THE PERFORMANCE OF MBFGS WITH DIFFERENT INEXACT LINE SEARCH RULE

Manish Kumar Sahu, Suvendu Ranjan Pattanaik and Santosh Kumar Panda

ARTICLE HISTORY
Compiled April 26, 2022

ABSTRACT
The modified BFGS optimization algorithm is generally used when the objective function is non-convex. In this method, one has to move in a specific direction such that the value of the objective function reduces. Therefore, the different inexact line search or exact line search plays an important role in optimization. Here, we have studied Modified BFGS with different inexact line searches methods and compared them in some test problems. Numerical results show that MBFGS with Armijo line search methods is efficient for solving non-convex non-linear unconstrained optimization problems.

KEYWORDS
Unconstrained Optimization, Quasi Newton Algorithm, Modified Broyden–Fletcher–Goldfarb–Shanno (MBFGS) and Inexact Line Search

1. Introduction

The Quasi-Newton method is the most effective optimization algorithm when the objective function is non-linear and involves millions of variables. In this method, we approximate the inverse-Hessian using gradient information iteratively. If one compares the Quasi-Newton method with the Newton method (NM) or the steepest descent method in terms of computational cost and storage space, then the quasi-Newton method has a clear advantage over the other two methods (Nocedal, J., Wright, S.J (2006)). The rate of convergence of the steepest descent method is linear, while the rate of convergence of the Newton method is quadratic (Nocedal, J., Wright, S.J (2006)). It is known that the computation of the Hessian matrix is quite challenging and time-consuming for large scale problems. Therefore, Quasi-Newton is a useful method where one has to approximate the Hessian or the inverse of the Hessian only.

Depending on the different ways of approximation to the Hessian, various methods, i.e., Symmetric Rank 1 (SR1) (Nocedal, J., Wright, S.J (2006)), Davidon–Fletcher–Powell (DFP) (Nocedal, J., Wright, S.J (2006)) and Broyden–Fletcher–Goldfarb–Shanno (BFGS) (Nocedal, J., Wright, S.J (2006)) updates are introduced to approximates Hessian matrix. Among all of them, the BFGS update formula performs better than the other two methods. However, standard BFGS with exact as well as inexact line search fails to converge in some nonconvex problems (G. Yuan, Z. Wang, and P. Li (2006); Y. Dai (2006)). Therefore, the modified BFGS (MBFGS) method is developed to handle the nonconvex problems (Y Yuan (1991)).
Moreover, the modified BFGS algorithm performs better than BFGS for some of the test problems (Pengyuan Li, Junyu Lu and Haishan Feng (2021)). MBFGS has many applications in machine learning, deep learning, artificial intelligence (AI) and data science. Also, it has been observed that for nonconvex objective functions having large number of variables, MBFGS optimization algorithm with inexact line search gives better results than other methods. Therefore, it is necessary to identify the best line search rule in the MBFGS optimization algorithms to minimize the objective function. Here, we construct a sequence of updates through inexact line search methods with the step length that satisfies some criterion which assures that the updated steps are neither too long nor too small. For the inexact line search, we have implemented Armijo, Wolfe and Goldstein line search methods. We present the performance of the modified BFGS method with the above said inexact line search rule and provide a comparative results.

1.1. Notation

Let $R$ denotes the set of real number, $D = [d_1, ..., d_m] \in R^{n \times m}$ denotes as the difference of iterate displacement, $H = [h_1, ..., h_m] \in R^{n \times m}$ denotes the difference of iterative gradient and $S^n$ denotes the symmetric element of $R^{n \times n}$. We study the following unconstrained optimization problem

$$\min_{x \in R^n} f(x)$$

where $f : R^n \rightarrow R$ is a continuously differentiable function. We define the gradient function $g : R^n \rightarrow R^n$ and Hessian function $B : R^n \rightarrow S^n$. Here, $r = ||x_0 - x^*||$ where $x_0$ is the initial guess to minimize the objective function, $x^*$ is the exact solution of the objective function and $||.||$ denotes the standard Euclidean norm in $R^n$ and $a_k$ denotes step length at $k$th iteration.

