A Hybrid of Quasi-Newton Method with CG Method for Unconstrained Optimization

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Abstract. The quasi-Newton is a well-known method for solving small to medium-scale unconstrained optimization problems due to its simplicity and convergence. This leads to many modifications to improve its performance, and one of them is by hybridizing it with another optimization method. In this study, the quasi-Newton method is combined with the ARM method, which is a type of conjugate gradient method. The resulting hybrid algorithm is globally convergent under exact line search.

1. Introduction
In this study, we first consider the unconstrained optimization function as formulated by

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

where $$f : \mathbb{R}^n \to \mathbb{R}$$ is a smooth function whose gradient $$g_k$$ at point $$x_k$$ is available. The iterative scheme used to obtain the solution of (1) is defined by

$$x_{k+1} = x_k + \alpha_k d_k, \quad k = 0,1,2,\ldots$$

where $$\alpha_k > 0$$ denotes the step size, $$x_k$$ is the iterate and $$d_k$$ is the direction of search. The exact minimization rule is used in this study to determine the step size is given by

$$f(x_k + \alpha_k d_k) = \min_{\alpha \geq 0} f(x_k + \alpha d_k)$$

The exact line search calculates the optimal step size which provides the best possible reduction of the objective function [27]. However, this approach is often very slow and can be ineffective when the starting point chosen is far from the solution point [24, 26]. Therefore, inexact line search methods like Goldstein [1], Armijo [9] and Wolfe [22] are more preferable as they are easier to implement. In recent years, the development of faster processors has successfully curbed the “slowness” of exact line search as demonstrated in [17] and [18]. Hence, more and more studies start to return to this approach to
determine the step size such as [19] and [21].

Unlike Newton’s method that uses Hessian matrix in its calculations, quasi-Newton generates a series of Hessian approximations while maintaining a fast rate of convergence [7]. Several different types of quasi-Newton method were developed, that is, Davidon-Fletcher-Powell (DFP), symmetric rank 1 (SR1), Broyden-Fletcher-Goldfarb-Shanno (BFGS), though it is generally accepted that the BFGS algorithm is the most effective method amongst them [5],[23]. Chong and Zak [7] explained that SR1 method does not preserve the positive definiteness of $kH$ whereas DFP algorithm tends to get “stuck” in cases of large nonquadratic problems. The BFGS method actually manages to avoid these problems, hence why it is preferable. The search direction for BFGS method is given by

$$d_k = H_k g_k$$

where the term $H_k$ represents the positive definite $n \times n$ inverse Hessian approximation matrix of the objective function $f$ at $k$th iteration while $g_k$ is the gradient of $f$ at point $x_k$. The update equation of the approximate inverse Hessian matrix is written as

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

with $s_k = x_{k+1} - x_k$ and $y_k = g_{k+1} - g_k$. Many studies were made on the convergence properties of this particular method. If the minimization problem is convex, then the BFGS method is globally convergent under exact line search [11] and Wolfe line search [15]. However, Dai [25] proved that this method may fail when applied to non-convex functions. Further studies have been conducted for the purpose of improving the efficiency of BFGS method in solving unconstrained optimization problems. This includes the application of hybrid method which has been garnering more attentions lately.

The concept of hybrid quasi-Newton method has been around for some time. The general idea is to combine about a quasi-Newton method with another optimization method to produce a hybrid method that incorporates the advantages of its ‘parent’ methods. One of the earlier hybrid methods is the QN-SD method proposed by Han and Neumann [10] who combined the quasi-Newton method and the steepest descent method. After that, more papers cropped up that focused on hybridization of quasi-Newton and steepest descent method like [2],[3] and [14]. Although quasi-Newton is efficient in solving unconstrained optimization problems, the inverse Hessian matrix in its algorithm makes for slow progress when encountering large-scale problems due to its high memory requirement. In order to make up for this problem, some researchers suggested combining quasi-Newton with conjugate gradient (CG) method, which is an optimization method well-known for its fast-computational capability in solving problems with high number of variables. Ibrahim et al. [12] combined the search direction of BFGS and CG, leading to a new $d_k$ shown by

$$d_k = \begin{cases} 
-H_k g_k, & k = 0 \\
-H_k g_k + \eta (-g_k + \beta_k d_{k-1}), & k \geq 1
\end{cases}$$

