FEDERAL STATE AUTONOMOUS EDUCATIONAL INSTITUTION OF HIGHER EDUCATION

ITMO UNIVERSITY

Report

on the practical task No. 2

“Algorithms for unconstrained nonlinear optimization. Direct methods”

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Goal

Direct methods are used in unconditional nonlinear optimization problems (one-dimensional exhaustive search methods, bisection method, search for the golden section; multidimensional exhaustive search methods, Gaussian (coordinate descent), Nelder-Mead).

Formulation of the problem

1. Use the one-dimensional methods of exhaustive search, dichotomy and golden section search to find an approximate (with precision $\mathcal{E}$ = 0.001) solution $x: f(x) \rightarrow min$, then calculate the number of f-calculations and the number of iterations performed in each method and analyze the results.

2. Use the methods of exhaustive search, Gauss and Nelder-Mead to solve the minimization problem. by means of least squares through the numerical minimization (with precision $\mathcal{E}$ = 0.001) of the following function:$D(a,b) = \sum_{k=0}^{100}(F(x_k, a, b) - y_k)^2$. Visualize the data and the approximants obtained in a plot separately for each type of approximant.

Brief theoretical part

Task Overview:

The main objective of this study is to analyze the performance of various algorithms for nonlinear unconstrained optimization, in particular, direct methods, through the observation of the iterations they perform to obtain the result, as well as the number of times they perform the evaluation on the function. We will use these methods for both one-dimensional and multidimensional tasks. The tasks can be broadly classified into mathematical operations on functions using the fundamentals of the different algorithms and the use of graphs to observe the behavior of the algorithms.

Theoretical Background:

1. Algorithms for unconstrained nonlinear optimization:
   - One of the main fields of nonlinear programming is unconstrained optimization or free optimization, which deals with the problem of minimizing or maximizing a function in the absence of any constraint.
   - There are methods for finding the optimal value of a function f(x) that can be applied for functions of one or several variables, using derivatives or without using derivatives.
   - Direct search methods: which use only values of the objective function.
   - Exhaustive search: It is a univariate optimization method, where it is assumed that the function to be optimized meets the requirements of concavity/convexity, unimodal and continuous. It is the simplest method among the rest of the univariate optimization methods, so it is a good starting point.
   - Dichotomy method: is a search algorithm that works by selecting between two different alternatives (dichotomies) at each step. It is a specific type of divide-and-conquer algorithm. A well-known example is binary search.
   - Golden Section Search: is a technique for finding the extrema (minimum or maximum) of a unimodal function by successive reductions of the range of values in which the extrema are known to lie. The technique owes its name to the fact that the algorithm keeps the values of the function in trios of points whose distances form a golden ratio.
   - Gauss (coordinate descent) method: is an optimization algorithm that successively minimizes along coordinate directions to find the minimum of a function. At each iteration, the algorithm determines a coordinate or a coordinate block by a coordinate selection rule, then exactly or inexactly minimizes the corresponding coordinate

hyperplane while fixing all other coordinates or coordinate blocks. A line search along the direction of the coordinates in the current iteration can be performed to determine the appropriate step size.

- Nelder-Mead method: this technique is based on the use of polygons with different geometric shapes (reflection, expansion, reduction and contradiction). geometric shapes (reflection, expansion, reduction and contradiction), which uses the inclination of the plane found to direct the search to direct the search and thus obtain an approximation to the local optimum.

2. Least Squares Method:
   - Is a method used in a regression model to minimize the error obtained when calculating the regression equation.
   - The main characteristic of the least squares method is that the longest distances between the observed values and the regression function are minimized.

Methodological Approaches:

The task used One-Dimensional Optimization Methods, Least Squares Approximation, Data Visualization, etc.

this study combines theoretical insights with practical experimentation to provide a comprehensive understanding of algorithmic efficiency and performance. It sheds light on how different algorithms behave in different dimensions, as well as their speed.

Results

1. Exhaustive search

```
cube_exhaustive: 0.0
cube_Function calls: 1001
cube_iterations: 1001
abs_exhaustive: 0.0
abs_Function calls: 1001
abs_iterations: 1001
sine_exhaustive: -0.2172296012912312
sine_Function calls: 1001
sine_iterations: 1001
```

Figure 1 - results of exhaustive search

In the same number of iterations, we found the minimum values of three different functions with the same precision range in their respective domains. They are 0.0, 0.0, -0.21723.

