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Development of The Steepest Descent Method for Unconstrained Optimization of Nonlinear Function

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Abstract. The q-gradient method used a Yuan step size for odd steps, and geometric recursion as an even step size (q-GY). This study aimed to accelerate convergence to a minimum point by minimizing the number of iterations, by dilating the parameter q to the independent variable and then comparing the results with three algorithms namely, the classical steepest descent (SD) method, steepest descent method with Yuan Steps (SDY), and q-gradient method with geometric recursion (q-G). The numerical results were presented in tables and graphs. The study used Rosenbrock function $f(\boldsymbol{x}) = (1 - x_1)^2 + 100(x_2 - {x_1}^2)^2$ and determined $\mu = 1, \sigma_0 = 0.5, \beta = 0.999$, the starting point ($\boldsymbol{x_0}$) with a uniform distribution on the interval $\boldsymbol{x_0}$= (-2.048, 2.048) in $\mathbb{R}^2$, with 49 starting points ($\boldsymbol{x_0}$) executed using the Python online compiler on a 64bit core i3 laptop. The maximum number of iterations was 58,679. Using tolerance limits as stopping criteria is 10^{-4} and the inequality $f(x^*) > f$ to get numerical results. q-GY method downward movement towards the minimum point was better than the SD and SDY methods while the numerical results of the Rosenbrock function showed good enough performance to increase convergence to the minimum point.

INTRODUCTION

Optimization is a branch of applied mathematics that studies the process of obtaining the best decision that gives the maximum or minimum value of a function. Optimization problems can be categorized into constrained optimization and unconstrained optimization. Optimization problems can be solved analytically or numerically. For unconstrained optimization of nonlinear functions with many variables requires a numerical method to solve this problem. Numerical methods are iterative and one of them is the steepest descent method or also called the gradient descent method. This method is also one of the simplest minimization methods for unconstrained optimization problems, because it uses a negative value gradient to find the direction (gradient). In terms of finding the direction (gradient) does not require a second derivative, resulting in low computational costs and low matrix storage requirements. For a function f which is defined $\mathbb{R}^n$and has a real value, namely $f: \mathbb{R}^n \rightarrow \mathbb{R}$ the method of finding the minimal form of the nonlinear equation$f(\boldsymbol{x})$ = 0, for $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$ introduced by (Mitrinovic & Keckic, 1984) using gradients. The disadvantage of steepest descent is that it has a slow convergence to reach the optimal value, due to the zigzag step (Silalahi et al., 2015). For this reason, there is a need for development, using the Yuan step size as a step search, also shown by (Silalahi et al., 2015) and q-calculus called q-Jackson by (Jackson, 1909) he provides generalizations from special numbers, sequences, functions, q-integral and used in this research is q-derivative. (Soterroni et al., 2011) introduced the q version for the steepest descent method, called the q-gradient method or the (q-G) method which is a tool to solve the global minima unconstrained problem. The main idea of the method (q-G) is to use a negative q-gradient objective function that is used as a direction finding, the q-gradient is

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calculated based on the q-Jackson and requires a dilation with the parameter q which is a real number not equal to. By using the Rosenbrock function, the algorithm will be analyzed in the form of numerical results and graphs of the movement of the function to the minimum point.

It can be seen in Figure 1 below q_1 and $q_2$the sign of the q derivative is positive and the q-G method will move to the left as did the steepest descent method. However, for q_3 the sign of the negative q derivative could potentially allow the q-G method to move in the right direction, towards the global minimum f.

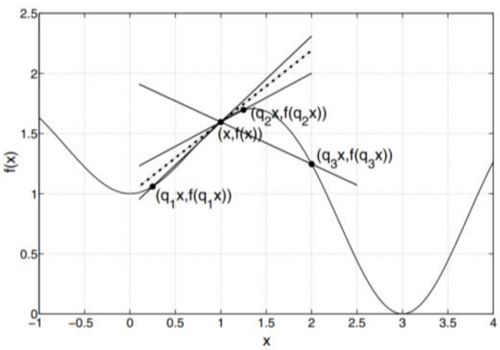

Figure 1. Point movement with q dilation (Soterroni et al., 2011)

In this paper, we are interested in developing a steepest descent method to accelerate convergence by combining the q-G method with the Yuan and geometric recursion step size (q-GY).

q- Derivative

$f(x)$ is a real-valued continuous function with a single variable, the q-derivative of f is given as follows

$$D_q f(x) = \frac{f(x) - f(qx)}{(1-q)x}$$

With $x \neq 0$ dan $q \neq 1$. And in the finite case, $q = 1$, the q-derivative is equal to the classical derivative with f differentiable at x. The parameter q is taken from the interval $0 < q < 1$, but q can be a real number different from 1. For a real-valued continuous function is differentiable at $x = 0$, the derivative of q can be given by

$$Dq_i, x_i f(\boldsymbol{x}_i) = \begin{cases} \dfrac{f(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n) - f(x_1, \dots, x_{i-1}, q_i x_i, x_{i+1}, \dots, x_n)}{(1-q_i)x_i}, x \neq 0\ q \neq 0 \\ \dfrac{\partial f}{\partial x_i}(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_n), \qquad x_i = 0 \\ \dfrac{\partial f}{\partial x_i}(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n), \qquad q_i = 0 \end{cases}$$

For a real-valued continuous function of n variables $f(x)$, the gradient vector is a vector of n first-order partial derivatives of f provided that the function has first-order partial derivatives with respect to all independent variables $\boldsymbol{x_i}$ =($i = 1, 2, \cdot\cdot\cdot, n$). Similarly, the gradient vector q is the vector of n first-order partial derivatives of f. Before introducing the gradient vector q, it is convenient to define the first-order partial derivative q of a real-valued continuous function of n variables with respect to the variable x_i.

$$\nabla_q f(\boldsymbol{x}) = [Dq_1, x_1 f(\boldsymbol{x}_1), Dq_2, x_2 f(\boldsymbol{x}_2), \dots, Dq_n, x_n f(\boldsymbol{x}_n)]$$

and in limit, $q_i \rightarrow 1$, for all i =(1,..,n) [3]

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q-Gradient Method

A general optimization strategy is to consider an initial set of independent variables $\boldsymbol{x_0}$ and apply the iterative procedure given by $\boldsymbol{x_k}$ = $\boldsymbol{x_k}$ −1 +$\alpha_k \boldsymbol{s_k}$, where k is the iteration number, x is the variable vector, α is the step length and s is the search direction vector. This process continues until no additional reduction in the value of the objective function can be made or the solution point has been approached with sufficient accuracy. In the steepest descent method, the search direction s_k is given by the negative gradient vector Because it uses a negative gradient as the search direction, it is also known as the gradient method (Djordjevic, 2019). at the point x_k , $f\ (x_k)$, and the step length k can be found by a one-dimensional search performed in the s_k direction. Similarly, the search direction for the q −steepest descent method is given by the negative gradient vector q at the x_k , $q\ f\ (x_k)$.

At the start of the iterative procedure, $\sigma_k \neq 0$ with μ= 1, this strategy implies that the parameter q_i can be any positive real number with more occurrences around the mean, but with the same probability of occurring in the interval (0,1) or (1,∞) . At that point, the gradient vector q can point in any direction. This gives the method the possibility of looking in other directions different from the steepest descent direction and escaping the local minimum for multimodal functions, or reducing the zigzag motion to the minimum for poorly scaled functions. At the end of the iterative procedure, when σ_k tends to 0 with μ = 1, the parameter $q_i$tends to 1 and the gradient vector q tends to the regular gradient vector. In other words, when $\sigma \rightarrow 0$ this strategy makes the q −steepest descent method reduces to the classical steepest descent method. The optimization algorithm for the classic q −steepest descent method is given below.

q-Steepest Descent Algorithm

Step 1: at random $x_0 \in \mathbb{R}^n$, set μ = 1, take σ_0 and β.
Step 2: Set $k := 1$.
Step 3: Generate the parameter q = $(q_1, \ldots, q_i, .., q_n)$ with log-normal distribution or a gaussian distribution in (Gouvêa et al., 2016; Soterroni et al., 2015) with μ and standard deviation σ_k.
Step 4: Calculate the search direction $s_k = -\nabla f(x_k)$.
Step 5: Find the step length α_k with *geometric recursion*
Step 6: Calculate $x_{k+1} + 1 = x_k + \alpha_k s_k$
Step 7: If the stopping criteria is reached, then stop; else, continue with step 8.
Step 8: Subtract the standard deviation $\sigma_k = \beta.\sigma_{k-1}$ and $\alpha_k = \beta.\alpha_{k-1}$,
Step 9: Set $\boldsymbol{k := k+1}$, and go to step 3. (Soterroni et al., 2011)

Yuan Step Size

The steepest descent method is the simplest iterative optimization technique that does not need to calculate the Hessian of the objective function, but has a slow convergence, the theoretical convergence rate was first studied by Hestenes and Stiefel in 1952 where it was recognized that the degree of convergence is highly dependent on the value distribution. The eigenvalues of a positive definite matrix (Mishra et al., 2021), the eigenvalues are denoted by , which is the magnitude of the change in vector length that occurs, in the steepest descent method the small step length makes the gradient descent converge to the minimum very slowly (Watt et al., 2016).

(Yuan, 2006) introduced the Yuan method in his original paper using alternating step sizes as in the AM method. However, the Yuan method uses a new step size. Yuan's method uses exact line search on odd iterations, and then uses the following step size on even iterations (Silalahi et al., 2015):

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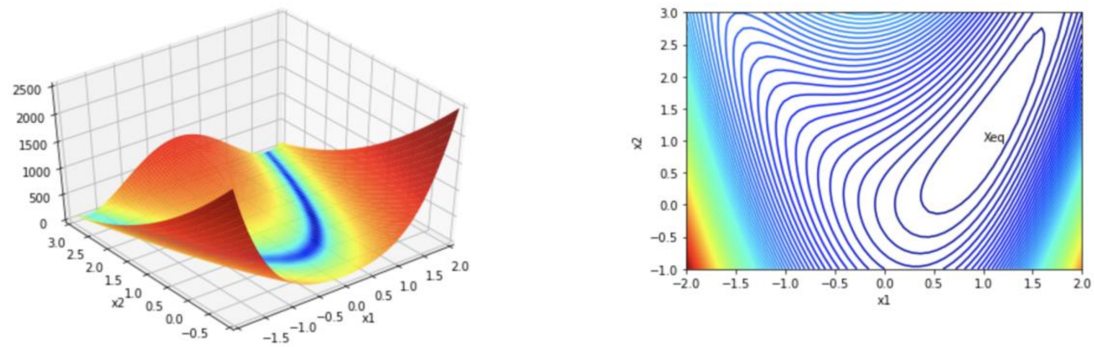
$$\alpha^k = \begin{cases} \dfrac{g_k^T g_k}{g_k^T A g_k}, if\ \ k\ odd \\ \dfrac{2}{\sqrt{\left(\dfrac{1}{\alpha_{2k-1}} - \dfrac{1}{\alpha_{2k}}\right)^2 + \dfrac{4\|g_{2k}\|^2}{\|s_{2k-1}\|^2}} + \dfrac{1}{\alpha_{2k-1}} + \dfrac{1}{\alpha_{2k}}}, \qquad if\ \ k\ even \end{cases}$$

Rosenbrock function

The Rosenbrock function is a unimodal function having an optimal solution 0 to (0, 0, …, 0) (Soterroni et al., 2015) $f(\boldsymbol{x}) = (1 - x_1)^2 + 100(x_2 - {x_1}^2)^2$ dengan $\mu = 1, \sigma_0 = 0.5$ as a variable to find the parameter q , $\beta = 0.995$ as a reduction factor to find the standard deviation value in each iteration at the interval x_0= (-2.048, 2.048). The following is a graph of the Rosenbrock function and the contours of the Rosenbrock function:



a **b**

Figure 2. Rosenbrock Function Form (a) and Contour (b) (Shang & Qiu, 2006)

Shows the 2-dimensional contour of the Rosenbrock function which has one global minimum at x_{eq}.

q-GY Algorithm

The q-GY algorithm is an algorithm with q-Jackson direction search or also called q-gradient with Yuan and geometric recursion step size (q-GY), following the q-GY algorithm, determined starting $x_0, \sigma^0 > 0, \beta\ \epsilon\ (0,1)$ or $0 < \beta < 1$.

Step 1 : Set k=0

Step 2 : $x^* = x^k$

Step 3 : If the stopping criteria is not reached, then continue:

Step 4 : Make $\boldsymbol{q}^k\boldsymbol{x}^k$ of the Gaussian distribution with σ^k and μ^k

Step 5 : Calculate vector q- gradient $\nabla f\left(\boldsymbol{x}^k\right)$

Step 6 : Determine $\boldsymbol{d}^k = -\nabla_q f\left(\boldsymbol{x}^k\right)$ (Soterroni et al., 2015)

Step 7 : Calculate α^k with Yuan step size

$$\alpha^k = \begin{cases} \dfrac{(d^k)^T d^k}{(d^k)^T A d^k}, if\ \ (k, 4) = 0\ or\ \ 3\ even \\ \dfrac{2}{\sqrt{\left(\frac{1}{\alpha^{k-1}} - \frac{1}{\alpha^k}\right)^2 + \frac{4\|d^k\|^2}{\|s\|^2}} + \frac{1}{\alpha^{k-1}} + \frac{(d^k)^T A d^k}{(d^k)^T d^k}} \end{cases}, others \text{ (Silalahi et al., 2015)}$$

$$\boldsymbol{s} = \boldsymbol{x}^k - \boldsymbol{x}^{k-1} = -\alpha^{k-1}\boldsymbol{d}^{k-1}$$

Step 8 : Do the following iteration $x^{k+1} = x^k + \alpha^k . d^k$

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Step 9 : if $f\left(x^{k+1}\right) < f(x^*)$, set $x^* = x^{k+1}$
Step 10 : Define $\sigma^{k+1} = \beta.\sigma^k$ (Soterroni et al., 2015)
Step 11 : Set $k = k + 1$
Step 12 : And back again to step (3.1)

RESEARCH METHODS

In this study, the search for the direction of the q-gradient with the Jackson derivative or also called the (q-G) method was carried out, namely the dilatation of the q parameter to the independent variable by comparing the numerical results of three algorithms, namely the classical steepest descent (SD) method, the steepest descent (SDY) method with steps Yuan (Yuan, 2006), q-gradient method with geometric recursion (Gouvêa et al., 2016). The method in this study used a direction search using the q-gradient method and a Yuan or q-GY step size, also included an initial search with geometric recursion. The numerical results were in the form of tables and graphs of convergence to see the improvement of the q-GY method on the level of convergence and the number of iterations, using a unimodal function, namely the Rosenbrock function at $\mathbb{R}^2$with 49 starting points $(\boldsymbol{x_0})$and a predetermined limit on the function. Run using Python online compiler on a 64bit core i3 laptop to see numerical results. For the Rosenbrock function $f(\boldsymbol{x}) = (1 - x_1)^2 + 100(x_2 - {x_1}^2)^2$ given $= 1, \sigma_0 = 0.5, \beta = 0.999$, the starting point was returned from the interval x_0= (-2.048, 2.048) using a uniform distribution on the selection of starting points (Soterroni et al., 2011). The maximum number of iterations in python was 58,679 or 2MB and used a tolerance limit as the stopping criteria, which is 10^{-4} in 10 iterations of search, while $f\left(\boldsymbol{x}^{k+1}\right) > f(\boldsymbol{x}^*)$ stopping criteria was used to find minimum point in the algorithm.

Data Input:

$\boldsymbol{x}_0$= initial point

$\sigma^0 > 0$ the reduced standard deviation with the parameter $\beta \, \epsilon \, (0,1)$ in the iteration process

q^k= parameter whose value is close to 1, or q→1 is searched with a Gaussian distribution

Gaussian distribution when $\mu = 1, \sigma^k > 0, \mu^k = \boldsymbol{x}^k, \pi = 3.14 \ or \ \frac{22}{7}$

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

$\boldsymbol{d}^k$ direction finding (downward direction) using q-derivative

α^k step size k

$\boldsymbol{g}_k$ = $\boldsymbol{d}^k$

A= Hessian matrix

$$A = \begin{bmatrix} \frac{\partial^2 f}{\partial x \partial x} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y \partial y} \end{bmatrix}$$

$\nabla_q f(\boldsymbol{x}^k)$ = q-Gradien

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$$D q_i, x_i f(\boldsymbol{x}_i) = \begin{cases} \dfrac{f(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n) - f(x_1, \dots, x_{i-1}, q_i x_i, x_{i+1}, \dots, x_n)}{(1-q_i)x_i}, x \neq 0\ q \neq 0 \\ \dfrac{\partial f}{\partial x_i}(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_n), \qquad x_i = 0 \\ \dfrac{\partial f}{\partial x_i}(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n), \qquad q_i = 0 \end{cases}$$

$$\nabla_q f(\boldsymbol{x}) = [D q_1, x_1 f(\boldsymbol{x}_1), D q_2, x_2 f(\boldsymbol{x}_2), \dots, D q_n, x_n f(\boldsymbol{x}_n)]$$

$$\left\|\nabla_q f(\boldsymbol{x}^k)\right\| = \sqrt{(D q_1, x_1 f(\boldsymbol{x}_1))^2 + \left(D q_2, x_2 f(\boldsymbol{x}_2)\right)^2 \dots + (D q_n, x_n f(\boldsymbol{x}_n))^2}$$

RESULTS AND DISCUSSION

The numerical result table for each algorithm showed the number of iterations for each algorithm with the Rosenbrock function, and the graph showed the level of convergence to the minimum point. The iteration process to see the number of iterations reached the minimum point will continue as long as $f\left(\boldsymbol{x}^{k+1}\right) < \boldsymbol{f}$ but to see the level of convergence of the graph form, $f\left(\boldsymbol{x}^{k+1}\right) > 10^{-4}$ and only took the first 10 iterations, as long as the stopping criteria were not met then $i = i + 1$, $\sigma_{k+1} = \beta . \sigma_k$ and β were constant and then returned to the direction finding step. The search for the first 10 iterations aimed to see the average $f(x^*)$ at a certain point, so that in this study 14 starting points were taken randomly among 49 points evaluated on the Rosenbrock function in intervals (-2.048, 2.048).