2. Background on MBFGS

The global convergence of the BFGS method for convex function under Wolfe line search is first proved by Powell (Powell, M. J. D. (1976)). Then many results on global convergence of BFGS method for convex function are thoroughly studied in (Richard H. Byrd, Jorge Nocedal, Ya-Xiang Yuan (1987)). However, Y.Dai (Y. Dai (2006)) proposes a counterexample to illustrate that the standard BFGS may not be applicable to nonconvex function with Wolfe line search. Nonconvergence of the BFGS method with the exact line search is studied by W.F.Mascarenhas (W. F. Mascarenhas (2004)). For handling the nonconvex function, the modified BFGS is introduced in (Yuan (1991)). For obtaining a better approximation of the Hessian matrix, G. Yuan and Z. Wei (G. Yuan and Z. Wei (2010)) propose a new modified BFGS method which is stated below

$$B_{k+1} = B_k - \frac{B_k d_k (d_k)^T B_k}{(d_k)^T B_k d_k} + \frac{y_j (y_j)^T}{d_j^T y_j}.$$ \hspace{1cm} (2)

where $D = [d_1, ..., d_m] \in R^{n \times m}$, $H = [h_1, ..., h_m] \in R^{n \times m}$. The search direction $p_k$ of the quasi-Newton method is generated by the following equation $p_k = -M_k g_k \ \forall k \geq 0$
where $M_0$ is any $n \times n$ symmetric positive definite matrix and $M_k = B_k^{-1}, y_j = h_j + \max(C_j, 0)/|d_j|d_j$ and $C_j = 2[f(x_j) - (f(x_j + \alpha_j p_j)] + (g(x_j + \alpha_j p_j) + g(x_j))^T d_j$. It is clear that if $C_j > 0$ holds, then the Quasi-Newton method reduces to (2); otherwise, it is the standard BFGS method. The global convergence of the MBFGS with the inexact line search is proved in (Qiang Guo, Jian-Guo Liu, Dan-Hong Wang (2008)). Here, we will demonstrate the performance of the modified BFGS (MBFGS) method for the nonconvex functions with Wolfe line search, Goldstein line search, and Armijo line search.

3. Line Search Rule

In the first step, the line search rule finds the direction in which function reduces and then computes the step size that determines how far $x$ should move along that direction. We can compute the step size either exactly or inexactly. Here, we discuss the inexact line search. $g(x_k)$ denotes the gradient of $f(x)$ at $x_k$. The step size estimation plays an important role in the problems having large number of variables. Therefore, the initial step size estimation and extending the range of acceptable step sizes are very important in the line search algorithm design.

3.1. Backtracking Wolfe Line Search:

(1) Given $a_{init} > 0, a_0 = a_{init}, t = 0, 0 \leq c_1 \leq c_2 \leq 1$

(2) Until $f(x_k + a tp_k) \leq f(x_k) + a_t c_1 [g(x_k)]^T p_k$ and $-p_k^T [g(x_k + a_k p_k)] \leq c_2 p_k^T [g(x_k)]$

- $a_{t+1} = \tau a_t$ where $\tau \in (0, 1)$ is fixed.($\tau = 0.5$)
- increment $t$ by 1

(3) Set $a_k = a_t$

3.2. Backtracking Armijo Line Search:

(1) Given $a_{init} > 0, a_0 = a_{init}, t = 0$

(2) Until $f(x_k) + (1 - c_1) a_t [g(x_k)]^T p_k \leq f(x_k + a_t p_k)$

- $a_{t+1} = \tau a_t$ where $\tau \in (0, 1)$ is fixed.($\tau = 0.5$)
- increment $t$ by 1

(3) Set $a_k = a_t$

3.3. Backtracking Goldstein Line Search:

(1) Given $a_{init} > 0, a_0 = a_{init}, t = 0, 0 \leq c_1 \leq 0.5$

(2) Until $f(x_k) + (1 - c_1) a_t [g(x_k)]^T p_k \leq f(x_k + a_t p_k)$

- $a_{t+1} = \tau a_t$ where $\tau \in (0, 1)$ is fixed.($\tau = 0.5$)
- increment $t$ by 1

(3) Set $a_k = a_t$

4. Numerical Experiment

In this section, we discuss the performance of MBFGS with Wolfe, Armijo and Goldstein line search for the comparison purposes and implement the programme in Python.
Table 1. (Rosenbrock Function) MBFGS with the different line search in the term of iteration counter (EXAMPLE 4.1)
### Table 2.
(Rosenbrock Function) MBFGS with different line search in term of average time taken in second (EXAMPLE 4.1).