2. Dichotomy search

```
cube_dichotomy_search: 1.2056736854538035e-10
cube_Function calls: 23
cube_iterations: 11
abs_dichotomy_search: 0.0001011962890624385
abs_Function calls: 23
abs_iterations: 11
sine_dichotomy_search: -0.21723352556119732
sine_Function calls: 23
sine_iterations: 11
```

Figure 2 - result of dichotomy search

In the dichotomy search, the minimum values of three different functions are changed compared with exhaustive search, the minimal value of function $f(x) = x^3$, $x \in [0, 1]$ is getting bigger, and others are similar.

3. Golden section search

```
cube_golden section search: 4.92568008577283e-11
cube_Function calls: 31
cube_iterations: 15
abs_golden section search: 7.331374358568454e-05
abs_Function calls: 31
abs_iterations: 15
sine_golden section search: -0.21723232817753246
sine_Function calls: 31
sine_iterations: 15
```

Figure 3 - result of golden section search

In the golden section search method, the results show that, in the results obtained through 15 iterations, the minimum values of the first two functions are larger, and the minimum value of the third function is similar to the other two methods.

Comparing the three methods, it was found that the best way to find the minimum value is the Exhaustive search method, but it takes up too many computing resources, and the number of iterations is much more than the other two methods. The fastest way to find the minimum value is dichotomy. The search method ended after only 11 iterations, and the results were not very different.

4. The noise dataset

```
alpha = random.random()
beta = random.random()
x_data = []
y_data = []

for i in range(0, 101):
    x = i / 100
    noise = np.random.normal(0, 1)
    y = alpha * x + beta + noise
    x_data.append(x)
    y_data.append(y)
```

Figure 4 – the generation of noise dataset

α	Random variable between 0 to 1
β	Random variable between 0 to 1
k	Range from 1 to 100
δ k	Radom variable with standard normal distrubution
x	1/k
y	y=x* α + β +noise(variable to be fitted)
Minimumize function(error function)	$(a,b) = \sum_{k=0}^{100}(F(x_k,a,b) - y_k)^2$
The variable of Minimumize function	a and b from linear function and rational function

