values on computation performance.

Keywords: global search algorithms, methodological classification, computational experiment, computation performance, inverse problem of mathematical modelling, comparative analysis of algorithms, expert system designing.

1. INTRODUCTION

The global search theory originates as an extension of local optimization; the problems investigated within the framework of this theory have been examined in much less detail as compared to the local extremum seeking theory and methodology [15]. The growth of technology in the area of big data processing is a prerequisite for creation and development of this theory. On the one hand, the architecture of big data storages requires optimization with regard to any specific search task. On the other hand, global search algorithms must be based on a methodology other than steepest descent which is the basis of local methods. Discrete methods of the global optimization theory, as well as random search modifications, also known as "genetic algorithms", are among the technologies known under the common name Data Mining [11].

Academic interest to global optimization methods (GOM) is primarily a result of the importance of real-life problems in the area of data storage architecture. However, the following aspect is equally important: when the data comprise a result of a costly full-scale experiment, they form the basis of real-life object and process models. In such a case, modelling methodology involves a solution of the inverse problem. The inverse problem of mathematical modelling, which consists in matching somewhat optimal parameters, is inappropriate; in particular, because it has multiple solutions. When solving this problem, GOMs are used in accordance with their structure and with special aspects of the problem statement.

Software implementations of GOMs are quite wide-ranging. However, it should be noted that two classes can be obviously set apart from the whole variety of software:

- software implementation of popular algorithms (e.g. genetic algorithms or branch-and-bound algorithms) in the free software segment.
- professional information systems, where a certain GOM is implemented as a software module.

It makes systematic comparative analysis of algorithms of different classes more difficult when model problems are solved. This is why we have attempted to develop an application intended for comparison of GOM performance in computation schemes of common methods employed in mathematical modelling.

2. STATEMENT OF A GLOBAL OPTIMIZATION PROBLEM

Assume the following function is defined: F(x), $x \in X \subset \mathbf{R}^n$, $F: X \to \mathbf{R}$

Required: to find the $\mathbf{x}^*$ element among **x** elements of the **X** set, which affords the minimum value of the function F(x).

If the optimization set $X = \mathbf{R}^n$, then the unconstrained optimization problem can be solved, otherwise the constrained optimization problem can be solved.

Mathematical solution of the optimization problem means performance of one of the four operations:

1. To find $\vec{x}^* \in X$, such that $F(x^*) = \min_{x \in X} F(x^*)$
2. If there is not any minimum point, to find $\inf_X F(x^*)$
3. To show that X is an empty set;
4. To show that the target function is not bounded from below;

For steps 3 and 4 assume the optimization problem is degenerated.

Evidently the minimization requirement does not restrict the generality of the problem statement.

The following structural unit of the problem are important for the algorithm design:

- The optimization set - $X \subset R^n$
- The target function - the mapping $F:X \rightarrow R$;
- GOM classification is based on two different approaches to these concepts.

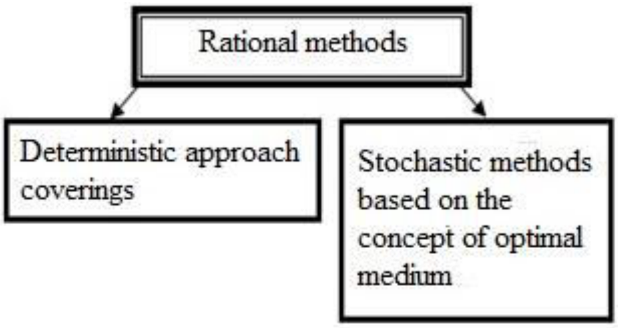
3. CLASSIFICATION OF GLOBAL OPTIMIZATIONS METHODS

Global minimum search methods are iterative methods, so the rule of transition to the next iteration and formulation of the algorithm stopping rule play a key role in their design.

Let us set apart two groups on the first stage of classification:

- Rational methods. Algorithms of this group are used in design of the rule of transition to the next iteration and are based on mathematical properties of the target function and the optimization set, which are considered already known. This approach ensures convergence of the iterative method; however, it is used less often than the methods of the second group due to severe restrictions of the set and the target function.
- Heuristic methods. The design of these algorithms employs a flexible rule (heuristics), which can be applied irrespective of fundamental properties, such as continuity and differentiability of the target function, convexity and simple connectivity of the optimization set.

Figure-1 illustrates the generalized classification of rational and heuristic methods [7, 8].