where where $\eta \in (0,1)$ and $\beta_k = \frac{g_k^T g_{k-1}}{g_k^T d_{k-1}}$. This method is called the BFGS-CG method. In the study, some numerical tests were executed with Armijo line search and the results showed that BFGS-CG method has the best performance compared to some classical conjugate gradient methods (FR, PR, HS) in terms of number of iterations and CPU time taken to complete the computation. Alternatively, Ibrahim et al.
[13] presented another hybrid BFGS and CG method which is referred as HBFGS method. The $d_k$ is defined by

$$d_k = \begin{cases} -H_k g_k, & k = 0 \\ -H_k g_k + \eta \beta_k d_{k-1}, & k \geq 1 \end{cases}$$

The numerical results obtained show that the HBFGS method is more efficient than standard BFGS method in solving unconstrained optimization problems. However, both hybrid methods in [12] and [13] cannot be applied with exact line search due to the equation of their $\beta_k$. For exact line search, the denominator of the $\beta_k$ will be equal to zero, hence making the calculation process not possible.

This paper is divided into five sections with the introduction as the first one. The second section contains our proposed hybrid quasi-Newton method and its algorithm. In the third section, we prove the global convergence of the new the hybrid method under exact line search. For the following sections, we provide some numerical results and discussion in section 4 plus a short conclusion in section 5.

2. Hybrid BFGS-CG Method

We extend the research in [13] by combining BFGS algorithm with a different CG method. The CG methods are usually characterized by the different formulas for $\beta_k$, also known as the conjugate gradient coefficient. In this study, we modify the search direction of the BFGS-CG method in [13] by substituting its $\beta_k$ with $\beta_k^{ARM}$ from [19] and use exact line search for calculating the step size. The ARM CG method is defined as follows:

$$\beta_k^{ARM} = -\frac{m_k \|g_k\|^2 - g_k^T g_{k-1}}{m_k (g_{k-1}^T d_{k-1})}, \quad m_k = \frac{\|d_{k+1} + g_k\|}{\|d_{k-1}\|}.$$ (7)

We set the value of the variable $\eta = 10^{-4}$ as was suggested by [12] and [13]. The resulting algorithm will be called the BFGS-ARM method.

The following algorithm will implement the BFGS-ARM method.

Step 1: Given an initial point $x_0 \in \mathbb{R}^n$, $H_0 \in \mathbb{R}^{n \times n}$, set $k = 0$.

Step 2: If the stopping criterion $\|g_k\| \leq 10^{-6}$ or $k = 10,000$ is fulfilled, stop.

Step 3: Compute the descent direction by (6) using (7) as $\beta_k$.

Step 4: Compute $\alpha_k$ by strong exact line search.

Step 5: Compute $x_{k+1} = x_k + \alpha_k d_k$.

Step 6: Set $s_k = x_{k+1} - x_k$ and $y_k = g_{k+1} - g_k$.

Step 7: Compute $H_{k+1}$ by (5).

Step 8: Set $k := k + 1$ and return to Step 2.

3. Convergence analysis of the hybrid method

In this section, we present the convergence analysis of BFGS-ARM method under exact line search. A convergent algorithm has to satisfy the sufficient descent and global convergence properties. The following assumptions are needed to aid the proving process.

Assumption 1

(i) The objective function $f$ is twice continuously differentiable.
(ii) In some neighborhood $N$ of $\ell$, $f(x)$ is continuously differentiable and its gradient is Lipschitz continuous; then, there exists a constant $L > 0$ such that for all $x, y \in N$, $\|g(x) - g(y)\| \leq L\|x - y\|$.

(iii) The level set $L$ is convex. There exist positive constants $c_1$ and $c_2$ satisfying
\[ c_1 \|z\|^2 \leq z^T F(x) z \leq c_2 \|z\|^2 \]
for all $z \in \mathbb{R}^n$ and $x \in L$ where $F(x)$ is the Hessian matrix of $f$.

A. Sufficient descent condition
For the sufficient condition to hold
\[ g_k^T d_k \leq -c \|g_k\|^2 \quad \text{for } k \geq 0 \quad \text{and} \quad c > 0 \quad (8) \]

Theorem 1
Suppose that the Assumption 1 holds true. Consider a hybrid BFGS method where the search direction is given as (6) and the step size $\alpha_k$ is determined by using exact line search, then the sufficient descent condition (8) holds for all $k \geq 0$.

