FEDERAL STATE AUTONOMOUS EDUCATIONAL INSTITUTION
OF HIGHER EDUCATION
ITMO UNIVERSITY

Report

on the practical task No. 3

« ***Algorithms for unconstrained nonlinear optimization. First- and second-order methods*** »

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Goal

The use of first- and second-order methods (Gradient Descent, Conjugate Gradient Descent, Newton's method and Levenberg-Marquardt algorithm) in the tasks of unconstrained nonlinear optimization.

Formulation of the problem

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:*

$$y = \alpha x_k + \beta + \delta_k \longrightarrow x_k = \frac{k}{100}$$

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. $F(x, a, b) = ax + b$ *(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 Gradient Descent, Conjugate Gradient Descent, Newton's method and Levenberg-Marquardt algorithm. If necessary, set the initial approximations and other parameters of the methods. Visualize the data and the approximants obtained ***separately for each type of approximant****. Analyze the results obtained (in terms of number of iterations, precision, number of function evaluations, etc.) and compare them with those from Task 2 for the same dataset.*

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.

In this laboratory work, first and second-order optimization methods, i.e. methods using to minimize of the function f on the set Q its values f (x) and the values of its first derivative and the values of f (x) and the values of its first and second derivatives (gradient, Hessian), respectively. Naturally, it is assumed that f is continuously differentiable on Q a sufficient number of times.

Results

Minimization by Levenberg-Marquart method

The initial approximations a and b for the Levenberg-Marquart method are equal to a =1, b =0. The values of the coefficients after minimization are a = 0.601 and b = 1.01, number of function evaluations: 34. When choosing such initial approximations, the graph of the function was approximated quite well (see Figure 1).

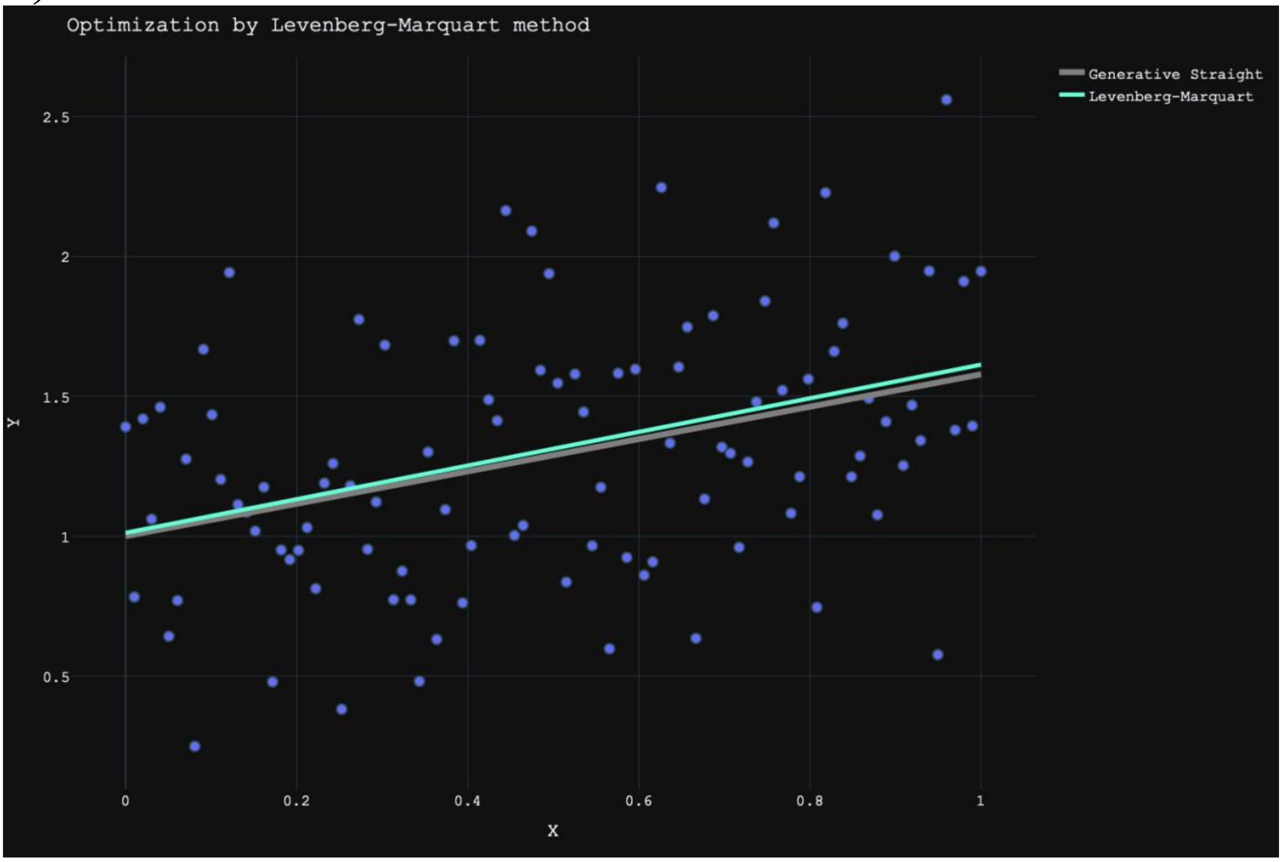

Figure 1: Linear function approximation of the least squares method with minimization by Levenberg-Marquart method

Minimization by Newton method

The initial approximations a and b for the Newton method are equal to a =0.001, b =0.5. The values of the coefficients after minimization are a = 0.4 and b = 1.097, number of iterations: 553. When choosing such initial approximations, thegraph of the function was approximated quite well (see Figure 2).

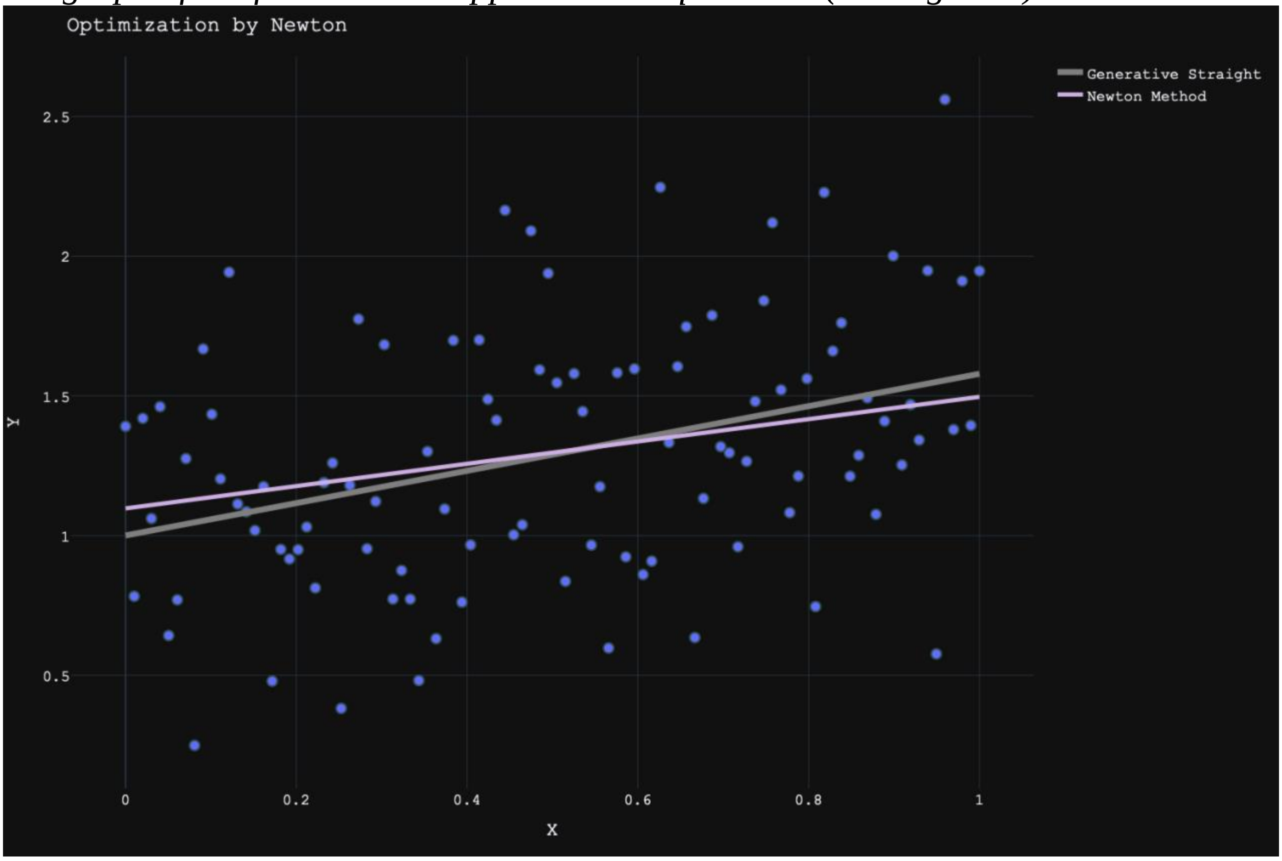

Figure 2: Linear function approximation of the least squares method with minimization by Newton method

Minimization by Gradient Descent method

The initial approximations a and b for the Gradient Descent method are equal to a =0.3, b =0. The values of the coefficients after minimization are a = 0.631 and b = 0.972, number of iterations: 100.

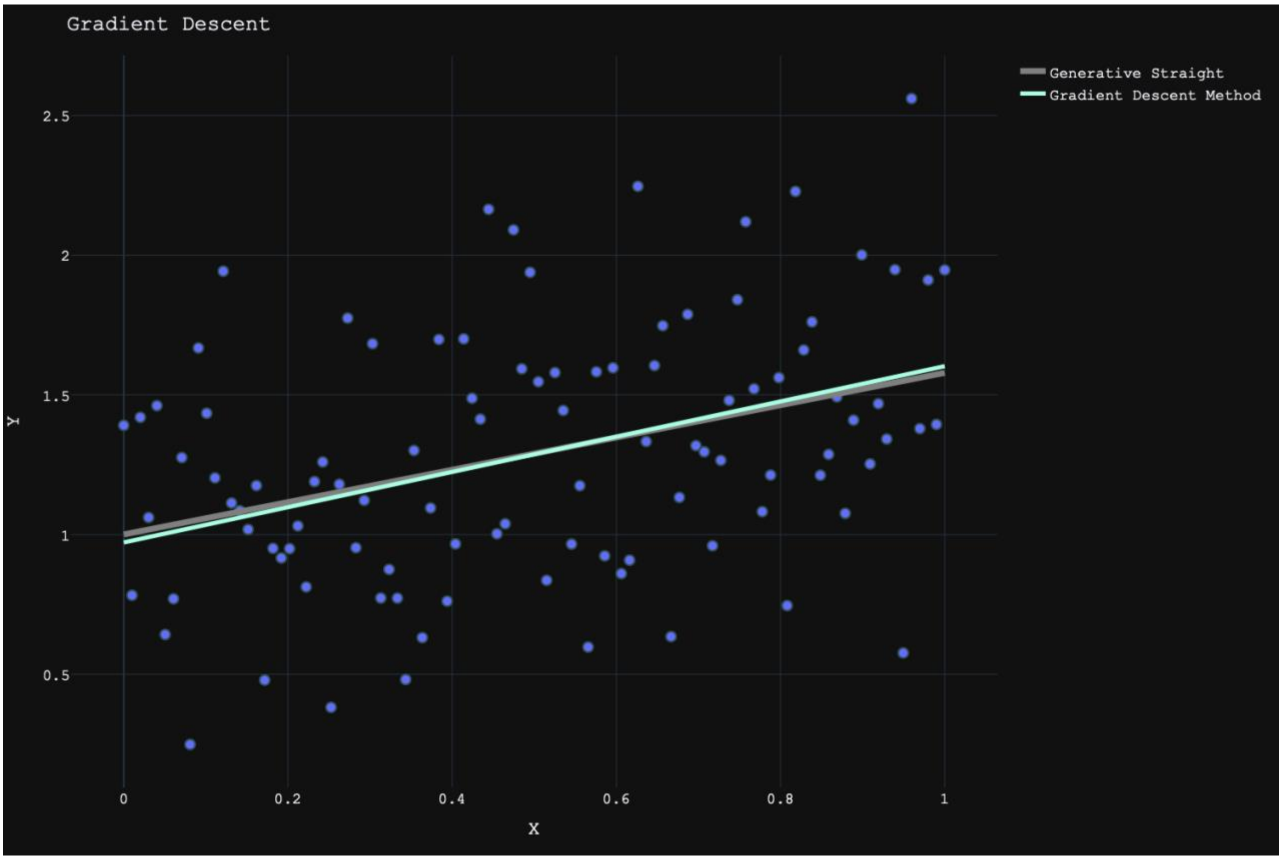

Figure 3: Linear function approximation of the least squares method with minimization by Gradient Descent method

Minimization by Conjugate Gradient method

The initial approximations a and b for the Conjugate Gradient method are equal to a =0.001, b =0. The values of the coefficients after minimization are a = 0.579 and b = 1, number of iterations:21, number of function evaluation 80. The graph for gradient descent almost coincided with the generating line (see Figure 4)

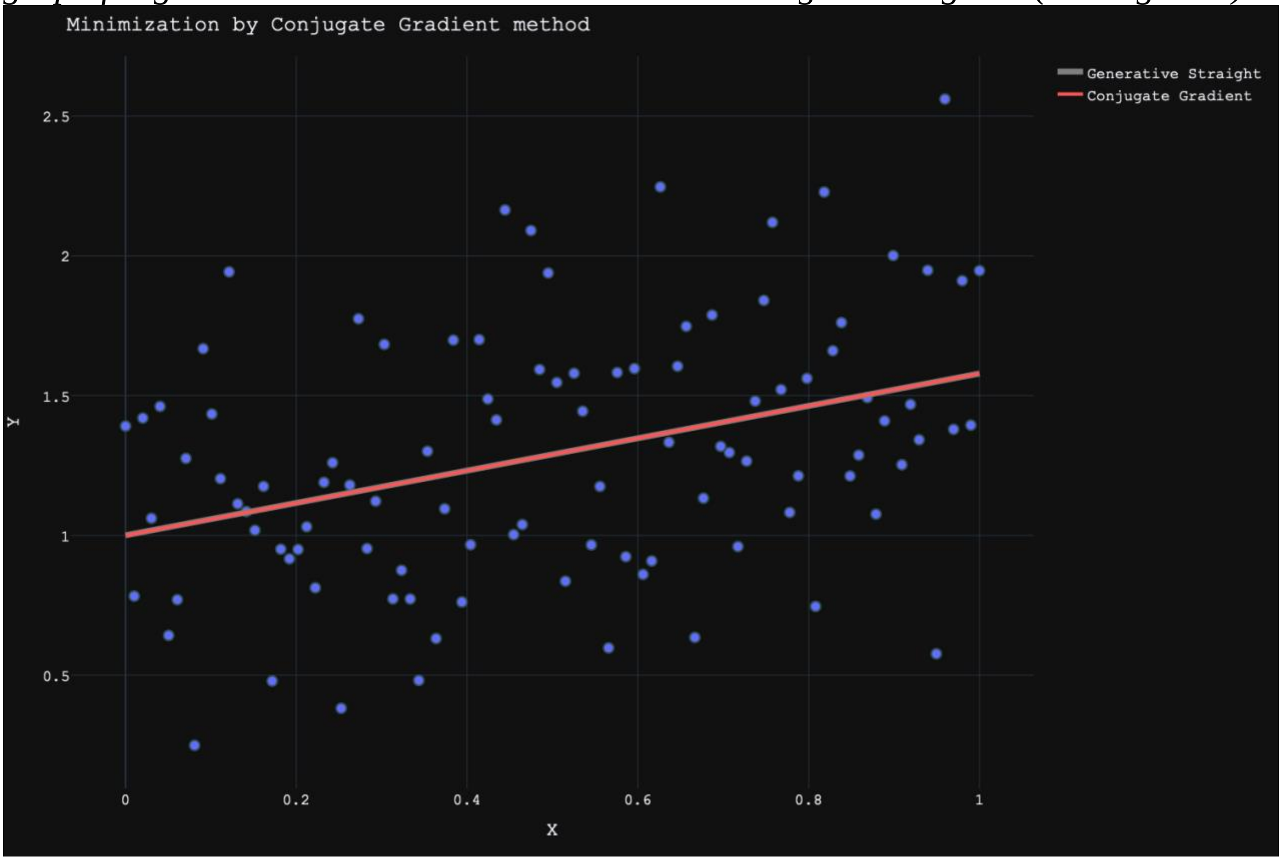

Figure 4: Linear function approximation of the least squares method with minimization by Conjugate Gradient method

Result of all methods on one plot

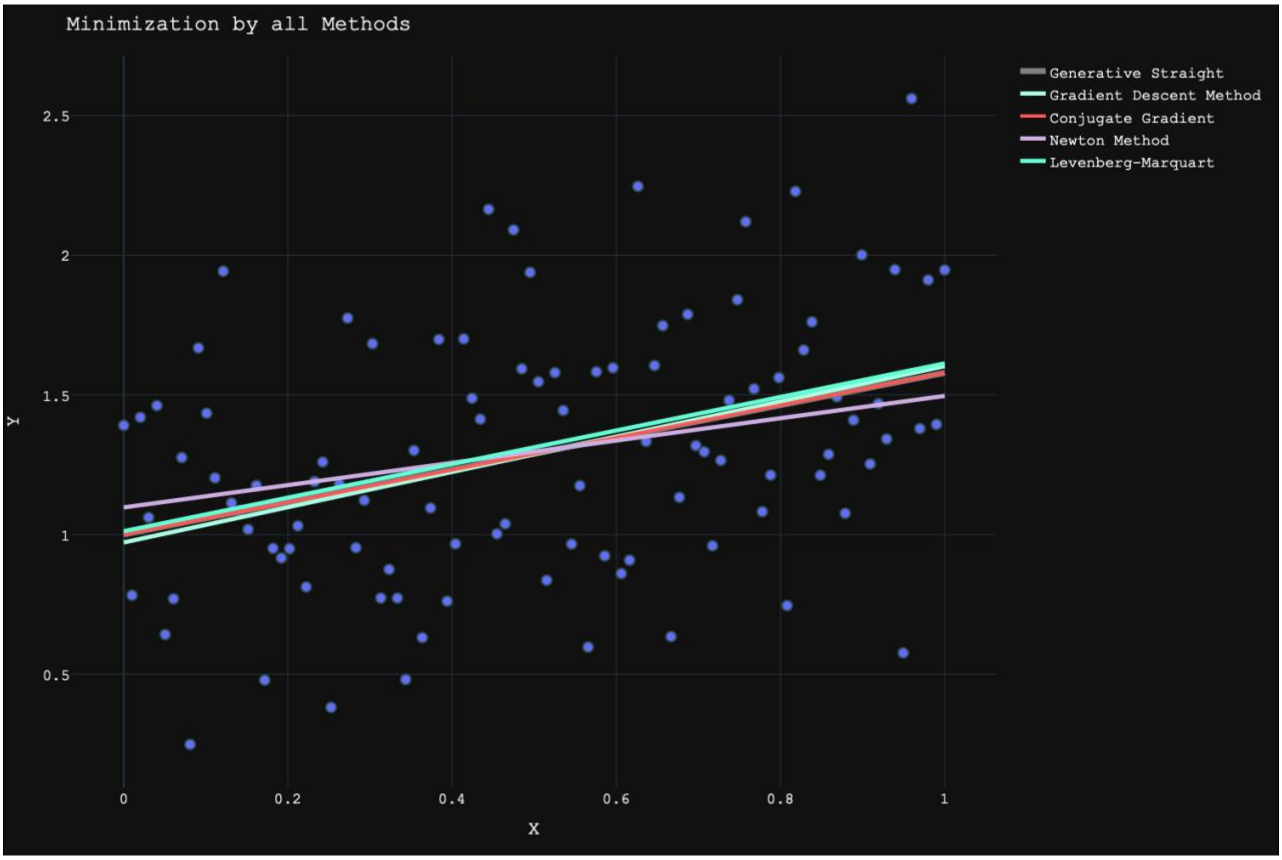

Figure 5: Linear function approximation of the least squares method with minimization by all method

Minimization by Levenberg-Marquart method

The initial approximations a and b for the Levenberg-Marquart method are equal to a =1, b =0. The values of the coefficients after minimization are a = 1.056 and b = -0.23, number of function evaluations:31. When choosing such initial approximations, the graph of the function was approximated quite well (see Figure 6).

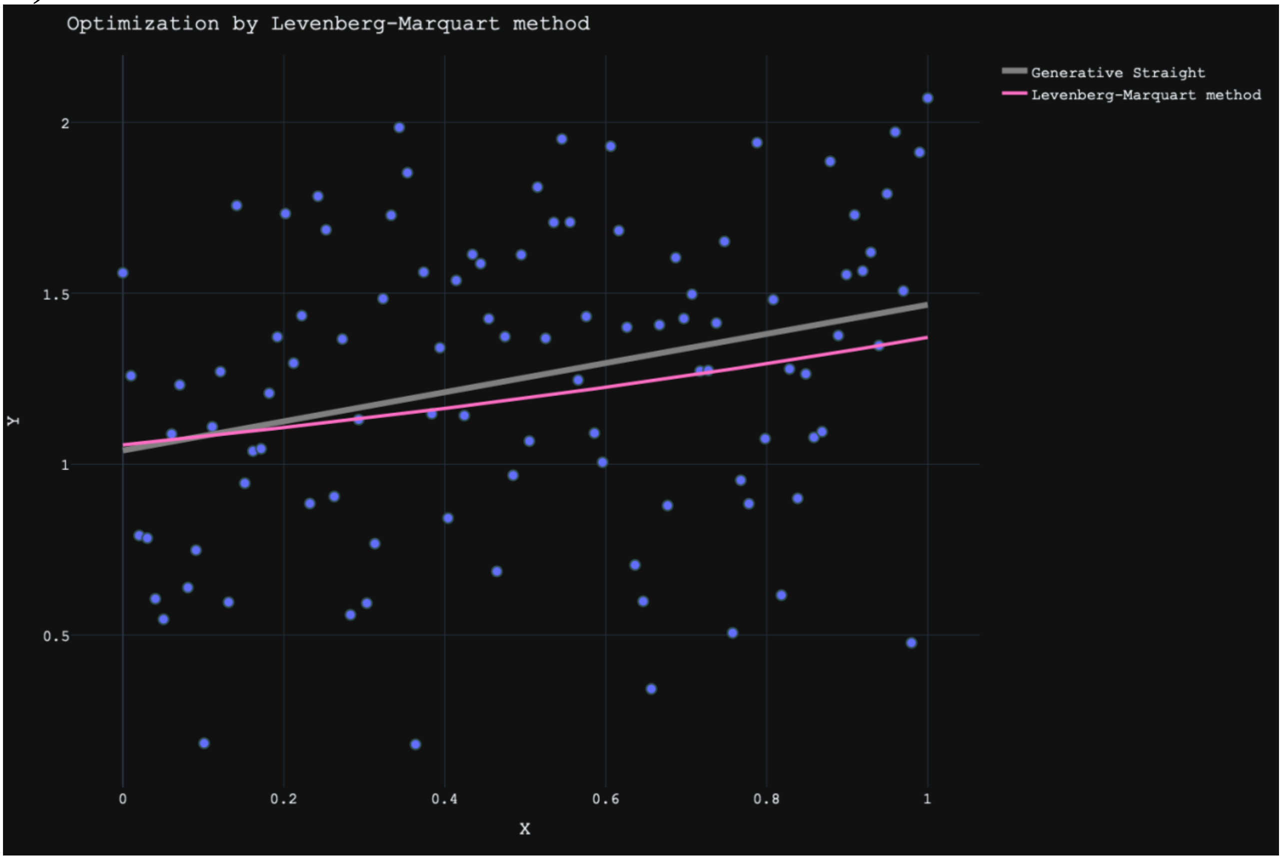

Figure 6: Rational function approximation of the least squares method with minimization by Levenberg-Marquart method

Minimization by Newton method

The initial approximations a and b for the Newton method are equal to a =0.5, b =0. The values of the coefficients after minimization are a = 1.967 andb = 0.978, number of iterations: 418. When choosing such initial approximations, the graph of the function was approximated (see Figure 7).