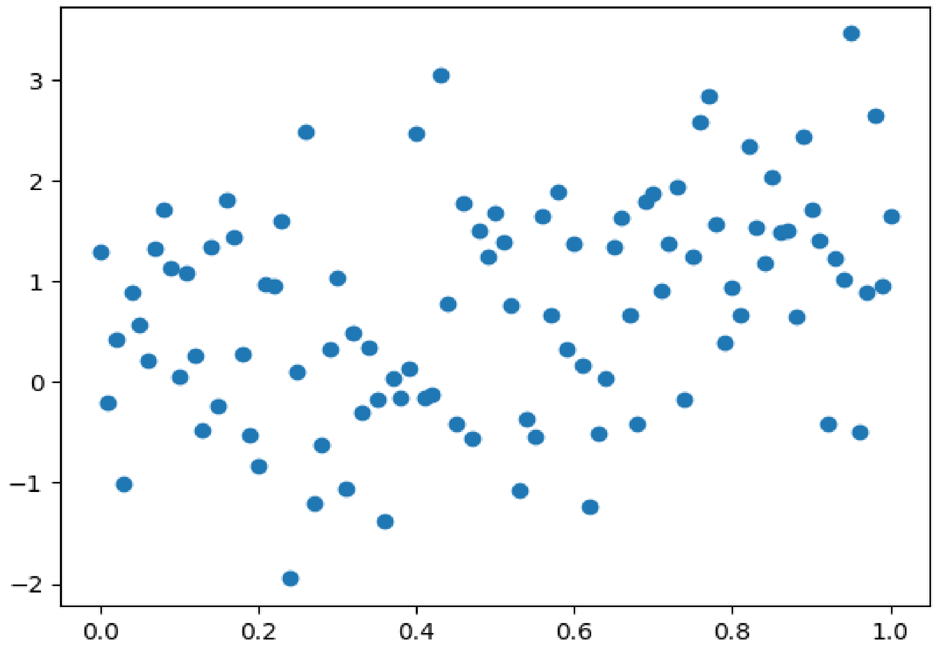
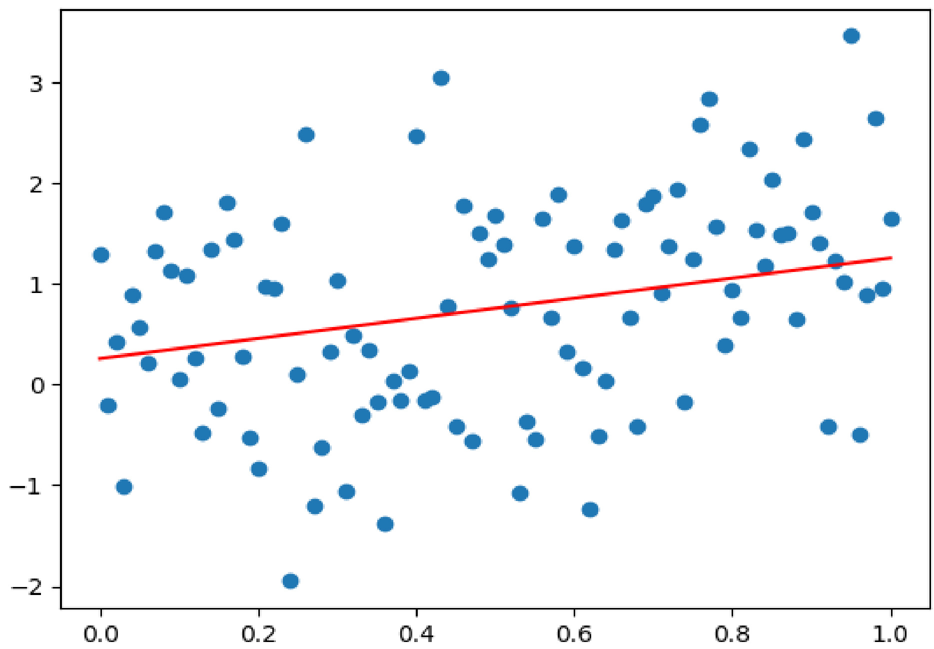


Figure 5-initial scatter plot

5. Exhaustive search linear function

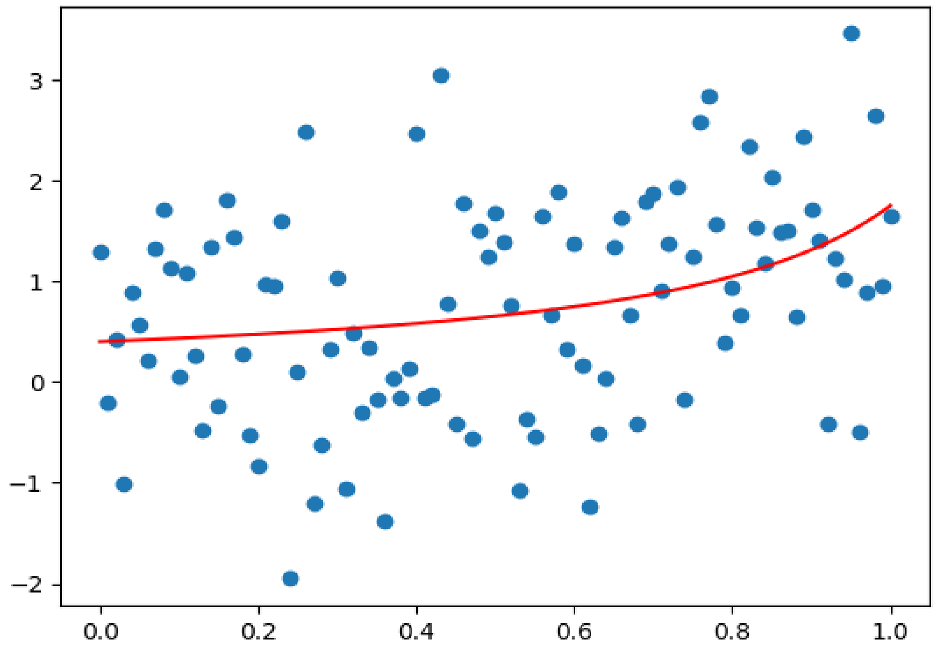



```
[a, b] = [0.999, 0.26]
Exhaustive Search-linear_function_f-calculations: 1000000
Exhaustive Search-linear_N of iterations: 1000000
```

Figure 6 - result of exhaustive search

In the result of exhaustive search,Since the dataset is randomly and uniformly,curve fitting distributed in the center of the scatter points.