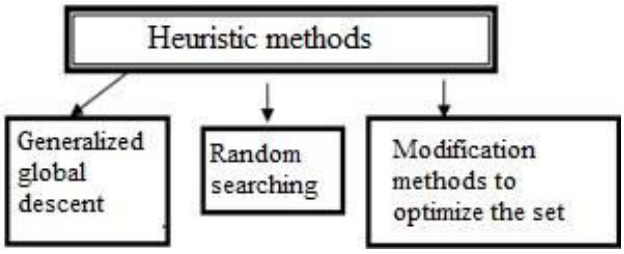


Figure-1. Classification of rational and heuristic GOMs.

On the next level the rational methods are divided into two groups on the basis of the target function construction. Deterministic methods are used for functions, where random distributions are not used for calculation of values. This group includes covering methods, based on convexity of the optimization set, and steepest multiple descent algorithms, based on calculation of a gradient of a continuously differentiable function.

Stochastic methods are used for functions, representing implementations of random processes. This group includes algorithms, based on the Bayesian concept, and the so-called Strongin information algorithms [13, 14]. However, the implied complexity of the theoretical framework involved in these methods holds off the experimenters.

Figure-2 illustrates the classification of heuristic algorithms under the common name of "random search". Convergence of this class is established by the respective theorem [15]. The methodology of these algorithms may be reduced to sequential modelling of random distributions in the whole optimization set.

Currently, the methods of the third group, i.e. various evolutionary algorithms and the simulated annealing method, are widely used. For example, natural selection process modelling is used in genetic algorithms, and the particle swarm optimization method (hereinafter PSO) is based on modelling a particle population behaviour over the optimization set.

These methods are appealing because their software implementation is simple and no calculation of a gradient is required during the search process.

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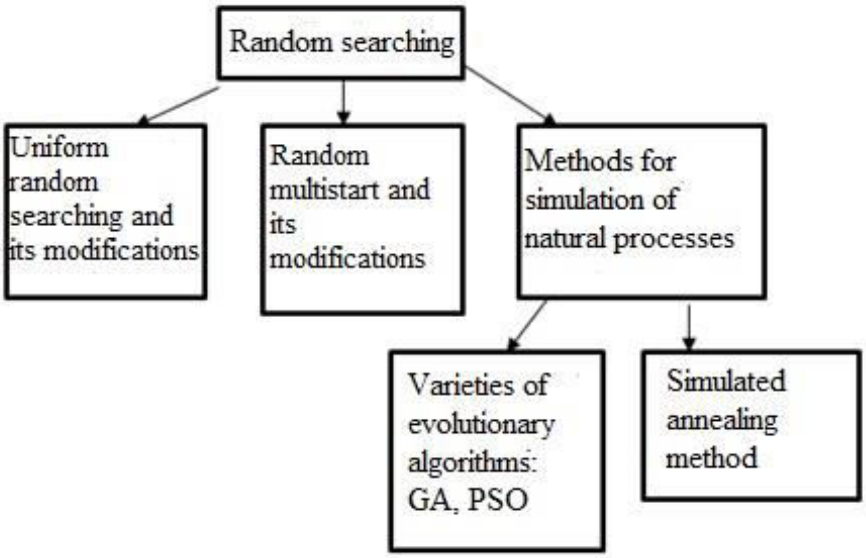

Figure-2. Classification of random search methods.

Figure-3 below illustrates the classification of methods, where the rule of transition to the next iteration is based on structuring of the search set. A number of special aspects shall be pointed out here:

- The design of transition rules for these methods also employs random distributions in the optimization set, which makes them akin to algorithms of the previous class.
- The difference between the groups of algorithms within this class is determined by the design of rules of splitting the set of acceptable solutions into subsets and carrying out a search by each iteration in each of such subsets.
- The issue of having these methods converge on a global minimum shall be resolved case by case, since no general methodology of proving convergence exists.