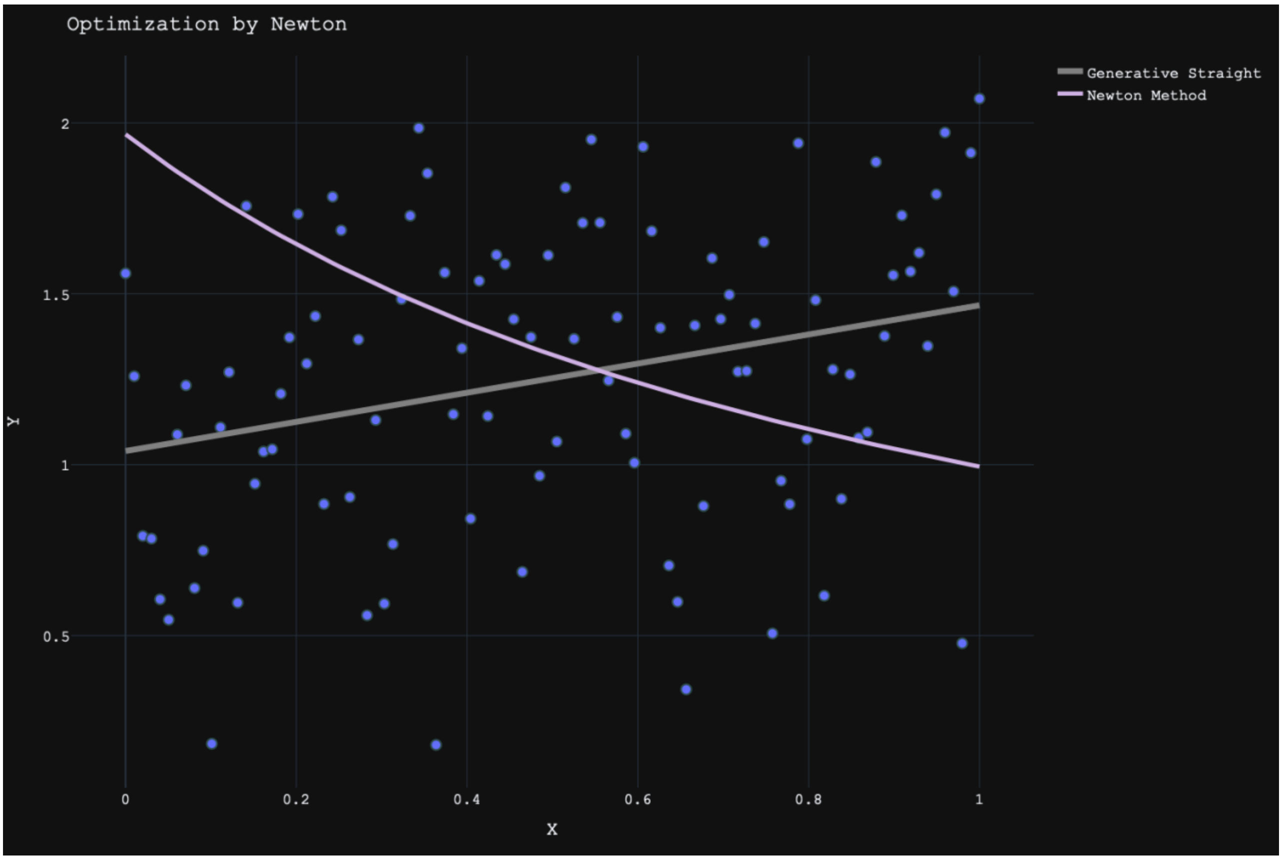

Figure 7: Rational function approximation of the least squares method with minimization by Newton method

Minimization by Gradient Descent method

The initial approximations a and b for the Newton method are equal to a =0.3, b =0. The values of the coefficients after minimization are a = 1.063 and b = -0.28, number of iterations: 150. When choosing such initial approximations, the graph of the function was approximated very well (see Figure 8).

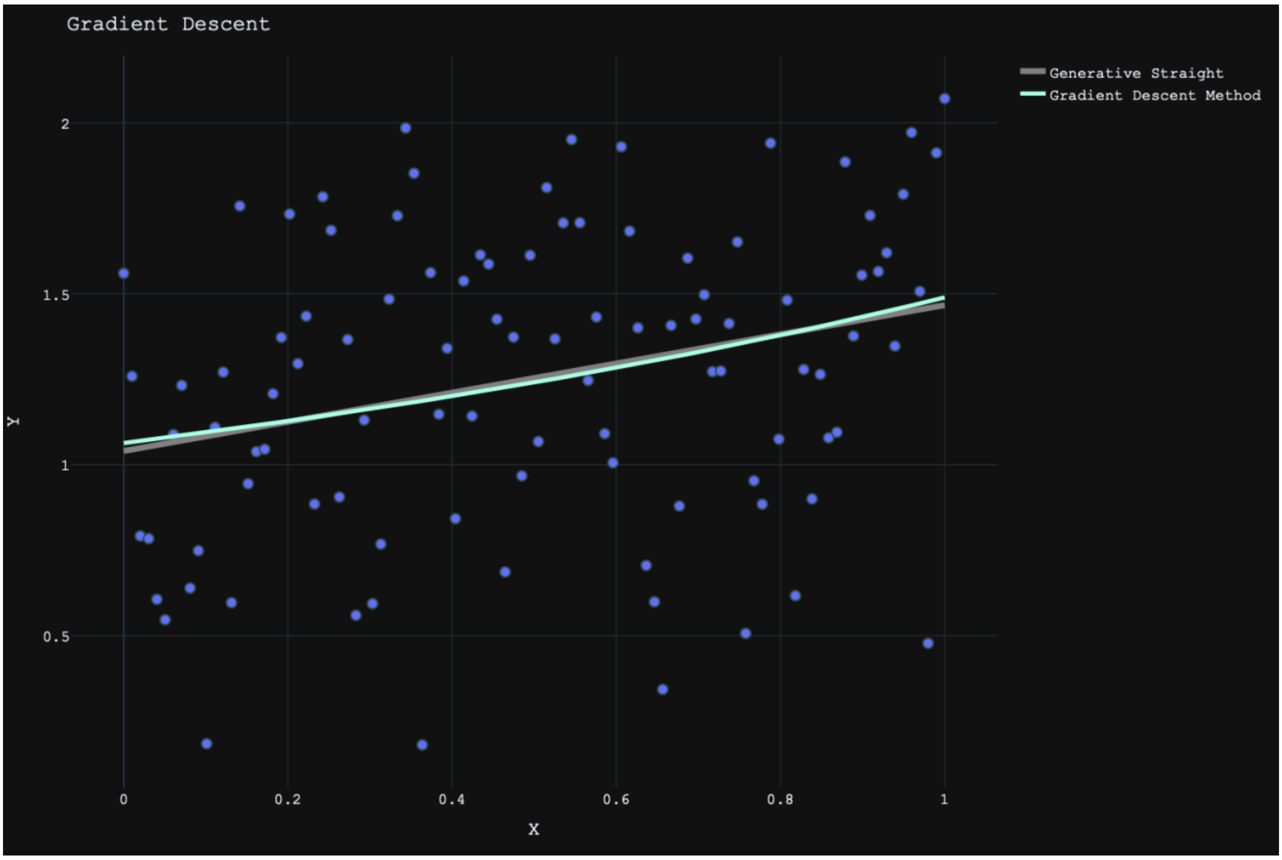

Figure 8: Rational function approximation of the least squares method with minimization by Gradient Descent method

Minimization by Conjugate Gradient method

The initial approximations a and b for the Newton method are equal to a =0.001, b =0. The values of the coefficients after minimization are a = 1.064 and b = -0.285, number of iterations:19, number of function evaluation 52. When choosing such initial approximations, the graph of the function was approximated very well (see Figure 9).

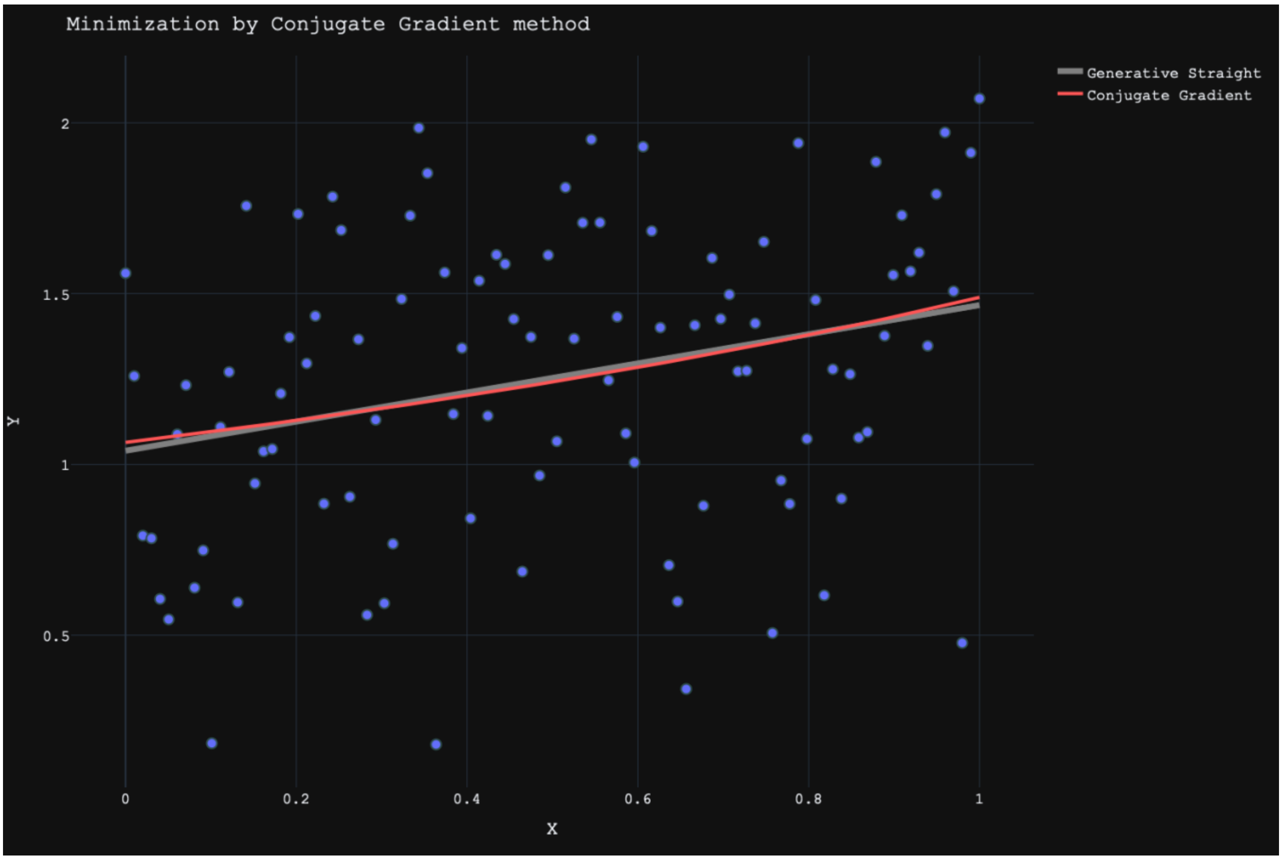

Figure 9: Rational function approximation of the least squares method with minimization by Conjugate Gradient method