6. Exhaustive search rational function

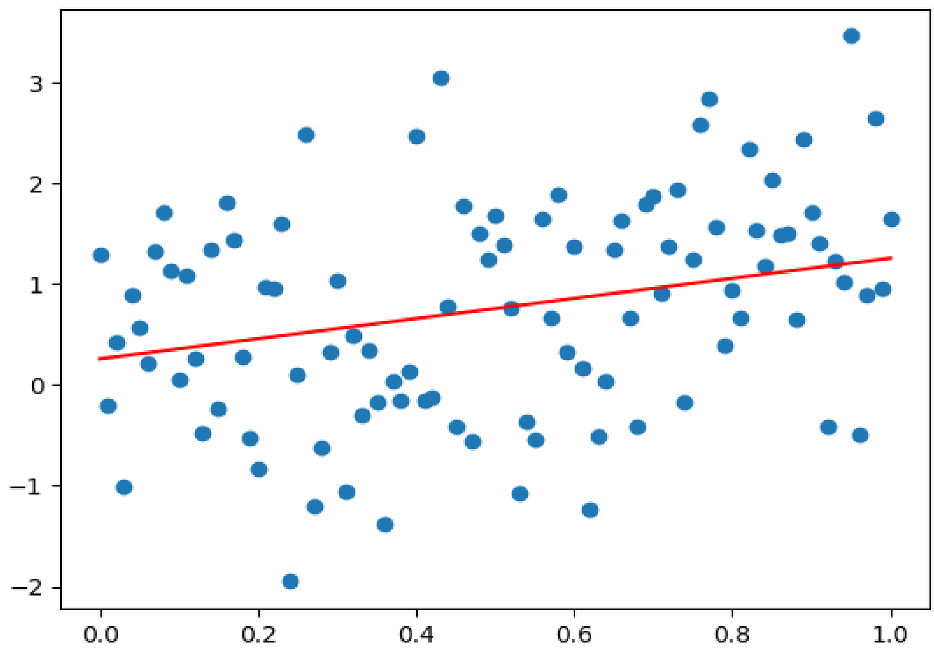



```
[a, b] = [0.404, -0.7697707707707708]
Exhaustive Search-rational_function_f-calculations: 1000000
Exhaustive Search-rational_function_N of iterations: 1000000
```

Figure 7 – exhaustive search rational function

Regarding exhaustive search rantional function, it will be miniuzed when the b of output is in negative . Detail discussion will be placed later.

7. Gauss method of linear plot




```
[a, b] = [0.999, 0.26]
Exhaustive Search-rational_function_f-calculations: 4000
Exhaustive Search-rational_function_N of iterations: 4
```

Figure 8 – Gauss method of linear plot

The Gauss method of linear plot and brute-froce have a similar outcome . Howerver,the Gauss method involves double function loop to minimize the value of a or b .So iteratins are the number of inner loop runs x the numbers of outer loop runs.