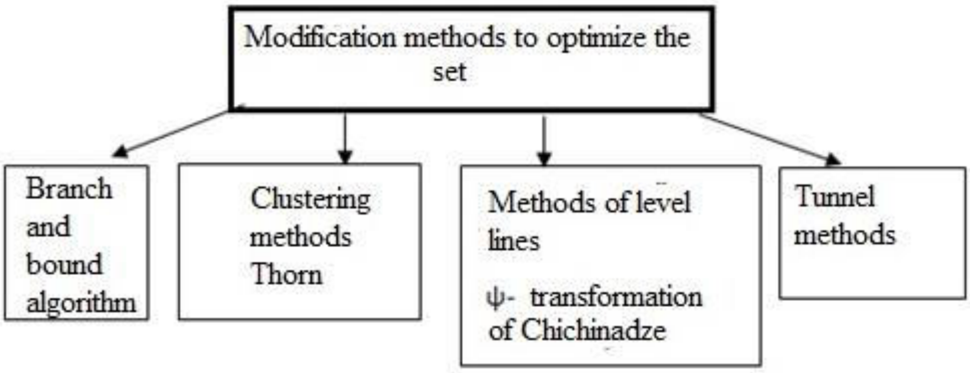

Figure-3. Classification of GOMs with transformation of an admissible set.

Branch-and-bound algorithms are based on sequential splitting of an acceptable solutions set, followed by elimination of subsets containing no solution. In order to evaluate a subset, it has to be tested against a certain condition. The list of conditions is formed in the process; initially it contains only one element that corresponds to the whole set of acceptable solutions defined by the original problem. Splitting (branching) one element on the list of conditions into several new problems and solving an estimation problem for each of them is performed on every stage of the branch-and-bound method.

4. REVIEW OF PROBLEMS SOLVED BY GOMs

As evident from the classifications provided, the method essentially depends on the nature of calculations performed during determination of the target function value, as well as on the optimization set structure. So, a certain method cannot be definitely recommended when solving a problem. A review of extremum problems common for the engineering practice is provided below, in order to identify their structure and facilitate the further search of a global solution.

4.1 The inverse problem of mathematical modelling (using the inverse problem of geological exploration as an example)

A mathematical description of laws determining the functioning of an object or process that is defined by given input variables and parameters is included as an operator in a direct problem. For example, if an object is described by a sorted list of numeric parameters p=(p_1, p_2, … p_n), i.e. p∈R^n, we can denote a direct problem operator (matrix, integral, differential, etc.) by D and apply this operator to the P parameter vector set in order to get the output set Y⊂R^m of all theoretical solution, i.e. implementations of a mathematical model DP=Y, at that y∈ Y is some solution of the direct problem.

Solution of the inverse problem in accordance with these notations will be represented by an operator equation in p

$$Dp=y \tag{1}$$

Solution of the inverse problem is clearly not the unique solution; this is one of the reasons why the inverse problem of mathematical modelling is inappropriate.

Furthermore, let $\tilde{Y}\subset R^m$ be the set of experimentally measured vectors of physical implementations of an object or process. Minimal residual condition

$$\left\| \tilde{y} - Dp \right\|_{R^m} \to \min_{p\in P} \tag{2}$$

defines a quasisolution of the operator equation (1) in a compact set P⊂R^n [1].

An integral operator of geophysical fields' calculation (gravity, magnetic, electrical, seismic velocity fields) represents operator D in the inverse problem of geological exploration. The set P is defined by the proposed shape of an object, responsible for experimentally measured anomalous values for these fields. Vector p is a vector of geometrical parameters of objects, for example, the radius and occurrence depth for a sphere.

Condition (2) defines the trial-and-error method, widely used in geophysical interpretation. Heuristic methods of global optimization are widely used during search of a quasisolution due to complicated structure of the P set and general inappropriateness of the inverse problem. Minimal residual function (2) is used as an optimization criterion.

4.2. The optimal system synthesis problem (using design of a chemical-engineering system as an example)

The optimal design problem differs from the problem discussed above by formulation of an optimality criterion. Apart from the residual norm (2), the optimality criterion includes functions with economic, technological, or environmental substance. The problem is multicriterion if a total of these criteria is considered.

Multiextremality in these problems is caused by a large number of recycles in the chemical-engineering process chart. The optimization set in all problems has a complicated structure due to equality constraints, representing the material and process balance conditions. The general statement of the economic criterion optimization problem is provided below [9].