__Result of all methods on one plot__

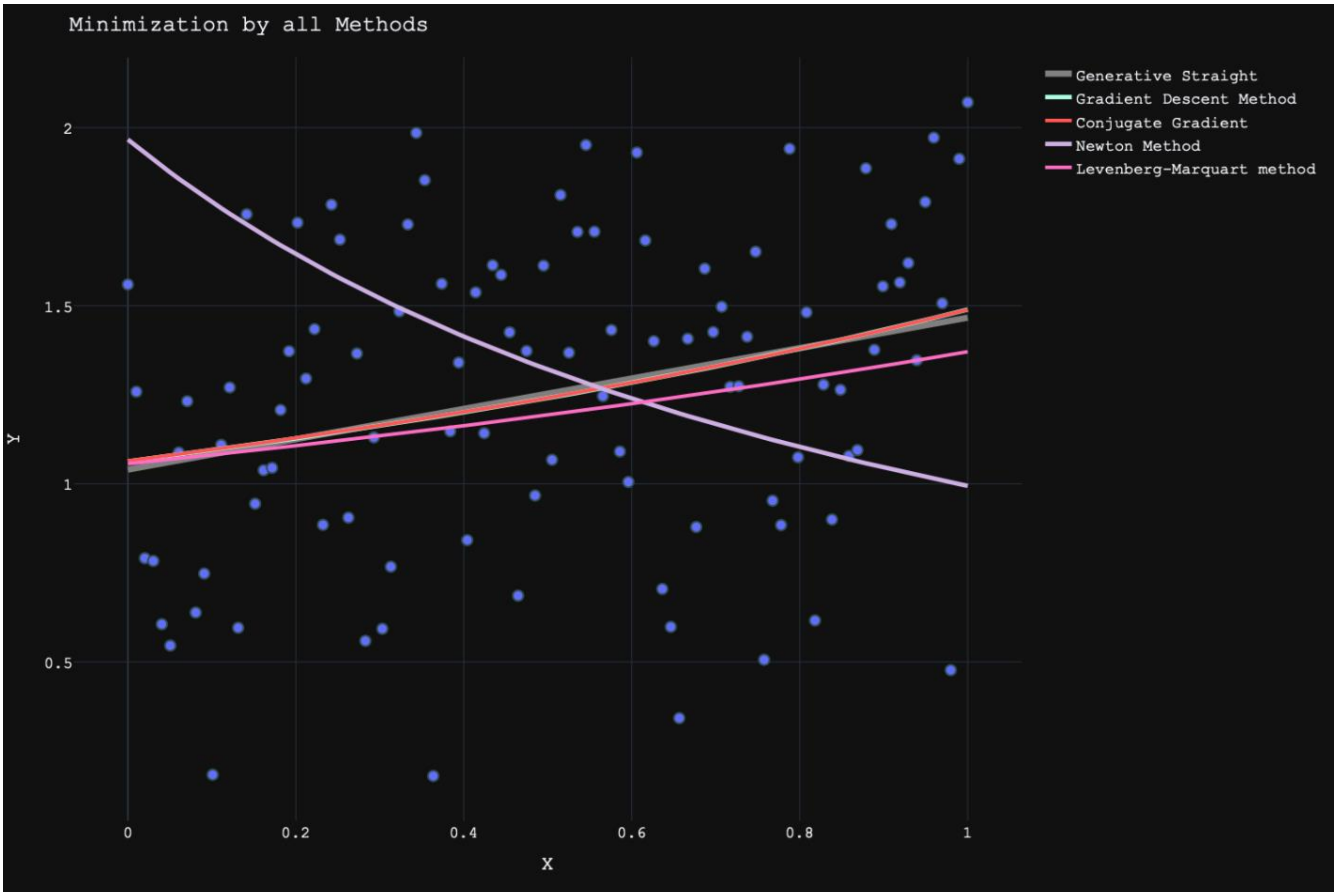

Figure 10: Rational function approximation of the least squares method withminimization by all methods.

Conclusions

In the course of the laboratory work use first- and second-order methods (Gradient Descent, Conjugate Gradient Descent, Newton's method and Levenberg-Marquardt algorithm) in the tasks of unconstrained nonlinear optimization. Research has shown that initial approximations play an important role in better optimization. Thenumber of iterations, the number of calculations of the function depends on them. The choice of optimization method also plays an important role in the quality of optimization and the number of calculations.

Appendix

Code Link