8. Gauss method of rational plot

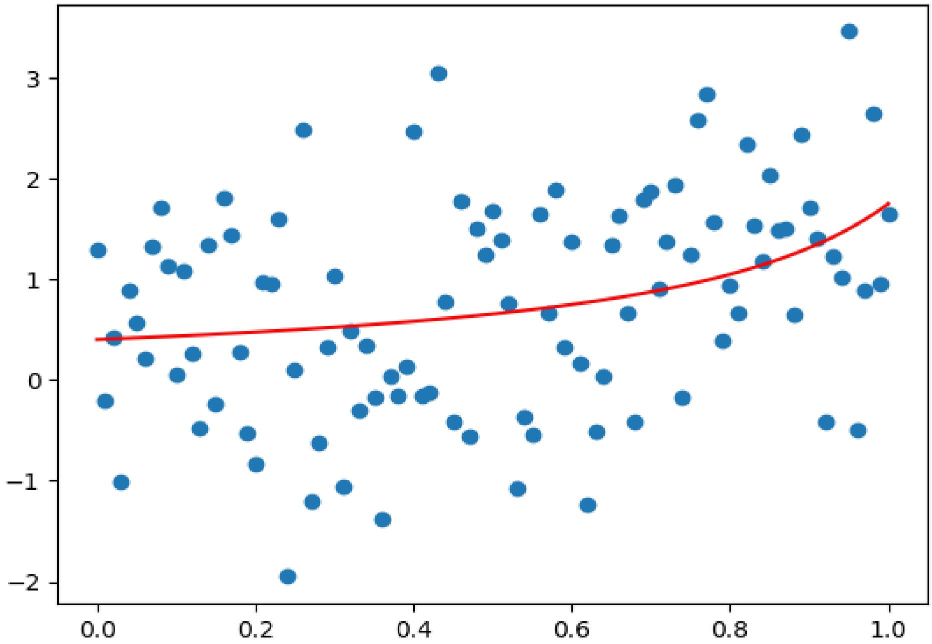


Figure 9 – Gauss method of rational plot

```
[a, b] = [0.405, -0.7689999999999998]
Gauss_Method_rational_f-calculations: 4000
Gauss_Method_rational_function_N of iterations: 32
```

9. Nelder -Mead method of linear method

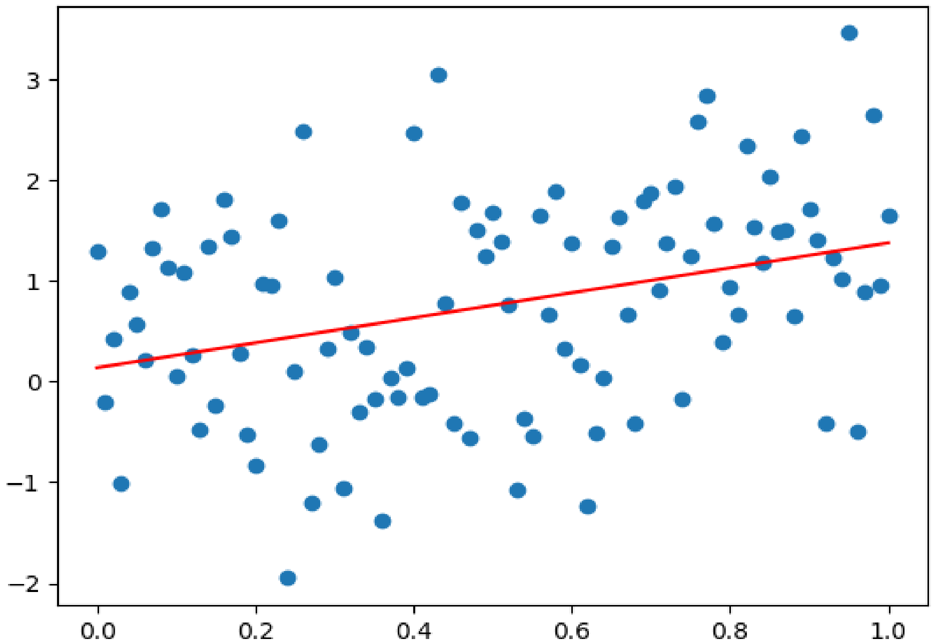


Figure 10 – Nelder mead method

Algorithms use existing function which cause b is negative number

```
Optimization terminated successfully.
         Current function value: 104.846924
         Iterations: 39
         Function evaluations: 70
[a, b] = [1.2408126672930704, 0.13887952398246772]
```

