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A MODIFIED BFGS METHOD VIA NEW RATIONAL APPROXIMATION MODEL FOR SOLVING UNCONSTRAINED OPTIMIZATION PROBLEMS AND ITS APPLICATION

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ABSTRACT. In this paper we present a new BFGS method for solving unconstrained optimization problems, using a modified rational approximation model. The idea is to improve the Barzilai and Borwein approximation (BBA) [27] by incorporating a new parameter. Under certain conditions the global convergent result of the proposed method is established. The numerical results have shown that, the new method is promising and outperforms other classical methods. Besides, the new method was used to solve data from Covid-19 and the performance was compared with Least Square Method (LSM). The outcome has shown that the new method has less relative error and can be used in place of LSM in regression analysis.

1. INTRODUCTION

For decade, the problem of finding the solution of unconstrained optimization has received a lot of attention, from different researches [11,19,24]. This is, due to the important role it plays, in many areas of human endeavors, such as science engineering and economics. Generally, this kind of problem is formulated as

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(1.1)
$$\min\{f(x): x \in \mathbb{R}^n\},\$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is a nonlinear function. The general iterative procedure for solving (1.1) is

$$(1.2) x_{k+1} = x_k + \alpha_k d_k,$$

where x_{k+1} and x_k are the previous and current iteration point, respectively; and α_k is the step size obtained using either an exact or inexact line search [11]. There are various inexact line searches. Popular among them is the Wolfe line search [9]. This line search provides a better step length compared to other procedures [5]. The line search is formulated as,

(1.3)
$$f(x_k + \alpha_k d_k) \le f(x_k) + \mu \alpha_k \nabla f(x_k)^T d_k$$
$$\nabla f(x_k + \alpha_k d_k)^T d_k \ge \sigma \nabla f(x_k)^T d_k,$$

with $0 < \mu < \sigma < 1$. Here d_k is the search direction, it ensure a sufficient decrease of the objective function [3]. Numerous search direction have been presented by many researchers, like Newton method, Quasi Newton and Conjugate gradient method [3,5,12,24]. The Quasi-Newton method was developed to reduce the cost of using the Newton direction [12, 13]. This search direction uses different approaches such as Davido-Fletcher-Powell (DFP), Broyden family, Symmetric rank one (SR1) and BFGS formula to approximate the Hessian matrix in the Newton iteration formula see [10,13,14,15]. Among all the variant of quasi newton method, the BFGS update is consider to be the best [25]. This update utilizes the identity matrix as the first approximation to the Hessian matrix, while in the subsequent iteration it uses the following approximation.

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{s_k^T y_k},$$

where $s_k = x_{k+1} - x_k$ and $y_k = g_{k+1} - g_k$. In each iterations B_k , must satisfy the standard secant condition [26]

$$B_{k+1}s_k = y_k.$$

For decade, different researchers, have provide the global convergent of BFGS method, when the objective function is convex and the line search is exact line search [17]. In case of non convex function convergence could be established

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when the line is search is inexact [17]. Discussion on this is still open. Recently, authors like Deng et al (2018), focused on proving the global convergent of BFGS method based on Wolfe line search, this is due to its good numerical performance compared to exact line search.

Several researchers have modified the standard secant equation (1.4) in order to improve the performance of BFGS method, some of the improvement includes; Al-Baali et al. [4] (1998), Zhang et al. [16] (1999), Wu and Liang [10] (2014), and recently Babaie-Kafaki [6] (2013). The main idea behind all, this improvement is to approximate the curvature of the objective function along the search direction more accurately, then in (1.4) [26]. Other disadvantage of (1.4) is, it only employs the gradient information, whereas the function and distance information were ignored [26]. To overcome this shortcoming researchers, like Wei et al (2006), Yuan and Wei (2010) have respectively present a new secant equation which utilized the function as well as gradient information at each stage. Leong et al. also gives a weaker secant equation as follow

$$s_{k-1}B_{k-1}s_{k-1} = y_k$$

Recently, Saheya et al. [21] proposed a new rational approximation model (RAM). This model was designed to improve the performance of the classical newton method while keeping it quadratic convergence rate. However, the model consists of computing the Jacobi matrix in every step. Because it was meant for solving system of nonlinear equations. To over comes this shortcoming Kamilu et al. have proposed number of approximation to reduce the cost of computing the Jacobian, detail can be found in [19,20]. Furthermore, the model has not been used to solve unconstrained optimization problems.

Motivated by this, in this paper we would use the RAM model, which consist of BB approximation and additional parameter, to approximate the hessian matrix. The idea is to improve the BB approximation, whenever it failed to give a descent dire action.

The paper is structured as follows, in section 2 we present the derivation of the new BFGS search direction as well as give the description of our new algorithm. Global convergence is presented in section 3. Section 4 consists of the numerical result generated by testing the new method on some benchmark test problems. Lastly, we present the application of the new method in regression analysis and the conclusion remark.

2. New Method

In this section, we present the new algorithm for solving (1.1), namely, A Modified BFGS Method via a New Rational Approximation Model for Solving Unconstrained Optimization Problems (MBFGS-RAM). This new method utilized the RAM approximation which consist of BB approximation and additional parameter to improve the iteration procedure in (1.2). Below we gives details of our new method.

Saheya et al. [21] improved the RALND function proposed by Sui et al [20, 19], so that it can be used to solve system of nonlinear equation. RALND function required finding function derivative in each step. However the model was never used to solve unconstrained optimization problems. In this paper we design a new RALND function. Our approach is similar to [21].

Let define the RALND function with the same horizon vector b_k for all nonlinear functions, $g_i(x)$, $i = 1, 2, \dots, n$ at x_k and approximate (1.1) by Rational function with linear denominator and numerator we get

(2.1)
$$g(x_k + s) \approx R(x_k + s) = g_k + \frac{B_k s}{1 + b_k^T s} = 0,$$

where $b_k, x_k \in \mathbb{R}^n$, $s_k = x_k - x_{k-1}$ and x_k is the current point. Equation (2.1) is quit different from RALND function and approximate function in [21]. Because, this new approximation (2.1) use the same vector b_k for all function $F_i(x)$, $i = 1, 2, \dots, n$ at each iteration step x_k and it does not require any gradient or hessian of the objective function at k iteration.

Using linear sation idea, we can derive a new iteration formula as follows, let $\omega_k = B_k \beta_k$

$$\omega_k s_k = -g_k,$$

where $\beta_k = y_k b_k^T$ Suppose $B_k \beta_k$ is define, then, using similar approach as in (1.2) we have

$$(2.2) x_{k+1} = x_k - \alpha_k d_k,$$

where $d_k = B_k \beta_k$ is the new RAM which will served as new Hessian approximation, updated in each step. Now we define $y_k b_k$. It is worth important to mention that at each step b_k is updated by requiring the following interpolation condition

(2.3)
$$R(x_{k-1}) = g(x_{k-1}),$$

with this the search direction in (2.2) would depend on the new RAM which will consist of information the gradient values of the preceding point $g(x_{k-1})$ as well as the current point.

Using the conic model [19, 21], equation (2.1) and (2.3) become,

(2.4)
$$g_{k-1} = g_k - \frac{B_k^+ s_{k-1}}{1 + b_k^T s_{k-1}}.$$

Let the denominator of (2.4) be α_k i.e. $\alpha_k = 1 - b_k^T s_{k-1}$ and $y_{k-1} = g(x_k) - g(x_{k-1})$, then, (2.4) become,

$$\alpha_k y_{k-1} = B_k^+ s_{k-1}.$$

Thus

(2.5)
$$\alpha_k = \frac{y_{k-1}^T B_k^+ s_{k-1}}{y_{k-1}^T y_{k-1}}.$$

From (2.1) we can write the vector b_k as follows

(2.6)
$$b_k = \frac{(1 - \alpha_k)c_k}{c_k^T s_{k-1}}$$

For any value of $c_k \in \mathbb{R}^n$ such that $c_k^T s_{k-1} \neq 0$. Assuming $c_k = s_{k-1}$, then (2.6) become

(2.7)
$$b_k = \frac{(1 - \alpha_k)s_{k-1}}{s_{k-1}^T s_{k-1}} = \frac{y_{k-1}(y_{k-1} - B_k^+ s_{k-1})s_{k-1}^T}{(y_{k-1}^T y_{k-1})(s_{k-1}^T s_{k-1})},$$

with (2.5) and (2.7) we have a new horizon vector $g_k b_k^T$ using similar linearisation approach (1.2)

$$y_k b_k^T = \frac{(1 - \alpha_k)s_{k-1}}{s_{k-1}^T s_{k-1}} = \frac{y_{k-1}(y_{k-1} - B_k^+ s_{k-1})}{y_{k-1}^T y_{k-1}} \frac{s_{k-1}^T y_k}{s_{k-1}^T s_{k-1}}.$$

In what follows we present our new algorithm.

Algorithm 1: (MBFGS-RAM)

Initialization, Given x_0 , let $\beta_0 = I$ for k = 0 choose ε_0 . **Step 1:** Compute $g(x_0)$ set $d_0 = -\beta_0 g_k$, $\varepsilon = \varepsilon_0$ and k = 0. **Step 2:** If $||g_k|| \le \varepsilon$ then stop. **Step 3:** Compute $\beta_{k+1} = y_{k+1}b_{k+1}^T$ and d_{k+1} by

$$y_k b_k^T = \frac{y_{k-1}^T (y_{k-1} - B_k^+ s_{k-1}) s_{k-1}^T y_k}{y_{k-1}^T y_{k-1} s_{k-1}^T s_{k-1}},$$

$$d_{k+1} = \begin{cases} -\beta_k g_k & \text{if} \quad s_k^T s_k \ge 0\\ -(\theta_k + \beta_k) g_k & \text{otherwise} \end{cases}$$

 B_k^+ is updated using $B_{k+1}^+ = \frac{s_k^T y_k}{s_k^T s_k}$ and $\theta_k = \frac{s_k^T s_k}{s_k^T y_k}$. **Step 4:** Compute α_k using (1.3) and update x_{k+1} using (1.2). **Step 5:** Set k = k + 1. Go to Step 2.

Unlike in BB method, MBFGS-RAM method utilizes a new approximation which consist of the RAM and BB approximation, based on the Wolfe line search

3. CONVERGENCE ANALYSIS OF THE NEW METHODS

In this section we present the global convergence of MBFGS-RAM method based on the Wolfe line search. For an algorithm to convergence the following assumption are important All the proof will be supported with Numerical results generated using different benchmark problems.

Assumption 1.

- (1) The level set $L = \{x \mid f(x) \leq f(x_0)\}$ is bounded with x_0 as initial point for Algorithm 1.
- (2) The objective function f is twice continuously differentiable and there is a constant M > 0, such as

$$||G(x) - G(y)|| \le M ||x - y||, \quad x, y \in L.$$

Now following the same way as in [15,17] with assumption that β_k is a good approximation to G(x) at x_k we add the following Assumption.

Assumption 2.

Assuming the β_k is a good approximation to G(x) at x_k , i.e,

$$\|\beta_k - G(x)\| \le \epsilon_k,$$

where $\epsilon_k \in (0, 1)$ similarly, we have

$$\|\beta_k\| - \|G(x_k)\| \le \|\beta_k - G(x_k)\| \le \epsilon_k.$$

Therefore, we can give

$$\|\beta_k\| \le \sigma, \ \forall k \ge 0.$$

Now with Assumption 1 and line search condition (1.3) the following equation is true

(3.1)
$$\lim_{k \to \infty} f(x_k) = f(x^*)$$

Before proving the convergence of Algorithm 1, we also need the following lemma.

Lemma 3.1. Let f satisfies the two assumption above and x_k be generated by the algorithm 1 there exist a constant c_1 and c_2 such that

(3.2)
$$\|\theta_k + \beta_k s_k\| \le \|B_k s_k\| \le c_1 \|s_k\|$$
 and $s_k^T \theta_k + \beta_k s_k \ge s_k^T B_k s_k \ge c_2 \|s_k\|^2$

for large number k. Then, we have,

$$\lim_{k \to \infty} \inf g(x_k) = 0$$

Proof. Suppose we change s_k with d_k then, $s_k = \alpha_k d_k$, is true holds by (3.2). Also from (3.2) and the relation $g_k = (\theta_k + \beta_k)d_k = B_k d_k$ we have

(3.4)
$$d_k^T(\theta_k + \beta_k)d_k \ge d_k^T B_k d_k \ge c_2 ||d_k||^2$$
 and $c_2 ||d_k|| \le ||g_k|| \le c_1 ||d_k||.$

Let ω be the set of indices k for which (3.2) is true. Based on the second condition of Wolfe line search and Assumption 2, we have

(3.5)
$$M\alpha_k \|d_k\|^2 \ge (g_{k+1} - g_k)^T d_k \ge -(1 - \sigma_2)g_k^T d_k.$$

This means that for any $k \in \omega$,

$$\alpha_k \ge \frac{-(1-\sigma_2)g_k^T d_k}{M\|d_k\|^2} = \frac{(1-\sigma_2)d_k^T(\theta_k + \beta_k)d_k}{M\|d_k\|^2} = \frac{(1-\sigma_2)d_k^T B_k d_k}{M\|d_k\|^2} \ge \frac{(1-\sigma_2)c_2}{M}$$

In addition, based on (3.1), we get

$$\sum_{k=1}^{\infty} (f_k - f_{k+1}) = \lim_{N \to \infty} \sum_{k=1}^{N} (f_k - f_{k+1}) = \lim_{N \to \infty} f_1 - f_N = f_1 - f^*,$$

which gives

$$\sum_{k=1}^{\infty} (f_k - f_{k+1}) < \infty.$$

Based on the first condition of Wolfe line search (1.3) leads to

$$\lim_{k \in \omega, \ k \to \infty} d_k^T (\theta_k + \beta_k) d_k = \lim_{k \in \omega, \ k \to \infty} d_k^T B_k d_k = \lim_{k \in \omega, \ k \to \infty} -g_k^T d_k = 0,$$

which along with (3.4) give rise to (3.3).

Theorem 3.1. (Global convergence) Let f satisfy the assumption 1 and 2 respectively, and $\{x_k\}$ be generated using Algorithm 1. Then, we have

$$\lim_{k \to \infty} \inf g_k = 0.$$

Proof. Based on Lemma 3.1 it is enough to show that condition (2.5) is true for infinitely many k. Using (3.1), we have

(3.8)
$$\|(\theta_k + \beta_k)s_k\| \le \|B_k s_k\| \le \|B_k\| \|s_k\| \le \sigma \|s_k\|.$$

from Algorithm, assuming B_k is positive definite. Then by (3.2),

(3.9)
$$s_k^T \theta_k + \beta_k s_k \ge s_k^T B_k s_k \ge c_2 \|s_k\|^2.$$

Therefore, Lemma 3.1 complete the proof.

4. NUMERICAL RESULTS

In this section, we present the numerical performance of MBFGS-RAM. We compared MBFGS-RAM with BB and classical BFGS methods in [7,26] respectively. We made use of the following benchmark test problems by Andrei [1,25], to test the efficiency and robustness of the methods.

The code was written on PC computer Intel core i3-3217u 4GB DDR3 Memory 500 GB HDD using a Matlab R2015b software.we choose the $||g_k|| \le \epsilon$ as our stooping condition or when the number of iteration exceed 1000 and report the method as failed. A popular performance profile, introduced by Dolan and More [2], was employed to analyses the numerical results. This profile, gives the performance of a solver efficiency and probability of success in a concise way.

Figure 1 and 2 shows that, MBFGS-RAM method is effective with a good numerical performance, that is, why, its curves appear at top and reach 1. BB and BFGS method have good convergent rate, but there numerical performance is not as good MBFGS-RAM. Hence, there curves appears below with 0.33 and 0.83 success respectively in term of number of iteration. The performance of MBFGS-RAM method is not surprising because it required a modified RAM, which keeps it, from going to a non-decent search direction as in the case of BB method.

Test problem	<i>n</i> -dimension
Six-hump camel back	2
Booth	2
Treccani	2
Zettle	2
Hager Function	2,4,10
Extended Penalty	2,4,10,50,100
Raydan 2 function	2,4,10,100
Generalised Quartic	2,4,100
Fletcher	2,4,10,100,500
Diagonal 4	2,4,10,100,500
Quadratic QF2	2,4,10,100,500
Extended Maratos	2,4,100,500,1000
Extended shallow	2,4,10,100,500,1000
Extended Beale	2,4,10,100,500,1000
Extended Trigonometry	2,4,100,500,1000
Extended Denschnb	2,4,100,500,1000

TABLE 1. A list of all the test problems



FIGURE 1. Performance Profile Based on the Number of Iteration



FIGURE 2. Performance Profile Based on CPU Time

5. Application In Regression Analysis

Regression Analysis is a statistical technique used to describe a relationship among different variables [28]. These variables are of two types, the dependent and independent variable. A simple regression analysis consist of two variable, Yand X, where Y is called a target variable and X is called a regressor. Furthermore, when solving real life problems, this kind of method may involve three or more variables. A general mathematical expression of a regression model is

(5.1)
$$y = g(x_1, x_2, x_3, \cdot, x_r + \epsilon),$$

where ϵ stands for error and r > 0.

The main idea when solving a regression model is to find a regression line. This line can be linear in a simple case or nonlinear. There are various approaches of finding this line [23]. Popular among them is the least square method. Detail can be found in [22,23]. In this paper, we consider a set of data from the number of infection and death by Covid-19 in Nigeria. The data is transformed into a linear and quadratic regression model. Both models were obtained with the help of Matlab software. We applied the MBFGS-RAM to solve all the models the performance is then compared with the LSM. Table 2 present the data. It was retrieve from Nigerian center of diseases.