Let X be the linear space over a field of real numbers with dimension n. x∈ X , $\vec{x}$ =(x_1, x_2,…, x_n); the optimization set X⊂X

$$X = \{\vec{x} : x_i \in [a_i; b_i], \quad \forall i = 1...n\}$$

x_i has economic or technological substance let us denote the chemical-engineering system sales income by L; let us denote the total chemical-engineering system costs by S.

$$L = f(\vec{x}), \quad S = g(\vec{x})$$

Equality constraints, represented by material and energy balance equations, are applied to the vector $\vec{x}$:

$$p_i(\vec{x}) = a_i \quad, i = 1...n$$

And conditions represented by inequalities $\varphi_i(\vec{x}) \geq b_i$ i=1…m

Required: to find

$$\vec{x}^* = \min_{x_i\in X} S(\vec{x}) \quad \text{or} \quad \vec{x}^* = \max_{x_i\in X} L(\vec{x})$$

under the given conditions.

4.3. Direct optimal control problems, based on the Lagrange maximum principle

Problems of this class are the most complicated problems within the optimization theory. The functional determined under initial-boundary conditions is used as an optimization criterion, and the acceptable solutions set represents a fixed-type set of control paths U.

The maximum principle is applied to the general control problem.

Let there be given two points x_0 and x_1 in the phase space X: it is required to choose from all admissible controls $u(t)$, as well as parameters t_0 t_1 , transferring the phase point from position x_0 to position x_1, in such a way as to assign the smallest possible value to the functional $\int_{t_0}^{t_1} f^{(0)}(x,u)dt$.

The review and calculation models of the approximate optimal control are provided in Gurman, VI, Racine, IV, & Blinov, AO. Evolution and prospects of approximate methods of optimal control [3].

Multiextremality in this problem is caused by complicated parameterization of the required control function and the phase space structure. The following is a classic example of the control optimization problem:

4.4 Maximization of atmospheric flight range of an aircraft

Let us consider an aircraft whose position is described by the following parameters: flight range and altitude, the value of velocity vector and the angle of its inclination to the horizon. The angle of attack and a function that corresponds to in-flight control of wing geometry (i.e. wing effective area) act as controls. It is required to find control functions which ensure a maximum flight range.

5. THE SOFTWARE SYSTEM ARCHITECTURE

The software system design is based on the methodological classification of GOMs discussed above. A software architecture which will simplify the systematic comparative analysis is required for investigation of computation performance of specific implementations of algorithms of different classes within the framework of generalized models of engineering problems.

So, development of the software system mainly intended to achieve the following: possibility of hassle-free scaling to a maximum number of problems and adding other global optimization methods.

A program structure corresponding to the specified requirements to scalability is necessary in order to achieve this goal. At the same time, it must be easily understandable for expert users, willing to extend the software system through adding other problems or implementing other methods.

6. THE CLASS DIAGRAM

The main classes, which implement the option "Solve a global optimization problem with manual input of parameters" and "Solve a global optimization problem by following a computational experiment plan", are presented on Figure-5. The UConrol control class is responsible for loading of the software system entity classes: RESEARCHER, TASK, METHOD, EXPR_PLAN, REPORT, and exercises control over running processes.

The RESEARCHER abstract class is responsible for user identification, its access level depending on the problem, selection of a method and a problem, as well as log keeping and saving of reports on activities of each user.

The global optimization problem solving process is described by the TASK and METHOD abstract classes, from which, in their turn, the classes that implement the aforesaid specific problems and methods derive.

The METHOD class has descendants, i.e. EMPIRIC and RATIONAL CLASSES, which are not presented on the diagram. Inclusion of these classes is necessary because of qualitative methodological differences between the algorithms. The EMPIRIC class has no attributes, determining the properties of the optimization set, as well as the method, determining the problem selection mode, i.e. restricting the properties of target functions. This is particularly useful for the methods that involve the so called "information algorithm" [13]. The RATIONAL class also includes a method based on the Bayesian approach to optimization, which requires stiff structuring. The classes presented on the diagram, implementing specific methods, are actually descendants of the EMPIRIC class.

In addition, the Consider abstract class implements representation of the target function estimation, which is specific to each problem, and describes the method of mutual comparison of objects, representing the search path elements.

It should be noted that detailed analysis during the first stage of the software system testing was performed using the RANDOM SEARCH class members. This is primarily due to relative algorithmic simplicity of these methods and their current popularity among the researchers.

The ψ-transformation method was considered because of its flexibility with regard to the target function relief and the original design.

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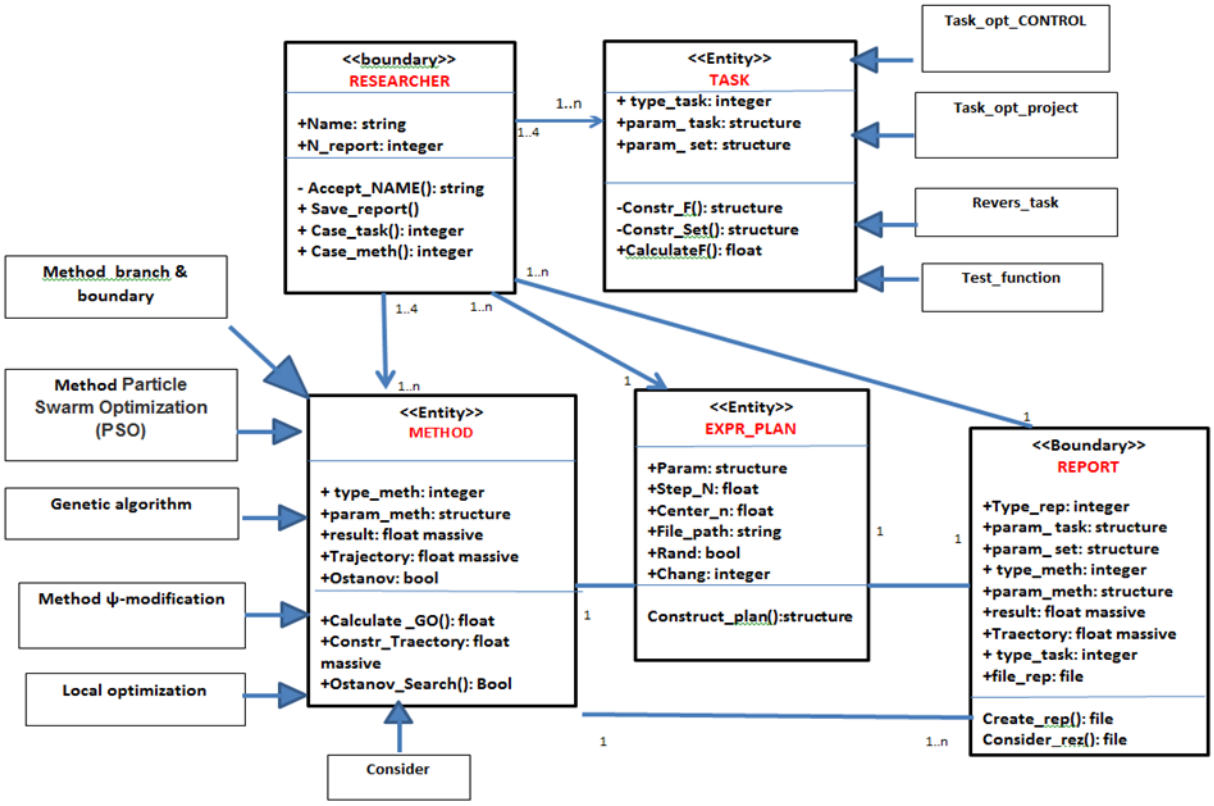

Figure-4. Class diagram.

CONCLUSIONS

This paper presented an approach to the software system design that preserves the integrity of the global search theory. The algorithms are classified according to the methodological criterion, i.e. the design is based both on the structure of the main problem units and the algorithm development method. Thus, a computation system developed on the basis of this design can effectively perform comparative analysis of algorithms by relying on common features and differences in their internal structure. It provides a basis not only for designing a computing system and implementing some global search algorithms, but also for designing an expert system intended to select a specific problem solution algorithm. This possibility offers great opportunities for further design.

The analysis of solved problems related to various areas of engineering made it possible to generalize and define the systemic issues of empirical global search algorithms:

- selection of an initial position for search paths;
- flexibility of paths, i.e. possibility to change the direction and numeric parameters during every stage, as well as to unite the paths;
- the computational algorithm stability with regard to its parameters, i.e. a path, leading to the global optimum point, must exist in case of any parameter variations;

The search process stopping problem, i.e. formulation of a clear path completion criterion.

These problems may be called "informational", as their solution decreases both the initial uncertainty and the uncertainty at every stage of the global search. It is the solution of these problems that is the subject of systematic comparative analysis of global search algorithms.

Extension and development is also possible within the framework of technical solutions of the software system implementation. The proposed software system architecture must be generalized for a distributed solution that involves client/server architecture. The structure of optimization algorithms allows implementation of parallel computing as well. Testing these solutions and determining their computational efficiency and time efficiency is a separate research task.

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