Classical SD method showed iterations will increase, the minimum point was at a large f value. The Rosenbrock function had one minimum value so that the cause of the increase in f was due to the increasing search direction in the running algorithm, such as at the point (-2.048, 0.061) there is f = 1717.71 with 1 iteration but at the point (-1.305,-2.048) and (- 1.305, -1.305) shows the opposite result, namely 1074 iterations and 1012 iterations with the minimum point being at f = 0.839 and f = 0.820 there was also one point with 1 iteration with f = 1.209, with the starting point (0.061, 0.061). The SD Yuan (SDY) method uses a Yuan step size where in even steps the step size is searched with a line search, and odd steps with a yuan step size, produced the same pattern in each iteration, i.e. a small number of iterations will produce a minimum point or f which large value, on the other hand if the minimum point was large, there is a small number of iterations, as in the value of f = (-2.048, -1.305) the number of iterations is 1234, f = (-1.305, -2.048) with1435 iterations and f= (-1.305, -1.305) with 1352 iterations, but there was also f = (0.061, 0.061) with 1 iteration. SD and SDY have similar results. The q-G method is a method that uses the search for the q-gradient direction and geometric recursion step size as in (Gouvêa et al., 2016). Returned to 20 out of 49 points with good results at the minimum point or towards the global minimum with small iterations, some of which were at f = {(-0.622, 0.061), (-0.622, 0.744), (-0.622, 2.048) , (1.305, 0.744), (-1.305, 0.744), (-1.305, 1.427), (-1.305, 2.048), (-2.048, -0.622), (-2.048, 0.061), (-2.048, -0.622) , (-2,048, 0.744), (-2,048, 1,427), ...} returns successive iterations = {4, 5, 2, 8, 4, 2, 1, 6, 5, 6, 3, 5, ...}, shows that q-G was very effective to reach the minimum point with faster convergence than the classical steepest descent (SD) method. The q-GY method uses an even or initial step search using geometric recursion with several provisions as mentioned in the research methods chapter, if it was adjusted to the research objectives, the results shown were quite satisfactory, it can be seen from the f values at several starting points $\boldsymbol{x_0}$= {(-2.048, -2,048), (-2,048),(0.744), (-2,048, 1,427), (-2,048, 2,048), (-1.305, 2.048), (-1.305, -1.305)} where f and the number of consecutive iterations were as follows , f = {972,338, 203,162, 117,683, 62.742, 2,922, 3,873}, number of iterations = {93, 91, 91,

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91, 8, 4}. From the results of the run the q-GY algorithm can be consistent in maintaining the average number of iterations at each starting point, but in this study, it was found that the use of the q-GY algorithm at several points can be used to accelerate convergence by changing the stopping criteria but will show different results. The cause of the instability of the minimum point is due to the stopping criteria using the inequality, $f^* > f$, so the iteration limit depends on the direction that the next step will take, each starting point has a different minimum point. The use of q-GY on Rosenbrock should use stopping criteria with a tolerance limit to get t*o* the minimum point but the results displayed do not always decrease. Using a simpler function can more clearly see the convergence to the minimum point.

Table 1. Recapitulation of the average value of $f(x^*)$ in each algorithm, there was Classic Steepest Descent (SD), Steepest Descent with Yuan step size (SDY), q-Gradien (q-G), q-Gradien with Yuan steps (q-GY). Next, the average result $f(x^*)$ was displayed in the form of a graph showing how each algorithm performed in the first 10 iterations in the specified interval. The following table shows a decrease in the value of f when using the SD, q-G and q-GY methods, while there was an increase and decrease in the value of f in SDY, more clearly seen in graph 1.

Table.1 Average $f(x^*)$ on Rosenbrock functions

Iterasi	SD	SDY	q-G	q-GY
1	770.4341	770.4341	727.7749	406.1857
2	766.0104	44906280	685.4928	336.62
3	761.6505	56594297	647.4297	286.8453
4	757.3552	3.37E+10	613.0453	267.6328
5	753.1256	2.78E+09	581.8847	250.8054
6	748.9636	1.97E+09	553.5622	243.2609
7	744.8726	5.73E+11	527.749	236.1797
8	740.8579	1.14E+11	504.163	232.8164
9	736.9286	1.54E+10	482.5615	229.5677
10	733.1006	2.47E+10	462.7341	227.9849

Graph 1. Shows the movement of an algorithm towards the minimum point, it can be seen in the SD method that the graph decreases starting at iteration 1 with f between 750 and 800, and in the 10th iteration the point f still has not reached the minimum point. In the SDY method, there is no change in iterations 1 to 6, but it shows that f which has a small value, it is a good step to reach the minimum point faster, but in the 7th iteration there is an increase in f, this is due to the stopping criteria used, namely the limit a tolerance of 10^{-4} causes the iteration to continue until it meets the stopping condition. The q-G method looked consistently down but was very slow. The initial iteration started with a large f value, namely f more than 6000 so that in the 10th iteration it has not reached the minimum point. The q-GY method had a decrease in the value of f and was smaller than SD and q-G, but unlike q-G which was slow in iteration, the q-GY method in the 10th iteration has f which was smaller than the 10th iteration in the q-G and SD methods.