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Number of	Data	Number of Infections y_1	Number of Death y_2
data x			
1	07-Aug	443	6
2	08-Aug	453	6
3	09-Aug	437	3
4	10-Aug	290	5
5	11-Aug	423	6
6	12-Aug	453	0
7	13-Aug	373	10
8	14-Aug	329	7
9	15-Aug	325	1

TABLE 2. A Data from Covid-19 Number OF Infections and Death in Nigeria

For each of the models we calculate the relative error using the following formula

(5.2) Realtive Error =
$$\frac{|\text{exact value} - \text{approximate value}|}{|\text{exact value}|}$$

At the end, we consider the regression model with less relative error, to be more efficient. In what follows, Table 3 presents the linear and quadratic least square method, for the number infections and death respectively.

TABLE 3. Approximation Function in Respect of Infections and Death Using LSM

Least Square method	Result Approximation Function	
Linear (Infec)	y = 459.194444444444 - 13.48333333333333 x	
Linear (Death)	y = 5.555555555556 - 0.1333333333333333333333333333333333333	
Quadratic (Infec)	y = 447.428571428572 - 7.065584415584 x -	
	$0.0641774891775 \ x^2$	
Quadratic (Death)	$y = 5.119047619 + 0.104761905 x - 0.023809524 x^2$	

The linear and quadratic model are then used to approximate the corresponding number of infections and Death. Next, using (5.2) we present the sum and average error for each of the model in Table 4. Detail of how we arrived at table can be found in [23,22].

	Linear Relative Error	Quadratic Relative Error
Sum of Error (Infec)	0.8592669242	1.0577542783
Average Error (Infec)	0.0954741027	0.1175282531
Sum of Error (Death)	5.3750264579	5.2223809412
Average Error (Death)	0.6718783072	0.6527976176

In the other hand, the set of the data in Table 2 was transformed into an unconstrained linear and quadratic regression mode using the following approach:

(5.3)
$$\min f(x) = \sum_{n=1}^{2} \{y_i - a(1, x_1)^T\}^2 \qquad (a \in \mathbb{R}^2),$$

(5.4)
$$\min f(x) = \sum_{n=1}^{3} \{y_i - a(1, x_1 x_2)^T\}^2 \qquad (a \in \mathbb{R}^3).$$

And the resulting function is solved using algorithm 1. The out come is presented in Table 5.

TABLE 5. Approximation Function in Respect of Infections and Death Using MBFGS-RAM

MBFGS-RAM Method	Result Approximation Function
Linear (Infec)	y = 459.19434432315 - 13.4833173890732 x
Linear (Death)	y = 5.55460481028 - 0.1331804609291 x
Quadratic (Infec)	y = 447.42857142857 - 7.0655844155847 x -
	$0.6417748917750 \ x^2$
Quadratic (Death)	y = 5.11045258237 + 0.184759943115 x -
	$0.0241402989881 x^2$

And the corresponding relative error using (5.2) is presented in Table 6.

Based on Table 4 and 6, the linear and quadratic model (Infections) solved by MBFGS-RAM method has a less relative error compare to the least square method (LSM). Even though, the quadratic model (Death) for MBFGS-RAM has higher relative error than LSM, however, the new model is comparable and a good method in describing the data set in Table 2. As a result, the Linear and Quadratic model

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TABLE 6. A Relative error in case of Infections and Death Using MBFGS-RAM

	Linear Relative Error	Quadratic Relative Error
Sum of Error (Infec)	0.85926661232	0.82676522675137
Average Error (Infec)	0.0954741020	0.09186280297237
Sum of Error (Death)	5.3750103836	5.80293189611362
Average Error (Death)	0.6717300479	0.72536648701420

(Infections) and linear (Death) are good methods in estimating the number of infection and death for next day. In general, the new method can serve as an alternative to LSM.

6. CONCLUSION

In this paper, we present a new algorithm for solving unconstrained optimization problems. It is a variant of Quasi newton method that utilize the modified RAM which consist of BB approximation formula and an additional parameter to form a new search direction based on Wolfe line search. Different standard test function have been used to generate the numerical results. The outcomes shows that MBFGS-RAM is efficient, reliable and effective. In addition, the MBFGS-RAM is used to solve the data set from Covid-19 in Nigeria. And the performance is attractive.

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