10. Nelder-Mead method of rational method

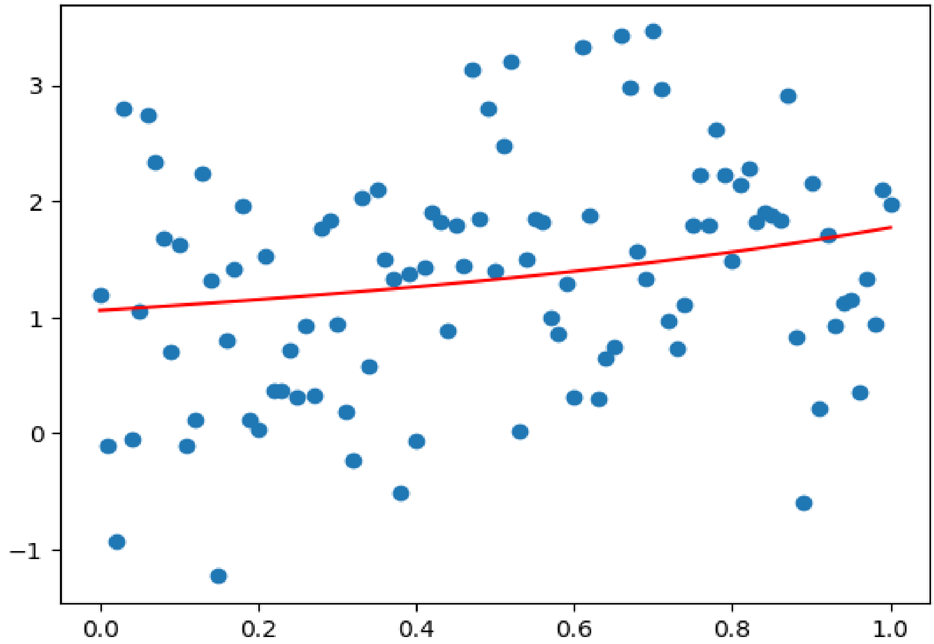


Figure 11 - Nelder mead method

```
Optimization terminated successfully.
         Current function value: 103.838132
         Iterations: 35
         Function evaluations: 68
[a, b] = [0.40368018512217707, -0.7697305319849139]
```