Proof:
If $k = 0$, then $g_0^T d_0 = -g_0^T H_0 g_0 \leq -c \|g_0\|^2$. Hence, condition (8) holds true.

We also need to show that for $k \geq 1$, condition (8) will also hold. From (6), we see that
\[ g_k^T d_k = -g_k^T H_k g_k + \eta \left( -g_k^T g_k + \beta_k g_k^T d_{k-1} \right) \]
\[ = -g_k^T H_k g_k - \eta g_k^T g_k + \eta \beta_k g_k^T d_{k-1} \quad (9) \]

For exact line search, we know that $g_k^T d_{k-1} = 0$. Therefore, we have
\[ g_k^T d_k = -g_k^T H_k g_k - \eta g_k^T g_k \leq -\eta \|g_k\|^2, \]
Taking $c = \eta$, we thus have
\[ g_k^T d_k \leq -\|g_k\|^2 \quad (10) \]

Hence, the sufficient descent condition holds true and the proof is complete.

B. Global convergence
We need to show that the hybrid BFGS algorithm with the new $\beta_k$ is globally convergent under exact line search. Firstly, we will simplify our $\beta_k$. From (6) we have
\[ \beta_k^{ARM} = -\frac{m_k \|g_k\|^2 - g_k^T g_{k-1}}{m_k \|g_k^T - g_{k-1} d_{k-1}\|}, \quad \text{where} \quad m_k = \frac{\|d_{k-1} + g_k\|}{\|d_{k-1}\|}. \]

We know that $g_k^T d_k \leq -c \|g_k\|^2$. Hence, the $\beta_k$ can be simplified to
Now, we establish the following theorem to prove the global convergence of the new hybrid method with exact line search.

**Lemma 1** (see [2])

Let \( B_k \) be generated by (5) where \( B_k \) is a symmetric and positive definite matrix with \( y_k^T s_k > 0 \) for all \( k \). Assume that \( \{ s_k \} \) and \( \{ y_k \} \) are such that

\[
\left\| \frac{(y_k - G_k) s_k}{s_k} \right\| \leq \epsilon_k.
\]

For some symmetric and positive definite matrix \( G(x) \) and for some sequence \( \{ \epsilon_k \} \) where \( \sum_{k=1}^{\infty} \epsilon_k < \infty \).

Then

\[
\lim_{k \to \infty} \left\| B_k - G_k \right\| d_k = 0,
\]

and the sequences \( \left\| B_k \right\| \) and \( \left\| B_k^{-1} \right\| \) are bounded.

**Lemma 2**

Let \( \alpha \) be generated by the exact line search and let Assumption 1 hold. Then

\[
\lim_{k \to \infty} \left\| g_k \right\| = 0.
\]

**Proof:**

For the exact line search, let \( \alpha \) be the solution. Then by the mean value theorem \( g_k^T d_k < 0 \) and Assumption 1(ii), let

\[
\alpha_k^* \in \left[ \frac{1}{3L} g_k d_k, \frac{2}{3L} g_k d_k \right].
\]

Then, we have

\[
f(x_k + \alpha_k d_k) - f(x_k) \leq f(x_k + \alpha_k^* d_k) - f(x_k)
\]

\[
= \int_0^1 g \left( x_k + t\alpha_k^* d_k \right)^T \left( \alpha_k^* d_k \right) dt
\]

\[
= \alpha_k^* g_k^T d_k + \int_0^1 \left[ g \left( x_k + t\alpha_k^* d_k \right)^T - g(x_k) \right]^T \left( \alpha_k^* d_k \right) dt
\]
By Cauchy-Schwartz inequality
\[
\alpha_k^* g_k^T d_k + \alpha_k^* \int_0^1 g\left(x_k + t\alpha_k^* d_k\right) - g(x_k) \|d_k\| dt \\
\leq \alpha_k^* g_k^T d_k + \frac{1}{2} L \alpha_k^2 \|d_k\|^2 \\
\leq - \frac{1}{3L} \left\| g_k^T d_k \right\| \left\| -g_k^T d_k \right\| + \frac{1}{2} L \frac{4}{9L^2} \left\| g_k \right\| \|d_k\|^2 \\
= - \frac{1}{9L} \left\| g_k^T d_k \right\|^2
\]

With Assumption 1(ii), we get
\[
\sum_{k=0}^{\infty} \left( g_k^T d_k \right)^2 < \infty.
\]
This implies that \( \lim_{k \to \infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} = 0 \) holds. By Theorem 2, \( \lim_{k \to \infty} \|g_k\| = 0 \) holds.

