FEDERAL STATE AUTONOMOUS EDUCATIONAL INSTITUTION

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**Report**

**on the practical task No. 2**

**“Algorithms for unconstrained nonlinear optimization. Direct methods”**

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# Goal

The use of direct methods (one-dimensional methods of exhaustive search, dichotomy, golden section search; multidimensional methods of exhaustive search, Gauss (coordinate descent), Nelder-Mead) in the tasks of unconstrained nonlinear optimization.

# Problem

**I**. Use the one-dimensional methods of exhaustive search, dichotomy, and golden section search to find an approximate (with precision ) solution for the following functions and domains:

1. ;

2. ;

3.

Calculate the number of f-calculations and the number of iterations performed in each method and analyze the results. Explain differences (if any) in the results obtained.

**II**. Generate random numbers Furthermore, generate the noisy data , where according to the following rule:

where are values of a random variable with standard normal distribution. Approximate the data by the following linear and rational functions:

1. (linear approximant),
2. (rational approximant),

by means of least squares through the numerical minimization (with precision ) of the following function:

To solve the minimization problem, use the methods of exhaustive search, Gauss and Nelder-Mead. If necessary, set the initial approximations and other parameters of the methods. Visualize the data and the approximants obtained in a plot separately for each type of approximant so that one can compare the results for the numerical methods used. Analyze the results obtained (in terms of number of iterations, precision, number of function evaluations, etc.)

# Theory

Optimization methods are numerical methods for finding optimal (in a sense) results of objective functions, for example, within the framework of mathematical models of certain processes. Optimization methods are widely used in data analysis and machine learning.

Let the objective function be given, where is, generally speaking, a multidimensional vector from some subset of the Euclidean space . The subset can be either limited or, in particular, coincide with the entire space . Below, for brevity, we will consider only the problem of minimizing the function f on the set (we can move from minimization to maximization by considering instead of ).

By solving the optimization (minimization) problem we mean finding such that . There is a special notation for . If is found, then, naturally, can also be found.

The stated formulation of the optimization problem implies the search for a global minimum of on . However, below we will also consider the search for a local minimum of on , when the value of is minimal only in a certain neighborhood of the point . Note that often the search for a local minimum is much simpler than a global one.

In this lab we work with direct optimization methods (zero order optimization methods). By definition, when searching for , they use only the values of the function f itself, but not its derivatives. These methods, in particular, are applicable for continuous (and not necessarily differentiable) functions of one variable x on the interval . Generally speaking, it turns out that direct methods can be used for a fairly wide class of functions f. This, however, is compensated by the rather low rate of convergence of the corresponding iterative processes.

Exhaustive search (brute force) is a method for solving mathematical problems. Refers to the class of methods for finding solutions using various options. The complexity of exhaustive search depends on the number of possible solutions to the problem. If the space solutions are very large, then a complete search may not yield results for several years.

Dichotomy method eliminates exactly half the interval at each iteration. When using the method, it is assumed that the function is continuous and has a different sign at the ends of the interval. After calculating the value of a function in the middle of the interval, one part of the interval is discarded so that the function has a different sign at the ends of the remaining part. Iterations of the bisection method stop if the interval becomes small enough.

The golden section method is a method of searching for the extremum of a real function of one variable on a given interval. The method is based on the principle of dividing a segment in the proportions of the golden section. It is one of the simplest computational methods for solving optimization problems.

The Nelder-Mead method is a method of optimizing (searching for the minimum) a function of several variables. A simple and at the same time effective method that allows you to optimize functions without using gradients. The method is reliable and, as a rule, shows good results, although there is no theory of convergence.

The algorithm consists in the formation of a simplex and its subsequent deformation in the direction of the minimum, through three operations: reflection; expansion; contract.

A simplex is a geometric figure that is an n-dimensional generalization of a triangle. For one-dimensional space it is a segment, for two-dimensional space it is a triangle. Thus, an n-dimensional simplex has n + 1 vertices.

# Materials and methods

In this task, all calculations were performed on the student's personal laptop. The work was performed in the Python programming language.

# Results

## The one-dimensional methods

Based on the task at hand, several one-dimensional methods were implemented. The results obtained for methods of exhaustive search, presented in Table 1. The results for methods of dichotomy, presented in Table 2. The results for methods of golden section search, presented in Table 3.

Table 1 – Data for methods of exhaustive search

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | f-calculation | number of iterations |
|  | 0 | 1000 | 1000 |
|  | 0 | 1000 | 1000 |
|  | -0.2172 | 990 | 990 |

Table 2 – Data for methods of dichotomy

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | f-calculation | number of iterations |
|  | 0 | 22 | 11 |
|  | 1.2056\*10-10 | 22 | 11 |
|  | -0.2172 | 22 | 11 |

Таблица 3 – Данные для methods of golden section search

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | f-calculation | number of iterations |
|  | 0 | 17 | 15 |
|  | 4.9256\*10-11 | 17 | 15 |
|  | -0.2172 | 17 | 15 |

Based on the data obtained, we can conclude that the fastest method is methods of golden section search since it has the least number of calculations. The slowest method is methods of exhaustive search, since it searches through all possible values.

Methods of dichotomy, although it outperforms methods of golden section search in terms of the number of iterations, methods of golden has a smaller number of calculations due to the fact that in the algorithm cycle two calculations are performed alternately, that is, one per cycle, and two actions are necessary before the beginning of the cycle.

In all algorithms, the values of are calculated almost identically.

## The multi-dimensional methods

Next, noisy data was generated for approximation by linear and rational functions, and brute-force, Gaussian, and Nelder-Mead methods were used to solve the minimization problem.

For linear approximation with methods of exhaustive search are presented in Figure 1, and for rational approximant in Figure 2.

Изображение выглядит как снимок экрана, текст, линия, диаграмма

Автоматически созданное описание

Figure 1 – Exhaustive search linear approximant  
Изображение выглядит как снимок экрана, линия, текст, диаграмма

Автоматически созданное описание

Figure 2 – Exhaustive search rational approximant

Изображение выглядит как снимок экрана, линия, диаграмма, График

Автоматически созданное описание

Figure 3 – Gauss linear approximant

Изображение выглядит как снимок экрана, линия, диаграмма, График

Автоматически созданное описание

Figure 4 – Gauss of rational approximant

Изображение выглядит как снимок экрана, текст, линия, диаграмма

Автоматически созданное описание

Figure 5 – Nelder-Mead linear approximant

Изображение выглядит как снимок экрана, текст, линия, диаграмма

Автоматически созданное описание

Figure 6 – Nelder-Mead rational approximant

Table 2 – Data of linear approximant

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| method | a | b | f-calculations | number of iterations |
| Exhaustive search | 0.722 | 0.722 | 1000000 | 1000000 |
| Gauss | 0.724 | 0.721 | 34034 | 34 |
| Nelder-Mead | 0.7222 | 0.7219 | 42 | 23 |

Table 3 – Data of rational approximant

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| method | a | b | f-calculations | number of iterations |
| Exhaustive search | 0.768 | -0.516 | 1000000 | 1000000 |
| Gauss | 0.999 | -0.999 | 38000 | 38 |
| Nelder-Mead | 0.7678 | -0.5163 | 71 | 37 |

# Conclusion

Thus, when performing this work, I studied and applied one-dimensional methods of enumeration, dichotomy and the golden section and multidimensional methods of enumeration, Gauss and Nelder-Mead in problems of unconditional nonlinear optimization.

Among one-dimensional algorithms, golden section search turned out to be the fastest, and among multidimensional algorithms Nelder-Mead with linear approximant.

# Appendix

GitHub link: