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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, Nelder-Mead) in the tasks of unconstrained nonlinear.

Formulation of the problem

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: $f(x) \to \min$ *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. $f(x) = x \sin(1/x)$, $x \in [0.01, 1]$.

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* $k = 0, \ldots, 100$, *according to the following rule:*

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

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

1. $F(x, a, b) = ax + b$ *(liner approximant)*
2. $F(x, a, b) = \frac{1}{1+bx}$ *(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****. Analyze the results obtained (in terms of number of iterations, precision, number of function evaluations, etc.).*

Brief theoretical part

Optimization methods are numerical methods for finding the optimal values 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 an objective function $f = f(x)$ *be given, where* x *is, generally speaking, a multidimensional vector from some subset* Q *of the Euclidean space* R^m*. The subset of* Q *can be either bounded or in particular, coincide with the whole space* R^m*. We will consider only the problem of minimizing the function* f *on the set* Q *(from minimization one can go to maximization by considering* $F(x) = -f(x)$ *instead of* $f(x)$*).*

By solving the optimization (minimization) problem $f(x) \to \min_{x \in D}$ *we mean finding* $x^* \in Q$ *such that* $f(x^*) = \min_{x \in Q} f(x)$*. For* x^* *there is a special notation:* $x^* = \arg\min_{x \in Q} f(x)$*. If* x^* *is found, then, naturally, one can also find* $f(x^*)$*.*

The specified formulation of the optimization problem implies the search global minimum of f *on* Q*. However, below we will consider also search for a local minimum of* f *on* Q *when the value* $f(x*)$ *minimum only in some neighborhood of the point* x^**. Note that often the search the local minimum is much simpler than the global one.*

If the optimization problem includes additional conditions on x^* *(in the form of a system of* S *equations and inequalities), then it is called conditional. Otherwise, the optimization problem is called unconditional. Note also that, depending on the type of* f *and* S*, problems of linear and nonlinear optimization. Here and below, we will consider only unconstrained nonlinear optimization problems. This means that the function* f *is generally nonlinear, and the conditions* S *are not imposed.*

Direct optimization methods (zero-order optimization methods). By definition, they search for x^* *only the values of the function* f*, but not its derivatives. These methods, in particular, are applicable for continuous (and not necessarily differentiable) functions* $f = f(x)$ *of one variable* x *on the interval* $Q = [0, 1]$*. Generally speaking, it turns out that direct methods can be used for a fairly wide class of functions* f*. This, however, is offset by the rather low-speed convergence of the corresponding iterative processes.*

Results

Part One

Find an approximate (with precision $\varepsilon = 0.001$*) solution* $x: f(x) \rightarrow min$ *for the following functions:*

1. $f1(x) = x^3,\ x \in [0, 1]$
2. $f2(x) = |x - 0.2|,\ x \in [0, 1]$
3. $f3(x) = x \sin(1/x),\ x \in [0.01, 1]$

	Method Name	X_min for f1	number of iterations	X_min for f2	number of iterations	X_min for f3	number of iterations
0	Exhaustive search	0.000000	1000	0.200000	1000	0.223000	900
1	Dichotomy method	0.000494	11	0.200101	11	0.222570	11
2	Golden section method	0.000367	15	0.200073	15	0.222593	15

Table 1. Number of iterations and Min value of functions for methods Exhaustive Search, Dichromia and Golden selection.

All functions have almost the same global minimum, with the exception of the last cubic function. The methods differ in the number of iterations, the method with the largest number of iterations is an exhaustive search. The result is shown in table 1.

Part Two

$$F(x, a, b) = ax + b \text{ (linear approximant)}$$

Minimization by exhaustive search

For the exhaustive search method, need to specify the initial approximations (the range of values on which you need to search for the coefficients for the least squares method and set the step equal to epsilon).

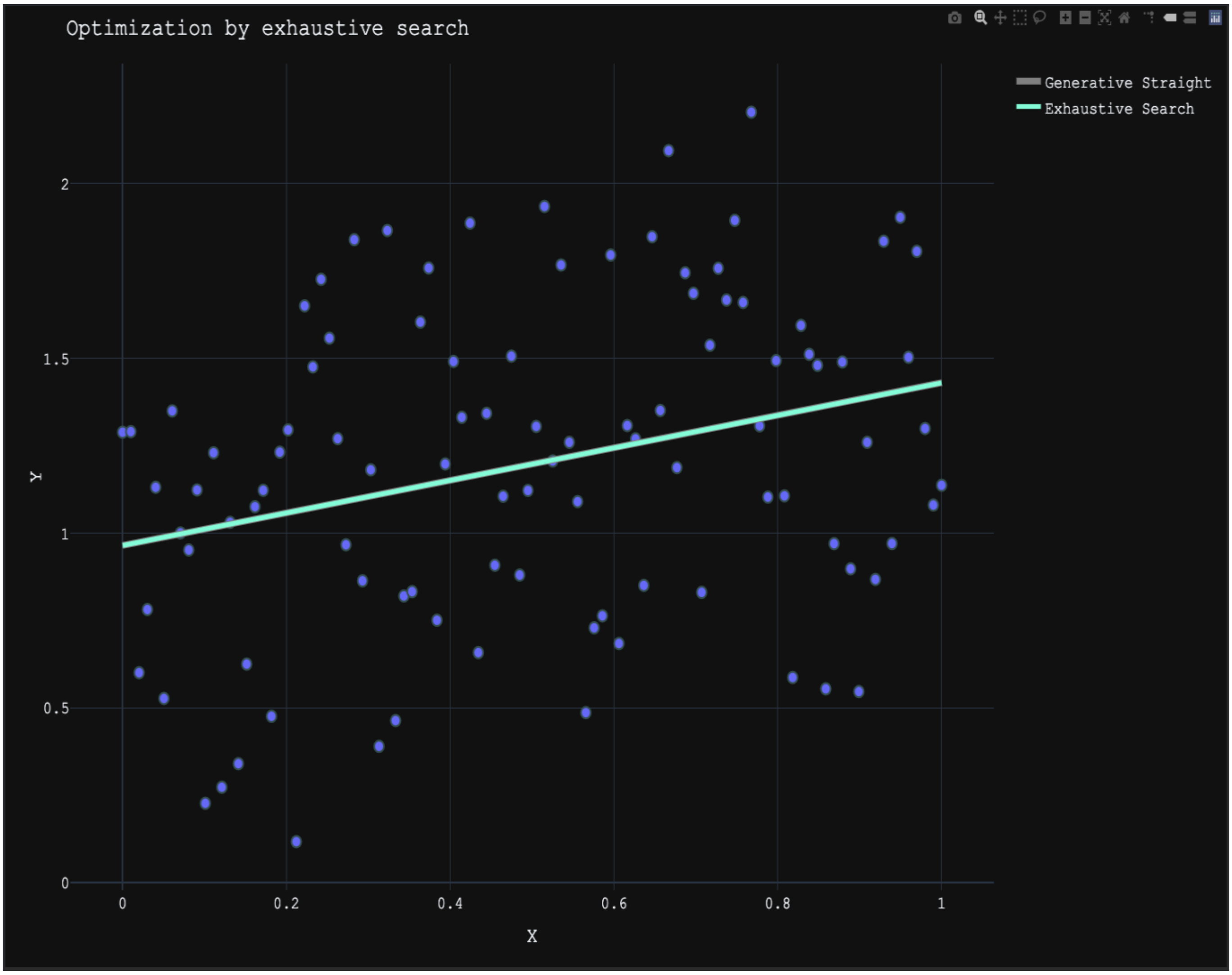

Figure 1: Linear function approximation of the least squares method with minimization by exhaustive search

The given initial approximations for this plot on the interval from 0 to 1 with step 0.001. The values of the coefficients are a = 0.461 and b = 0.964. When choosing such initial approximations, the graph of the function was approximated quite well.

Minimization by Nelder-Mead

The initial approximations a and b for the Nelder-Mead method are equal to zero. The values of the coefficients are a = 0.4649 and b = 0.964. The graph of the generating line coincided with the minimized line by the method Nelder-Mead (see Figure 2).

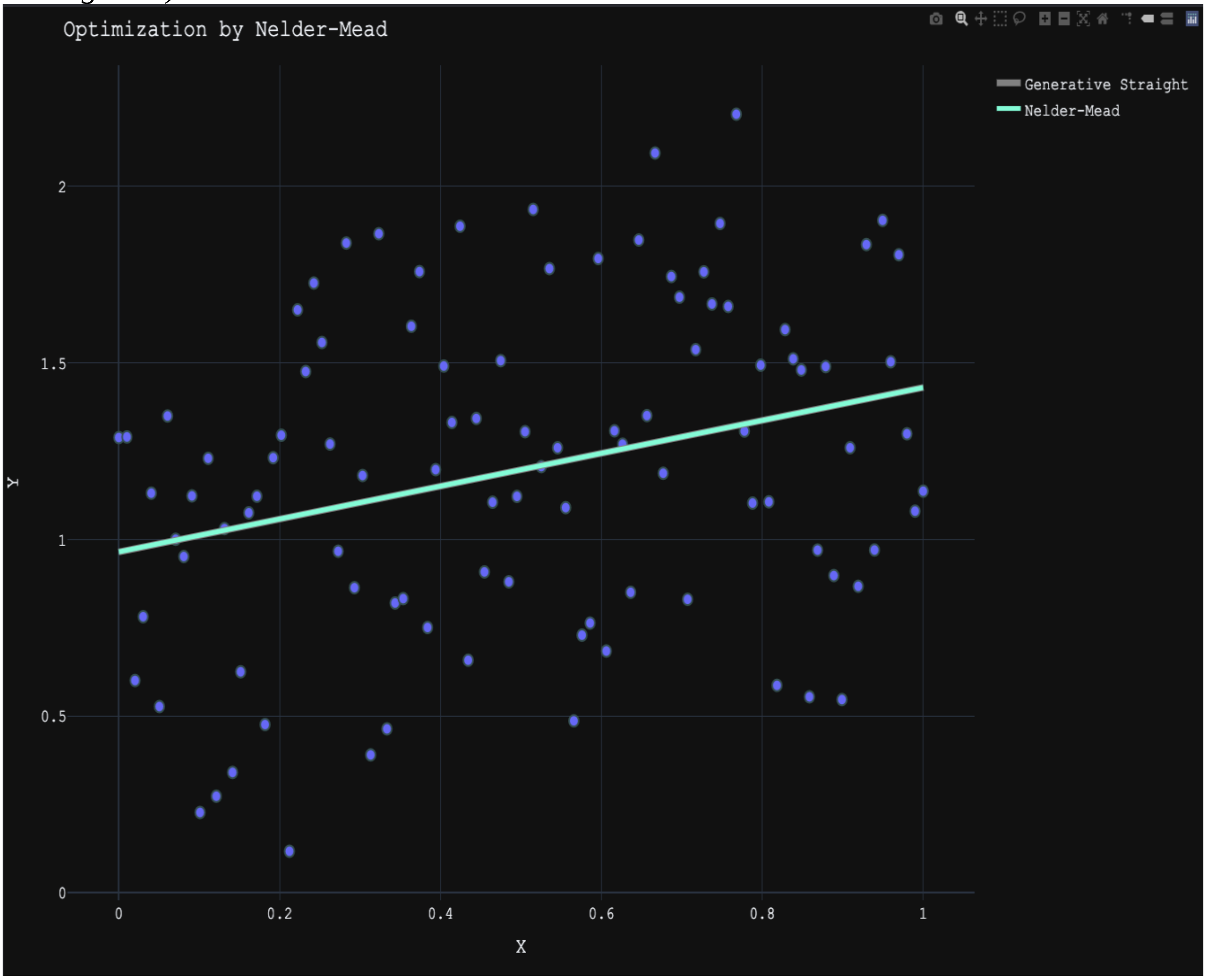

Figure 2: Linear function approximation of the least squares method with minimization by Nelder-Mead

Minimization by Gaussean

The initial approximations a and b for the Gaussean method are equal to a = 0.3, b =0.9. The values of the coefficients are a = 0.561and b = 0.916.). When choosing such initial approximations, the graph of the function was approximated quite well (see Figure 3).

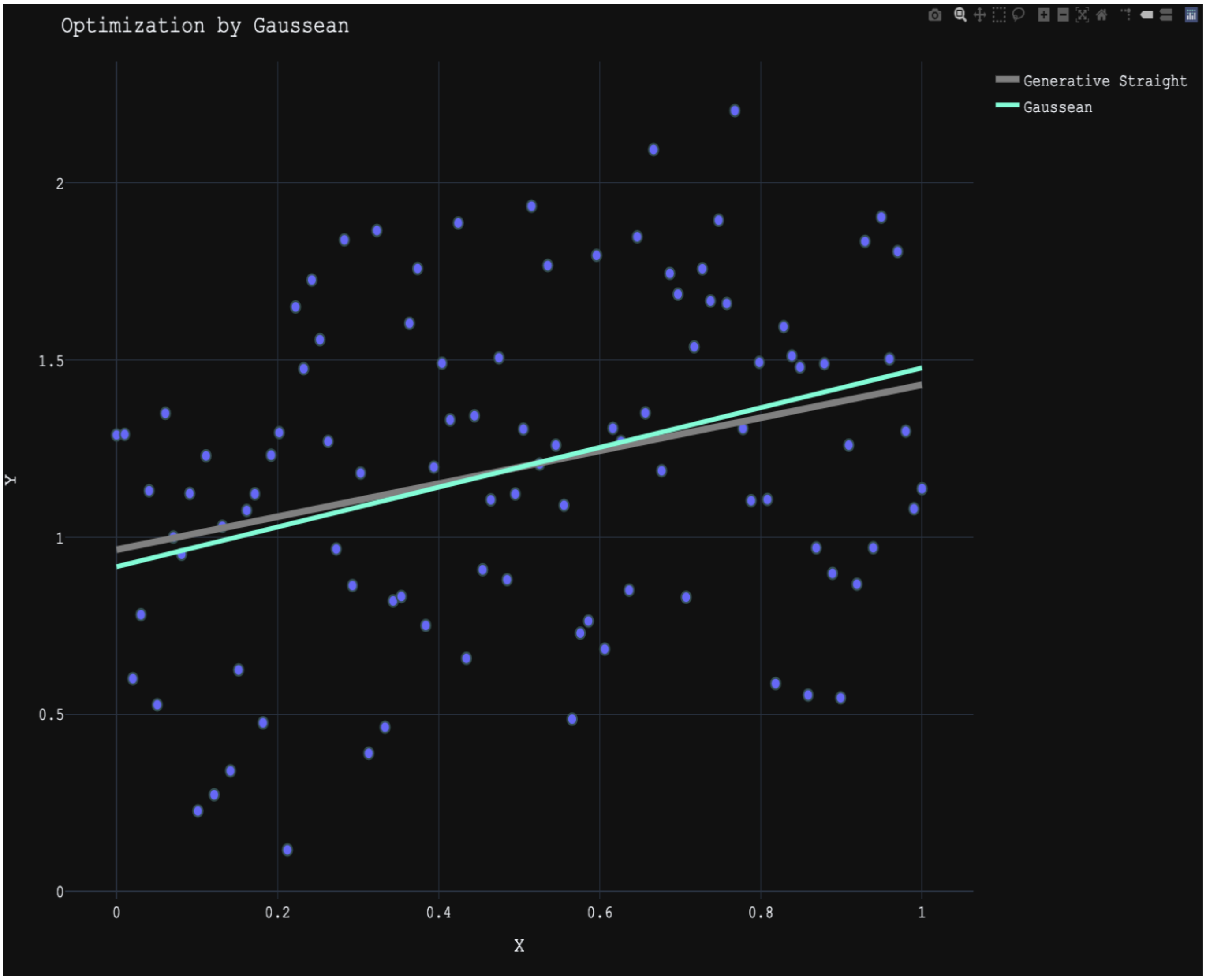

Figure 3: Linear function approximation of the least squares method with minimization by Gaussean.

$F(x, a, b) = 1/(1 + bx)$ *(rational approximant)*

Minimization by exhaustive search

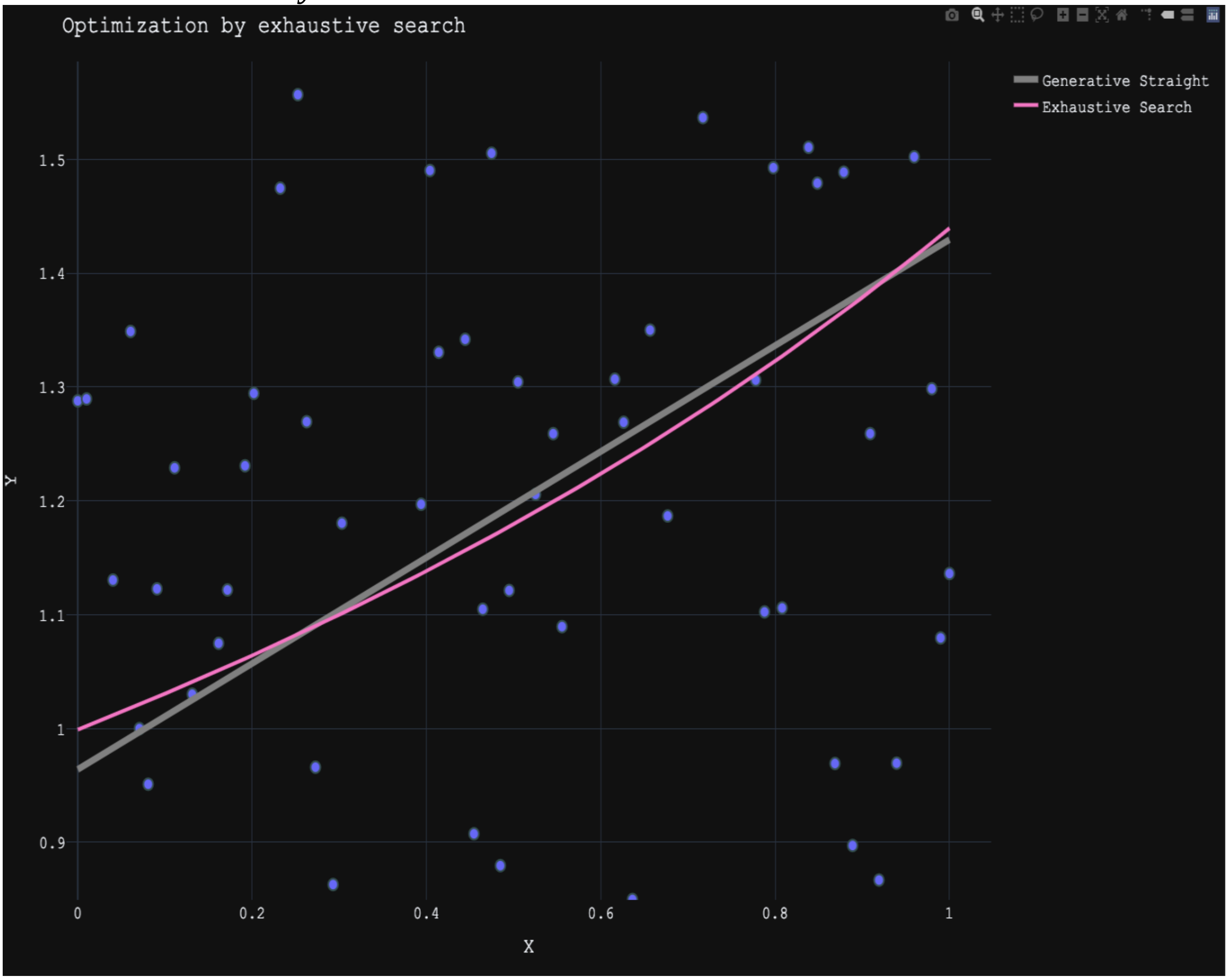

Figure 4: Rational function approximation of the least squares method with minimization by exhaustive search

The given initial approximations for this plot (see Figure 4) on the interval from -1 to 1 with step 0.001. The values of the coefficients are a = 0.999 and b = -0.302. When choosing such initial approximations, the graph of the function was approximated quite well.