Similiarily ,Algorithms use existing function which cause b is negative number

11 . The comparison of linear and rational

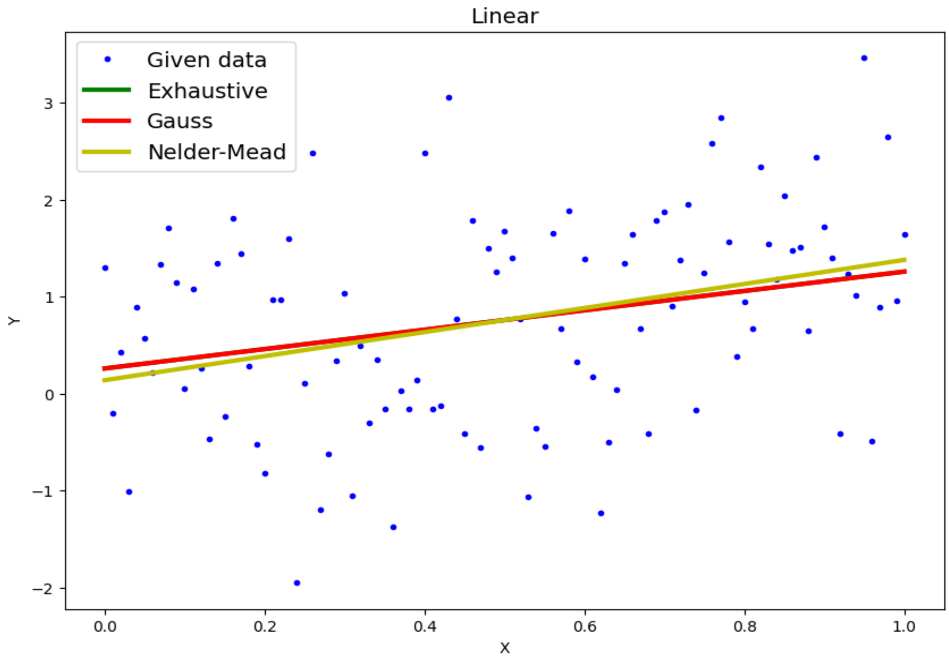


Figure 12 - comparison of linear

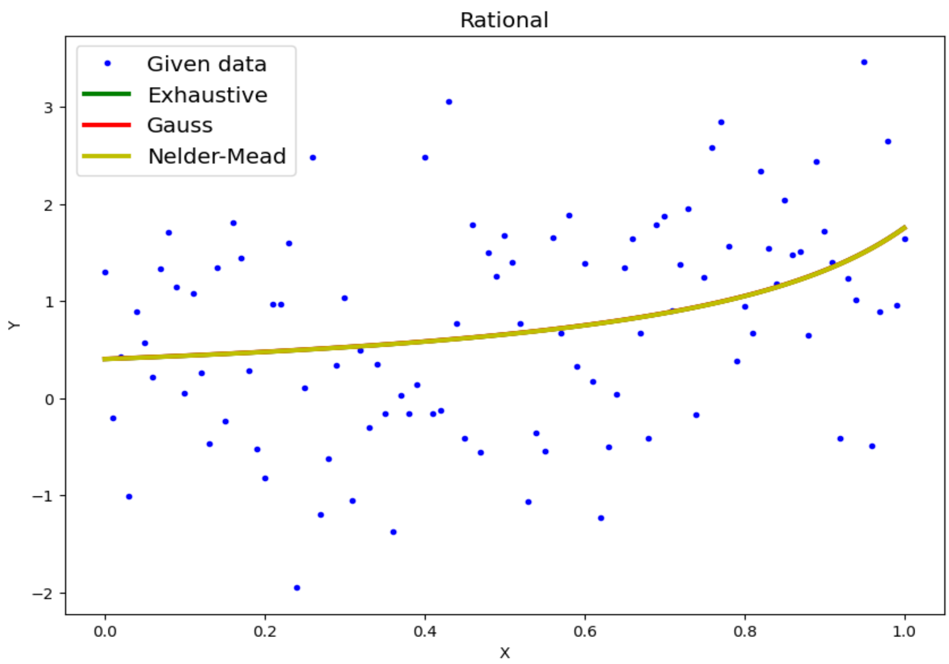


Figure 13 - comparison of rational

The image of Exhaustive , Gauss and Nelder-Mead is overlapped . I proved that the result was correct

11. Discussion on the value range of rational function parameter b

11.1 Theory

Regard to Talyor 's theorem

$$\frac{1}{1-x}=\sum_{n=0}^{\infty}x^{n}=1+x+x^{2}+x^{3}+\cdots+x^{n}+\cdots,x\in(-1,1)$$

Figure 14 - Talyor 's theorem

y = alpha * x + beta + noise (beta+noise∈（0，2）) alpha∈（0，1），y = alpha * x + beta + noise can be considered as y=1+x; Therefore, for a/(1+bx), b is a negative number and it is easier to obtain the minimum value.

