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.

Problems

I. Use the one-dimensional methods of exhaustive search, dichotomy and golden section search to find an approximate (with precision $\varepsilon = 0.001$) solution x: $f(x) \rightarrow min$ for the following functions and domains:

1. $f(x) = x^3, x \in [0, 1]$;
2. $f(x) = |x - 0.2|, x \in [0, 1]$;
3. $f(x) = x\, sin\frac{1}{x}, x \in [0.01, 1]$.

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 $\alpha \in (0,1)$ and $\beta \in (0,1)$. Furthermore, generate the noisy data $\{x_k, y_k\}$, where $k = 0, \dots, 100$, according to the following rule:

$$y_k = \alpha x_k + \beta + \delta_k, x_k = \frac{k}{100},$$

where $\delta_k \sim \mathrm{N}(0,1)$ are values of a random variable with standard normal distribution. Approximate the data by the following linear and rational functions:

1. $F(x, a, b) = ax + b$ (linear approximant),
2. $F(x, a, b) = \frac{a}{1+bx}$ (rational approximant),

by means of least squares through the numerical minimization (with precision $\varepsilon = 0.001$) of the following function:

$$D(a, b) = \sum_{k=0}^{100} (F(x_k, a, b) - y_k)^2$$

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.).

Brief theoretical part

Optimization methods are used in many areas of study to find solutions that maximize or minimize some study parameters, such as minimize costs in the production of a good or service, maximize profits, minimize raw material in the development of a good, or maximize production.

Brute-force search method, which try to calculate all possible solutions and decide afterwards which one is the best. This method is feasible only for small problems (in terms of the dimensionality of the phase space).

Algorithm:

Consider the following points in [a, b]:

$$x_k = a + \frac{k(b-a)}{n}, k = 0, \ldots, n,$$

where n is chosen so that $\frac{b-a}{n} \leq \varepsilon$.

Calculate $f(x_k), k\epsilon\{0, \ldots, n\}$, and find $\hat{x}$ such that

$$f(x_k) = min_{k=0,\ldots,n} f(x_k).$$

Then $|\hat{x} - x^*| \leq \varepsilon$, i.e. $\hat{x}$ is an approximant to x^*.

Dichotomy method. The idea of the method is to calculate at each next iteration two values of the objective function at points spaced by a value α in both directions from the middle of the uncertainty interval.

Algorithm:

Calculate $x_1 = \frac{a_0+b_0-\delta}{2}, x_2 = \frac{a_0+b_0+\delta}{2}, 0 < \delta < \varepsilon$, and $f(x_1)$ and $f(x_2)$.

Reduce the indeterminacy segment down to the segment $[a_1, b_1]$ as follows:

- if $f(x_1) \leq f(x_2)$, then $a_1 = a_0$ and $b_1 = x_2$;

- $a_1 = x_1$ and $b_1 = b_0$, otherwise.

Furthermore, by analogous formulas find x_1 and x_2 in the segment $[a_1, b_1]$ and repeat the reducing procedure down to a segment $[a_2, b_2]$, etc.

The search is stopped if at the current kth iteration it hold that

$$[a_k - b_k] < \varepsilon \; (x^* \in [a_k, b_k]).$$

Golden section search method in a one dimensional optimization method to find extremum value (minimum or maximum). The Golden Section Search method will try to find an extremum value with narrowing the searching interval in a golden ratio (φ) range. Golden ratio has value of 0.61803.

Algorithm:

Calculate $x_1 = a_0 + \frac{3-\sqrt{5}}{2}(b_0 - a_0), x_2 = b_0 + \frac{\sqrt{5}-3}{2}(b_0 - a_0), (\frac{x_1+x_2}{2} = \frac{a_0+b_0}{2})$ and $f(x_1)$ and $f(x_2)$ (the first iteration requires to calculate two points and two values of *f*).

Reduce the indeterminacy segment down to the segment $[a_1 - b_1]$ as follows:

- if $f(x_1) \leq f(x_2)$, then $a_1 = a_0, b_1 = x_2$ and $x_2 = x_1$;

- $a_1 = x_1, b_1 = b_0$ and $x_1 = x_2$, otherwise.

On the forthcoming iterations, calculate one point and one corresponding value of *f*: in the former case x_1 and $f(x_1)$, and in the latter one x_2 and $f(x_2)$.

The search is stopped if at the current kth iteration it holds that

$$|a_k - b_k| < \varepsilon \; (x^* \epsilon [a_k - b_k]).$$

Gauss (coordinate descent) method

Algorithm:

Let $x^0 = (x_1^0, x_2^0)$ be initial approximation. In the first iteration, find the minimum point of f as a function of the first variable, while others are fixed to get a new point $x^1 = (x_1^1, x_2^0)$.

Furthermore, using x^1, find the minimum point by varying only the second variable and get a new point $x^2 = (x_1^1, x_2^2)$. Start searching again by the first variable, etc.

The search is stopper under one of following criteria:

$$\left|x_i^{k+1} - x_i^k\right| < \varepsilon, i = 1,2, or \left|f\left(x_i^{k+1}\right) - f(x_i^k)\right| < \varepsilon$$

Nelder-Mead method

The Nelder-Mead method is a method of optimization (finding the minimum) of a function from several variables.

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

1) Reflection;

2) Expansion;

3) 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.

Results

I. To find approximate solutions (find the minimum of the function) one-dimensional methods of exhaustive search, dichotomy, golden section search were used.

The longest, as expected, was Exhaustive (brute force) method. It requires more f-calculating. It can be seen from the results obtained that the dichotomy method processes in fewer iterations than the golden section method. At the same time, all methods produced similar results with a given accuracy ($\varepsilon = 0.001$).

```
Exhaustive search (Brute-force)
<function cube_func at 0x000001ACF2292280>:      arg = 0.0000 Minimum: 0.0000 Number of f-calculations: 1000 Iterations: 1000
<function abs_func at 0x000001ACEF8754C0>:       arg = 0.2000 Minimum: 0.0000 Number of f-calculations: 1000 Iterations: 1000
<function sin_func at 0x000001ACEF875A60>:       arg = 0.2230 Minimum: -0.2172 Number of f-calculations: 990 Iterations: 990

Dichotomy search method
<function cube_func at 0x000001ACF2292280>:      arg = 0.0005 Minimum: 0.0000 Number of f-calculations: 25 Iterations: 12
<function abs_func at 0x000001ACEF8754C0>:       arg = 0.2001 Minimum: 0.0001 Number of f-calculations: 25 Iterations: 12
<function sin_func at 0x000001ACEF875A60>:       arg = 0.2226 Minimum: -0.2172 Number of f-calculations: 25 Iterations: 12

Golden section search method
<function cube_func at 0x000001ACF2292280>:      arg = 0.0004 Minimum: 0.0000 Number of f-calculations: 33 Iterations: 16
<function abs_func at 0x000001ACEF8754C0>:       arg = 0.2001 Minimum: 0.0001 Number of f-calculations: 33 Iterations: 16
<function sin_func at 0x000001ACEF875A60>:       arg = 0.2227 Minimum: -0.2172 Number of f-calculations: 33 Iterations: 16
```

Fig. 1 – Results

II. In the second part of the task, it was necessary to find the coefficients a and b of linear and rational approximate function x. To solve this problem brute force search, Gauss and Nelder-Mead methods were used. The obtained results are shown in figure 3 for linear approximation and in figure 5.

It is well known that the optimization problem associated with linear approximation has a single solution, and therefore it is expected that these methods will give similar optimal values for a and b, regardless of the choice of initial approximations. In the case of rational approximation, significant nonlinearities arise, and therefore the choice of the initial approximation can significantly affect the result.

But, as you can see in figure 2 and figure 4, we obtain similar results for all methods of each type of approximation.

```
Linear optimization (exhaustive search method):
 0.7978994967423588 0.7785930085573406

Linear optimization (Gauss search method):
    direc: array([[ 0.        ,  1.        ],
       [-0.8671978,  0.4335989]])
     fun: 95.8734584130468
 message: 'Optimization terminated successfully.'
    nfev: 101
     nit: 3
  status: 0
 success: True
       x: array([0.79790521, 0.77857019])

Linear optimization (Nelder-Mead method):
  final_simplex: (array([[0.79734907, 0.77868096],
       [0.79823092, 0.77817183],
       [0.7973442 , 0.77925076]]), array([95.8734639 , 95.87346493, 95.87347728]))
           fun: 95.87346389521713
       message: 'Optimization terminated successfully.'
          nfev: 113
           nit: 58
        status: 0
       success: True
             x: array([0.79734907, 0.77868096])
```

Fig. 2 – Results of data approximation by linear function

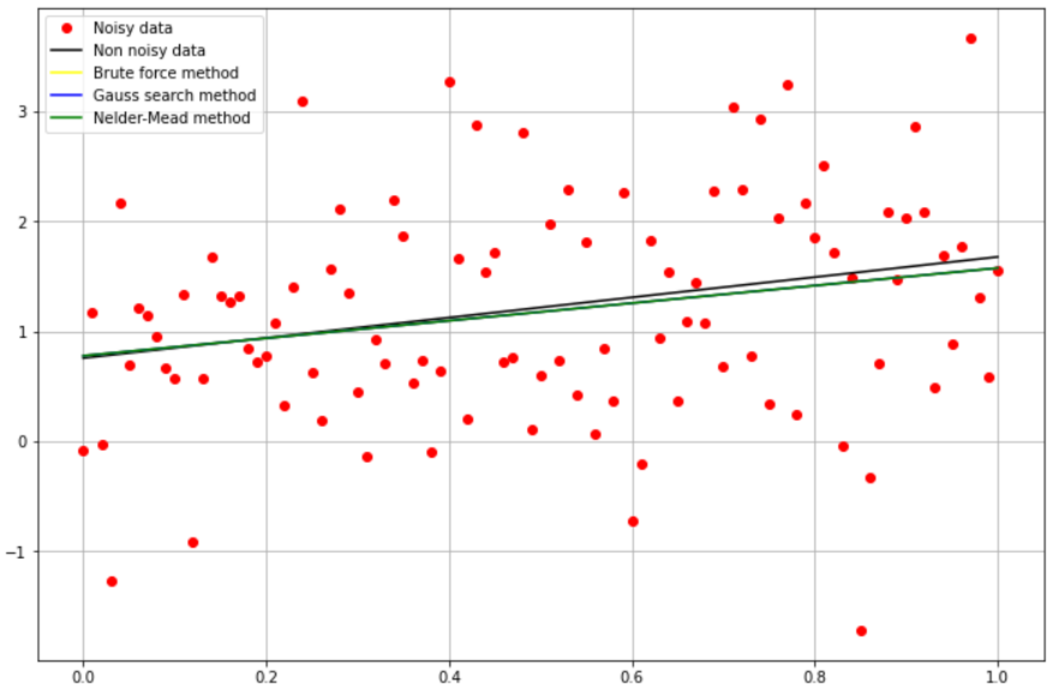

Fig. 3 - The results of applying exhaustive search, Gauss and Nelder-Mead methods to solve the linear approximation problem

```
Rational optimization (exhaustive search method):
 0.8797438118270169 -0.4601464603013651

Rational optimization (Gauss search method):
    direc: array([[ 0.        ,  1.        ],
       [-0.21163054, -0.21078657]])
     fun: 96.30677761419632
 message: 'Optimization terminated successfully.'
    nfev: 75
     nit: 3
  status: 0
 success: True
       x: array([ 0.87959991, -0.45972971])

Rationl optimization (Nelder-Mead method):
  final_simplex: (array([[ 0.87964361, -0.46032344],
       [ 0.88003429, -0.45970613],
       [ 0.87975407, -0.45982896]]), array([96.30673041, 96.30673805, 96.30674332]))
           fun: 96.30673041079261
       message: 'Optimization terminated successfully.'
          nfev: 111
           nit: 57
        status: 0
       success: True
             x: array([ 0.87964361, -0.46032344])
```

Fig. 4 - Results of data approximation by rational function

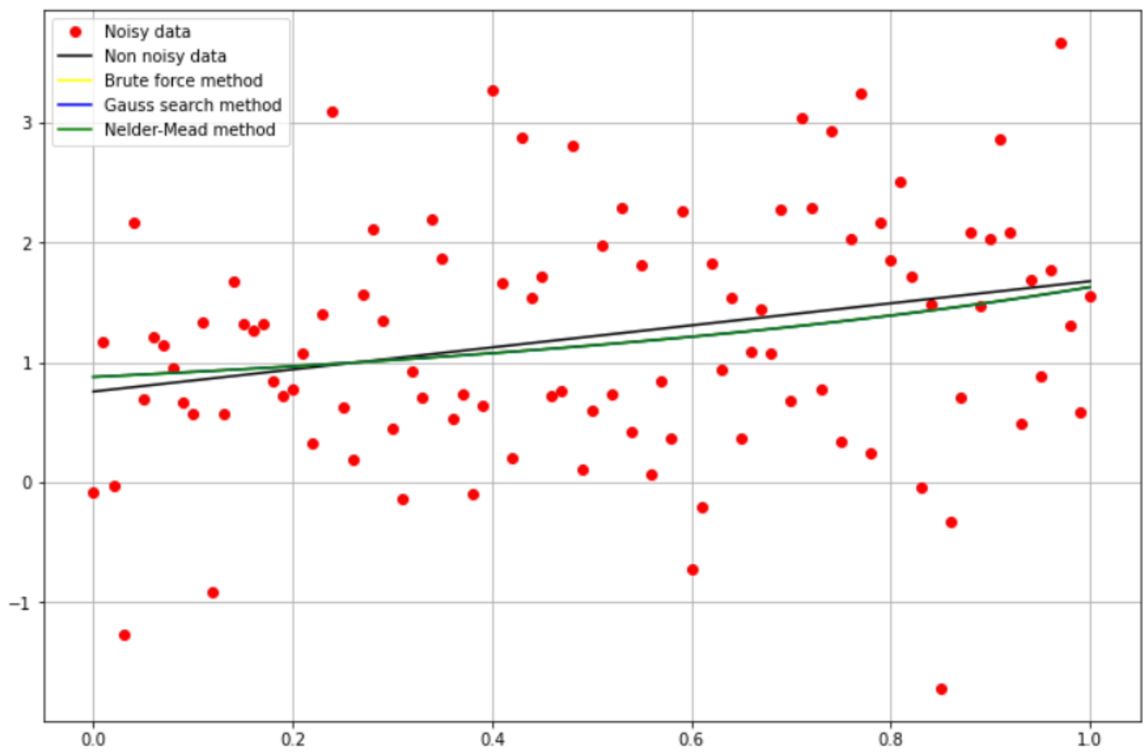

Fig. 5 - The results of applying exhaustive search, Gauss and Nelder-Mead methods to solve the rational approximation problem

Conclusion

During the execution of practical task, the approximate solutions x: $f(x) \rightarrow min$ was found. To complete this task the one-dimensional methods of exhaustive search, dichotomy and golden section search were used. We obtained the same results for each method. Also we solve the minimization problem, use the methods of exhaustive search, Gauss and Nelder-Mead. A detailed analysis can be found in the results section.

Appendix

GitHub Link: https://github.com/alex-mat-s/Algorithms/blob/main/Lab2.ipynb