Minimization by Nelder-Mead

The initial approximations a and b for the Nelder-Mead method are equal to zero. The values of the coefficients are a = 1.0110 and b = -0.29

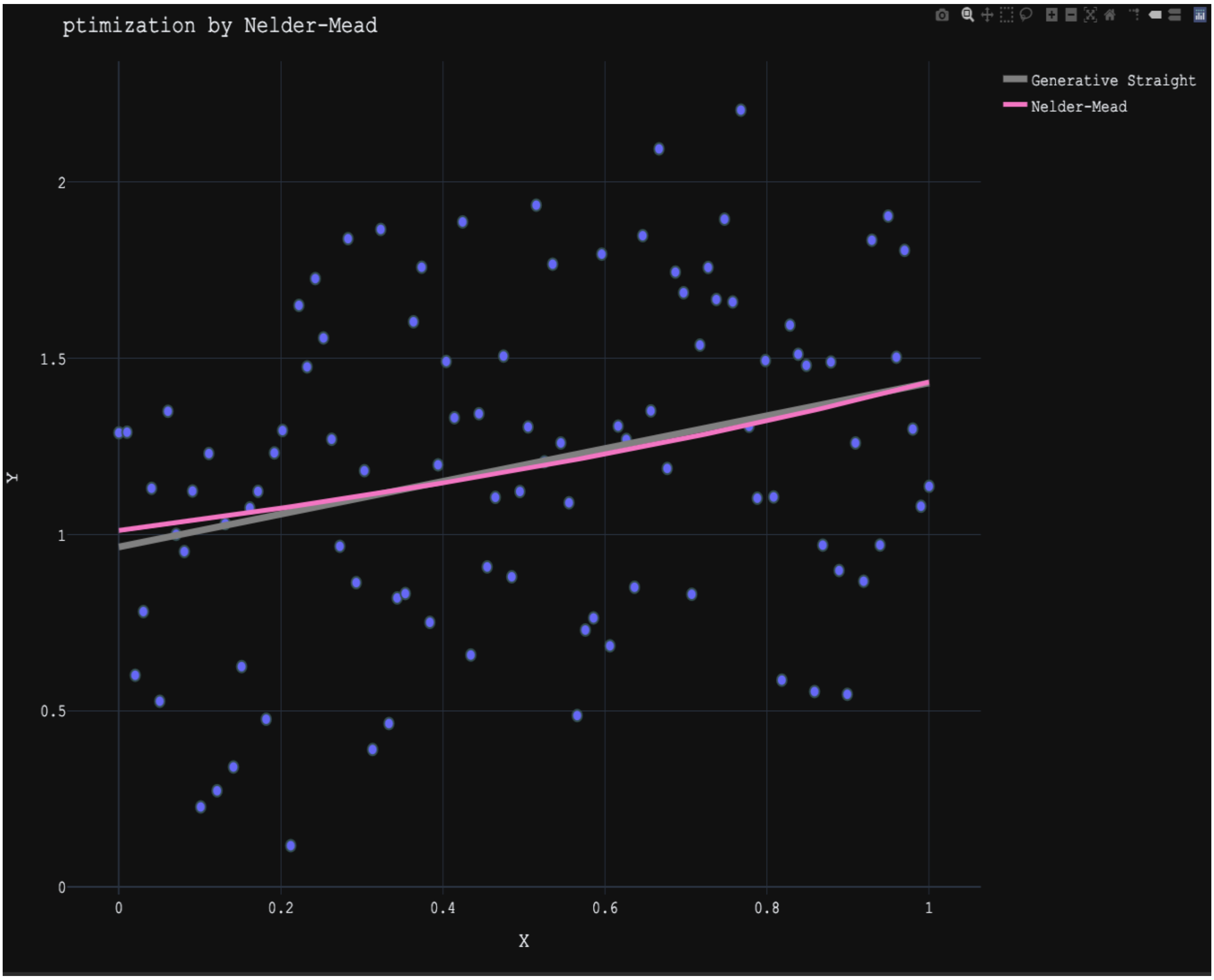

Figure 5: Rational function approximation of the least squares method with minimization by Nelder-Mead

Minimization by Gaussean

The initial approximations a and b for the Gaussean method are equal to a = 5,b =0. The values of the coefficients are a = 0.999 and b =-0.306.). When choosing such initial approximations, the graph of the function was approximated quite well (see Figure 6).

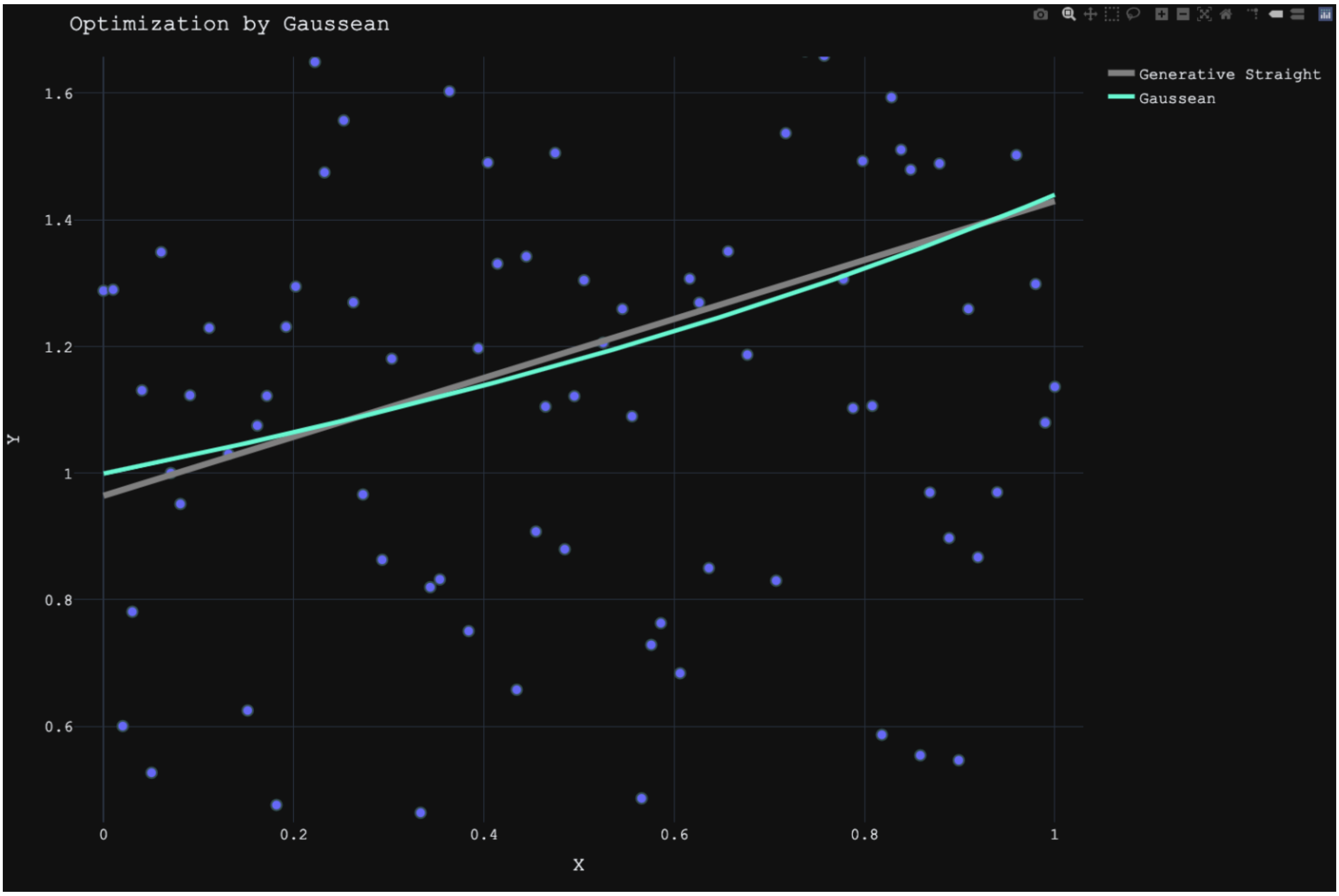

Figure 6: Rational function approximation of the least squares method withminimization by Gaussean

Conclusions

In the course of the laboratory work, direct methods were applied (one- dimensional methods of enumeration, dichotomy, golden ratio; multidimensional methods of enumeration, Gauss, Nelder Mead) in problems of unconstrained nonlinear optimization. One-dimensional methods generally differ in the number ofiterations performed. For multidimensional methods, an important role is played by the initial approximations

Appendix

Code Link