11.2 Image method

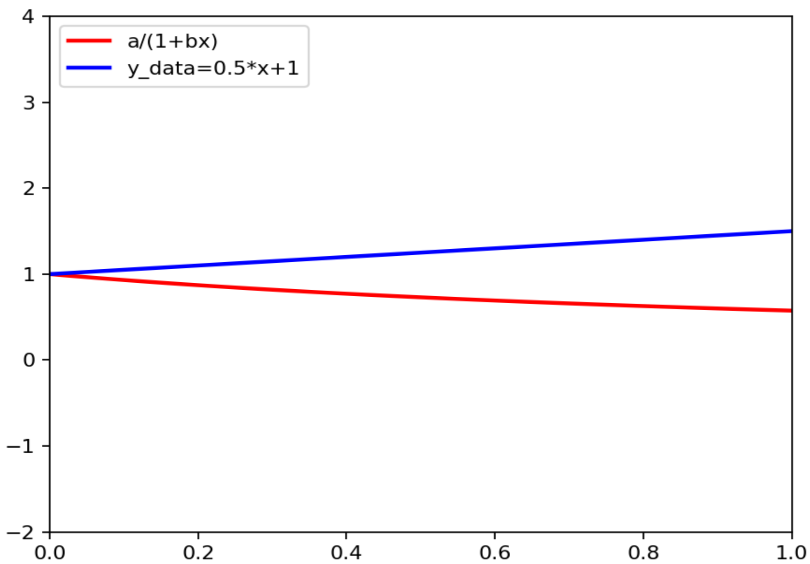


Figure 15 - Connection of a/(1+bx) and y_data=0.5*x+1

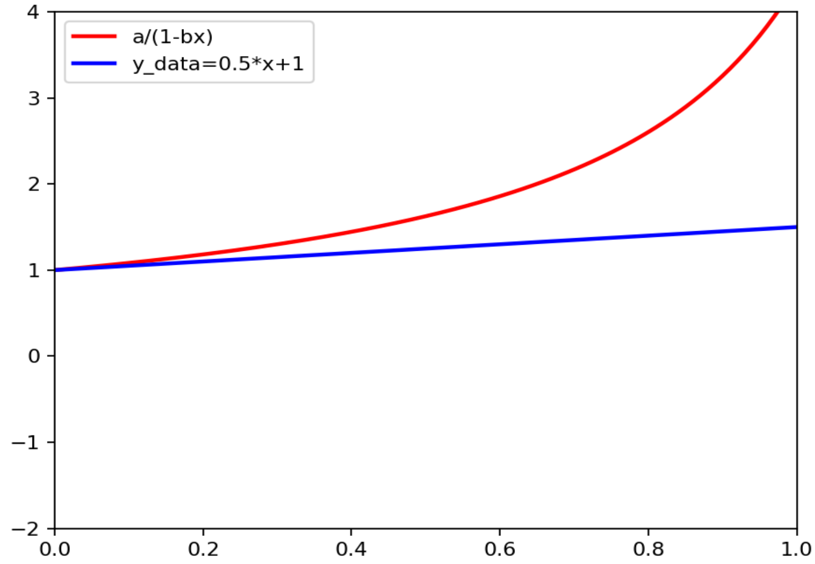


Figure 16 - Connection of a/(1-bx) and y_data=0.5*x+1

As shown in the figure, the trend of y_data is an image from the lower left to the upper right. The image of a/(1+bx) curves downward as b increases; the image of a/(1-bx) curves upward as b increases. Therefore, the image can be approximately fitted only when b takes a negative value.

Detailed animation: task2(add)

Conclusions

In conclusion, the task presented a comprehensive exploration of optimization and data approximation methods across various mathematical functions and domains. The following key points summarize the findings and insights gained from this task:

I. One-Dimensional Optimization Methods:
- The task introduced and compared three one-dimensional optimization methods: exhaustive search, dichotomy, and golden section search.
- It was observed that exhaustive search, while straightforward, can be computationally expensive due to its exhaustive evaluation of the objective function.
- Dichotomy and golden section search offered more efficient convergence, with golden section search typically converging faster.

II. Least Squares Approximation:
- The task applied the least squares methodology to approximate noisy data with mathematical functions.
- Linear and rational functions were employed as approximants, with the goal of minimizing the sum of squared differences between observed and predicted data points.

III. Optimization Methods:
- Three optimization methods were used to find the optimal parameters for the approximating functions: exhaustive search, Gauss optimization, and Nelder-Mead optimization.
- Gauss optimization, being a gradient-based method, tended to converge faster than exhaustive search, which performed a grid search.
- Nelder-Mead optimization, a derivative-free method, provided an intermediate solution in terms of convergence speed.

IV. Data Generation and Visualization:
- Random data generation techniques were utilized to create noisy data, mimicking real-world scenarios.
- Data and approximations were effectively visualized using Matplotlib, allowing for easy comparison of results.

V. Analysis of Results:
   - The results were analyzed in terms of the number of iterations, precision ($\varepsilon = 0.001$), and the number of function evaluations for each optimization method.
   - Trade-offs between computational cost and accuracy were considered, highlighting the importance of choosing an appropriate method for specific applications.

In summary, this task provided valuable insights into various optimization methods and their application in approximating real-world data. It emphasized the importance of method selection based on the problem's characteristics, computational resources, and desired precision. The task also showcased the power of data visualization in comparing and interpreting results. These methodological approaches are widely applicable and serve as valuable tools in fields such as engineering, science, and data analysis for finding optimal solutions and making data-driven decisions.