From the graph it can be concluded that the q-GY method had a better performance than the SD method on the large f and q-G values on the average number of iterations. The SDY method had a fairly good performance at the beginning of the iteration but it increased drastically in the 7th iteration, so the use of q-GY was more effective.

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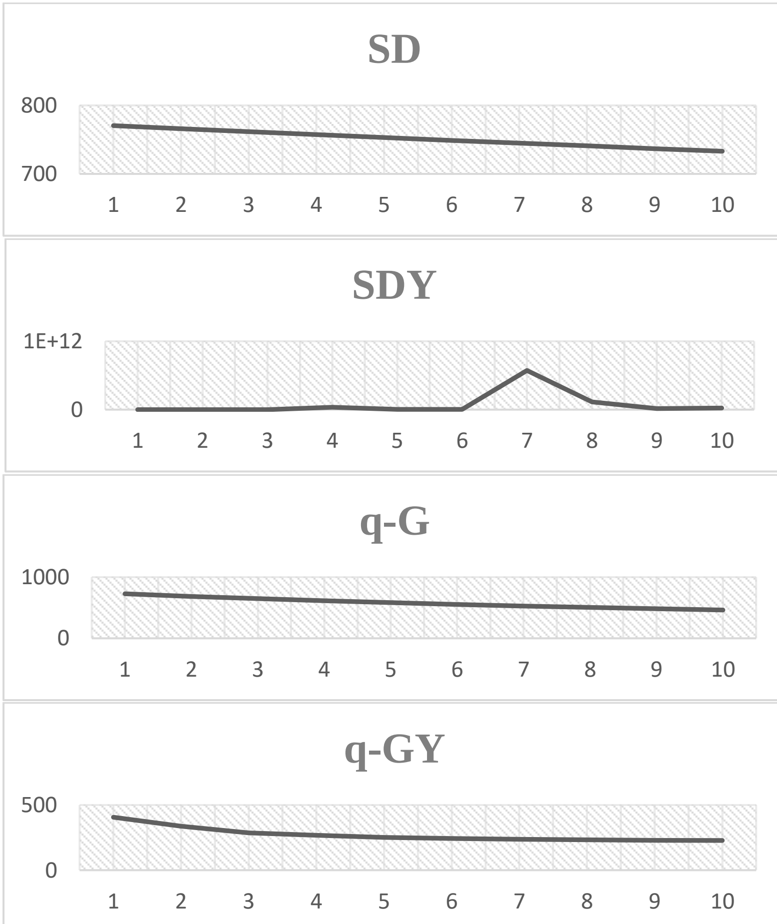

Graph 1. Convergence of the function to the minimum point in the SD, SDY, *q*-G and *q*-GY. methods

CONCLUSION

The *q*-GY method on the Rosenbrock function showed good enough results to accelerate convergence by reducing the number of iterations at several starting points, at intervals within the interval (-2.048, 2.048). From the numerical results, it was found that the *q*-GY method has a good performance compared to classical SD.

However, to see the performance of the method to achieve faster convergence to the minimum point, it would be better to use a simpler function to be able to display results that are in accordance with the research objectives or by changing the stopping criteria or using a tolerance limit of $f <10^{-4-}$. The graph of the average $f(x^*)$ of the Rosenbrock function with the SD method reached 1 – 1274 iterations, SDY reached 1 – 1702 iterations, *q*-G reached 1 – 258 iterations, and *q*-GY reached 1 – 93 iterations. The minimum point average was shown in table 4.1.1. The average value of $f(x^*)$ of the Rosenbrock function showed a decrease in the value of f when iterations run on the SD, *q*-G and *q*-GY methods, while an increase in SDY.

From the numerical results presented in the iteration table and the average f value, as well as a graph of convergence to the minimum point, it was concluded that the Rosenbrock function with the *q*-GY method could reach the minimum point with fewer iterations than the classical SD method. Improvement from the previous method (SD), and the *q*-G and *q*-GY methods had better results than the SD, SDY method by looking at the average f value.

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