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"

Performed by
Eugenia Khomenko
J4133c
Accepted by
Dr Petr Chunaev

St. Petersburg 2022

Goal

This work aims for the tasks of unconstrained nonlinear optimization using such first-order methods as Gradient Descent and Non-linear Conjugate Gradient Descent and Newton's and Levenberg-Marquardt algorithms known as second-order methods.

Formulation of the problem

Comparing the results for used numerical methods and finding approximate solutions for functions are the main goals of this paper. Work is required to solve the minimization problem of generated the noisy data by the first- and secon-order methods: Gradient Descent, Non-linear Conjugate Gradient Descent, Newton's method and Livenberg-Marquardt method. Data should be approximated by linear function $F(x,\ a,\ b) = ax + b$ and rational function $F(x,\ a,\ b) = \frac{a}{1+bx}$ by means of least squares.

Brief theoretical part

An algorithm is any well-defined computational procedure that takes some value, or set of values, as input and produces some value, or set of values, as output. An algorithm is thus a sequence of computational steps that transform the input into the output. Also an algorithm can appear as a tool for solving a well-specified computational problem.

Usually computer professionals use the method which is the easiest to implement. But at the same time bounded resources of computers should be taken into account because computers are not yet infinitely fast and memory is not free. Optimization methods which find optimal in some sense solutions for mathematical models will help us use these resouces wisely.

There are direct, or zero-order, first-order and second-order methods. This work includes first- and second-order methods.

First-order methods which are used in this paper:

1. Steppest gradient descent follows the rule, where at each iteration the value of function updates by the gradient at the current point and search will be continued in the new direction. The search can be stopped by two ways. Firstly, when modolus the gradient at the point is less than previously set constant epsilon. Secondly, algorithm can set certain amount of epochs for loop so the result will be calculated after definitive number of updates.

2. Non-linear conjugate gradient descent stops and obtains the minimum of function when the gradient is zero. Within a linear approximation, the parameters alpha and beta are the same as in the linear conjugate gradient method but have been obtained with line searches. The conjugate gradient method can follow narrow valleys, where the steepest descent method slows down and follows a criss-cross pattern.

Second-order methods which are used:

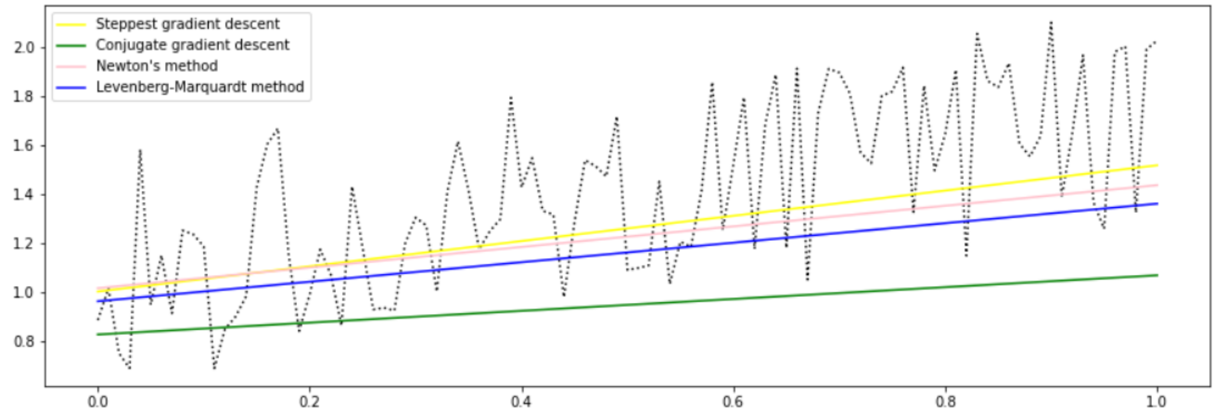
1. Newton's method uses the quotient of the value function and function's derivation for single-variable functions and the product of an inversed hessian matrix and the gradient for multidimensial case. This method requires that the derivative can be

calculated directly. Moreover, such process is not be easily obtainable and can be expensive to evaluate.

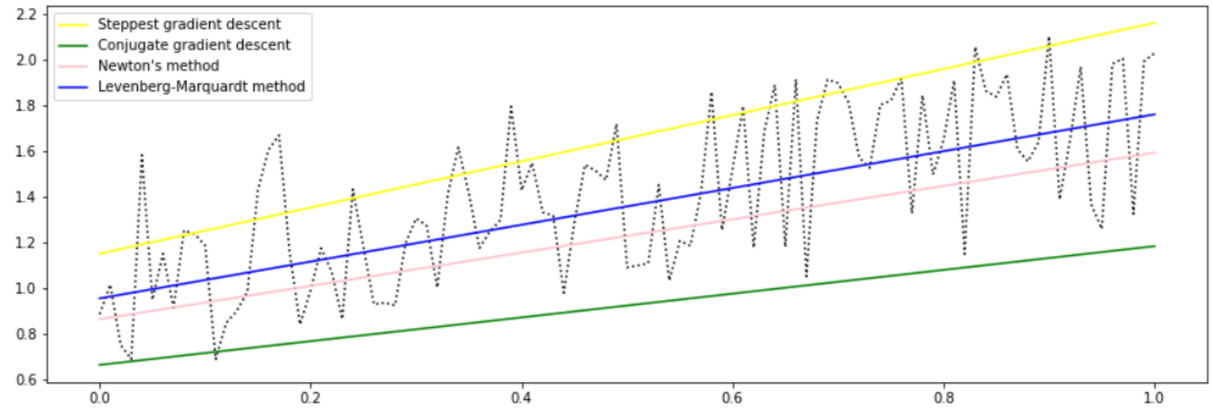
2. Levenberg-Marquardt method is not only preudo-second order algorithm but also is requared to solve non-linear least squares problems. It is a hybrid method which uses both steppest gradient descent and Gauss-Newton method for optimal solutions.

Results

1. Linear approximant.



2. Rational approximant.



Conclusions

In conclusion, in this work was considered varied algorithms of first- and secon-order algorithms and was visualized the results by matplotlib, Python library. On input data linear and rational approximants were minimized more effectively by Levenberg-Marquardt, which known as a kind of quasi-Newton method.

Appendix

https://github.com/JaneKKTTme/analysis-and-development-of-algorithms