| initial guess value of r | (Avg Time) Armijo | (Avg Time) Goldstein | (Avg Time) Wolfe |
|--------------------------|-------------------|----------------------|-----------------|
| (2.2,2.0)                | 1.562             | 0.0008704            | 0.0009176       |
| (2.0,2.0)                | 1.414             | 0.0008804            | 0.0011925       |
| (1.2,1.8)                | 0.825             | 0.0008648            | 0.000879        |
| (0.75,1.0)               | 0.25              | 0.0008723            | 0.0008813       |
| (0.0,1.8)                | 1.280             | 0.000862             | 0.0008713       |
| (1.8,2.0)                | 1.280             | 0.0008683            | 0.0009005       |

### Table 3.
(Powell’s quartic function) MBFGS with different line search rule in term of iteration counter (EXAMPLE 4.2).

| initial guess value of r | Iteration in Armijo | Iteration in Goldstein | Iteration in Wolfe |
|--------------------------|----------------------|------------------------|---------------------|
| (4,-1,0,1)               | 4.242                | 24                     | 24                  |
| (3,-1,1,1)               | 3.464                | 22                     | 22                  |
| (3,-1,0,1)               | 3.317                | 24                     | 24                  |
| (3,-1.5,0,1.5)           | 3.674                | 27                     | 27                  |

### Table 4.
(Powell’s quartic function) MBFGS with different line search rule in term of average time taken in second (EXAMPLE 4.2).

| initial guess value of r | (Avg Time) Armijo | (Avg Time) Goldstein | (Avg Time) Wolfe |
|--------------------------|-------------------|----------------------|-----------------|
| (4,-1,0,1)               | 4.242             | 0.00077              | 0.00032         |
| (3,-1,1,1)               | 3.464             | 0.00059              | 0.00063         |
| (3,-1,0,1)               | 3.317             | 0.00061              | 0.00064         |
| (3,-1.5,0,1.5)           | 3.674             | 0.00060              | 0.00064         |
| initial guess | value of r | Iteration in Armijo | Iteration in Goldstein | Iteration in Wolfe |
|---------------|------------|---------------------|------------------------|-------------------|
| (1.0,1.2,1.3,1.4) | 0.5385     | 14                  | 14                     | 14                |
| (1.3,1.2,1.3,1.4) | 0.6164     | 20                  | 20                     | 20                |
| (1.2,1.2,1.2,1.2) | 0.4        | 12                  | 12                     | 12                |
| (1.1,1.2,1.3,1.4) | 0.548      | 14                  | 14                     | 14                |

Table 5. (Wood Function) MBFGS with different line search rule in the term of iteration counter (EXAMPLE 4.3)

| initial guess | value of r | (Avg Time) Armijo | (Avg Time) Goldstein | (Avg Time) Wolfe |
|---------------|------------|-------------------|----------------------|-----------------|
| (1.0,1.2,1.3,1.4) | 0.5385     | 0.0006225          | 0.0007864            | 0.0006690       |
| (1.3,1.2,1.3,1.4) | 0.6164     | 0.0006290          | 0.0008083            | 0.0007815       |
| (1.2,1.2,1.2,1.2) | 0.4        | 0.0006286          | 0.001132             | 0.0009648       |
| (1.1,1.2,1.3,1.4) | 0.548      | 0.00063086         | 0.0007377            | 0.0006225       |

Table 6. (Wood Function) MBFGS with different line search rule in the term of average time taken in second (EXAMPLE 4.3)

The Table-4 represents the performance of MBFGS with Armijo, Goldstein, and Wolfe condition in the Powell’s quartic function in the terms of the average time taken by CPU to reach its optimal value.

**Example 4.3 (Wood Function).**

\[ f(x) = 100(x_1^2 - x_2)^2 + (x_1 - 1)^2 + (x_3 - 1)^2 + 90(x_3^2 - x_4)^2 + 10.1((x_2 - 1)^2 + (x_4 - 1)^2) + 19.8(x_2 - 1)(x_4 - 1). \]

The Table-5 represents the performance of MBFGS with Armijo, Goldstein, and Wolfe condition in the Wood function in terms of iteration counter to reach its optimal value.

The Table-6 represents the performance of MBFGS with Armijo, Goldstein, and Wolfe condition in the wood function in terms of the speed of the CPU to reach its optimal value.

**Example 4.4 (Schumer Steiglitz Function).**

\[ f(x) = x_1^4 + x_2^4 \]

![Figure 2](image-url) (Schumer Steiglitz Function) MBFGS with Armijo, Goldstein and Wolfe line search with initial guess (-0.4,0.6) respectively.
The Table-7 represents the performance of MBFGS with Armijo, Goldstein, and Wolfe condition in the Schumer-Steiglitz function in terms of iteration counter to reach its optimal value. Its performance can be seen in the Figure 2.

The Table-8 represents the performance of MBFGS with Armijo, Goldstein, and Wolfe condition in the Schumer-Steiglitz function in the terms of the speed of CPU to reach its optimal value.

**Example 4.5** (Schwefel function).

\[ f(x) = (x_1 - 1)^2 + (x_2 - 1)^2 + (x_1 - x_2^2)^2. \]

The Table-9 represents the performance of MBFGS with Armijo, Goldstein, and Wolfe condition in the Schwefel Function in terms of iteration counter to reach its optimal value. Its performance can be seen in the Figure 3.
Table 10. (Schwefel function) MBFGS with different line search rule in terms of average time taken in second

| initial guess value of r | (Avg Time) Armijo | (Avg Time) Goldstein | (Avg Time) Wolfe |
|-------------------------|------------------|----------------------|------------------|
| (4.0,8.0)               | 7.615            | 0.0008680            | 0.0009072        |
| (5.0,6.0)               | 6.403            | 0.0008422            | 0.0012093        |
| (6.0,6.0)               | 7.071            | 0.0008473            | 0.0009482        |
| (3.0,3.0)               | 2.828            | 0.0008499            | 0.0008564        |
| (8.0,6.0)               | 8.602            | 0.0008583            | 0.0009166        |

The Table 10 represents the performance of MBFGS with Armijo, Goldstein, and Wolfe condition in the Schwefel function in terms of the speed of the CPU to reach its optimal value.

5. Conclusion

We have demonstrated the performance of MBFGS with different line search rules in the Rosenbrock function, Wood function, Schumer Steiglitz function, Powell’s quartic function and Schwefel function. We observe that MBFGS with Armijo line search performs better than MBFGS with Wolfe or Goldstein line search in terms of number of iterations and Average time taken by CPU. When BFGS fails to optimize some nonconvex function, it is better to implement MBFGS with Armijo line search.
References

Pengyuan Li, Junyu Lu and Haishan Feng. 2021. “The Global Convergence of a Modified BFGS Method under Inexact Line Search for Non-convex Functions.” Mathematical Problems in Engineering, Hindawi, 1-9.

G. Yuan and Z. Wei. 2010. “Convergence analysis of a modified BFGS method on convex minimizations.” Computational Optimization and Applications, vol. 47, no. 2, pp. 237–255.

W. F. Mascarenhas. 2004. “BFGS method with exact line searches fails for non-convex objective functions.” Mathematical Programming, vol. 99, no. 1, pp. 49–61.

G. Yuan, Z. Wang, and P. Li. 2006. “A modified Broyden family algorithm with global convergence under a weak Wolfe Powell line search for unconstrained nonconvex problems.” Calcolo, vol. 57, pp. 1–21.

Y. Dai. 2006. “Convergence properties of the BFGS algorithm,” SIAM Journal on Optimization, vol. 13, pp. 693–701.

Bonnans, J.F., Gilbert, J.Ch., Lemaréchal, C., Sagastizábal, C.A. 1995. “A family of variable metric proximal methods.” Math. Progr. 68(1), 15–47

Broyden, C.G. 1970. “The convergence of a class of double-rank minimization algorithms.” J. Inst. Math.Appl. 6(1), 76–90

Dong-Hui Lia;1, Masao Fukushima. 2001. “A modified BFGS method and its global convergence in nonconvex minimization.” Journal of Computational and Applied Mathematics (2001)

Y Yuan. 1991. “A modified BFGS algorithm for unconstrained optimization.” IMA Journal of Numerical Analysis.

Richard H. Byrd, Jorge Nocedal, Ya-Xiang Yuan. 1987. “Global convergence of a class of quasi-Newton methods on convex problems.” SIAM J. Numer. Anal. 24(5), 1171–1189

Nocedal, J., Wright, S.J.: Numerical Optimization, 2nd edn. Springer, New York

Powell, M. J. D. 1976. “Some global convergence properties of a variable metric algorithm for minimization without exact line searches,” in Nonlinear Programming, SIAM-AMS proceedings, Vol. IX, R. W. Cottle and C. E. Lemke, eds., American Mathematical Society

Qiang Guo, Jian-Guo Liu, Dan-Hong Wang. 2008. “A modified BFGS method and its superlinear convergence in nonconvex minimization with general line search rule,” Korean Society for Computational and Applied Mathematics

Momin Jamil, Xin-She Yang. 2013. “A Literature Survey of Benchmark Functions For Global Optimization Problems,” International Journal of Mathematical Modelling and Numerical Optimisation, Vol. 4, No. 2, pp. 150-194