**Theorem 2**
Suppose that Assumption 1, Lemma 1 and 2 and Theorem 1 hold. Consider the hybrid BFGS-ARM method in the form of (2) and (6) with (7) as the \( \beta_k \) in addition to the step size \( \alpha_k \) obtained by exact line search. Then
\[
\liminf_{k \to \infty} \|g_k\| = 0
\]  
(12)

**Proof:**
To prove this theorem, we use the method of contradiction. Firstly, suppose that there exists a positive constant \( \delta > 0 \) such that
\[
\|g_k\| \geq \delta, \quad \forall k \geq 0.
\]  
(13)
Next, from (6), we have
\[
\frac{\|d_k\|}{\|g_k\|} \leq \frac{\|H_k + \eta \|g_k\| + \eta \|d_{k-1}\|}{\|g_k\|} \\
\frac{\|d_k\|}{\|g_k\|} \leq \frac{\|H_k + \eta \|g_k\| + \eta \|d_{k-1}\|}{\|g_k\|}.
\]
Substituting (12) into the equation, we get
\[
\frac{\|d_k\|}{\|g_k\|} \leq \frac{\|H_k + \eta \|g_k\| + \eta \|d_{k-1}\|}{\|g_k\|} + \frac{\|H_k + \eta \|g_k\| + \eta \|d_{k-1}\|}{\|g_k\|}.
\]
Since \( \|H_k\| \) is bounded, then there exists a positive constant \( u > 0 \) such that \( \|H_k\| \leq u \). Hence,
\[
\frac{\|d_k\|}{\|g_k\|} \leq \frac{\|H_k + \eta \|g_k\| + \eta \|d_{k-1}\|}{\|g_k\|} + \frac{\|H_k + \eta \|g_k\| + \eta \|d_{k-1}\|}{\|g_k\|}.
\]
From (10), note that \( c = \eta \)
\[
\frac{\|d_k\|}{\|g_k\|} \leq \frac{\|d_k\|}{\|g_k\|} + \frac{\|d_{k-1}\|}{c\|g_{k-1}\|} \leq \frac{\|d_k\|}{\|g_k\|} + \frac{\|d_{k-1}\|}{\|g_{k-1}\|}.
\]
Hence, for all \( k \), we have
\[ \frac{\|d_k\|}{\|g_k\|} \leq \sum_{i=1}^{k} \left( \frac{u + \eta}{\|g_{i}\|} \right), \]
\[ \frac{\|d_k\|}{\|g_k\|} \leq \frac{(u + \eta)k + 1}{\delta}, \]
\[ \|d_k\|^2 \leq \frac{(u + \eta)^{2}k + 1}{\delta^2}, \]
\[ \|g_k\|^2 \geq \frac{\delta^2}{(u + \eta)^{2}k + 1}, \]
\[ \sum_{k=0}^{\infty} \frac{\|d_k\|^2}{\|g_k\|^2} \geq \sum_{k=0}^{\infty} \frac{\delta^2}{(u + \eta)^{2}k + 1} = \infty. \]

From Theorem 3, it is implied that
\[ \sum_{k=0}^{\infty} \frac{\|g_k\|^4}{\|d_k\|^4} \geq \sum_{k=0}^{\infty} \frac{\delta^2}{(u + \eta)^{2}k + 1} \geq \infty. \]

This contradicts with Lemma 2. Hence the proof is completed.

4. Numerical Results

This section discusses the numerical tests of the BFGS-ARM method and the results obtained. The same tests are also applied on the BFGS and another hybrid BFGS method introduced in [3] which we will refer as BFGS-SD. While it should be more imperative to also compare BFGS-ARM’s performance with the current BFGS-CG method, the \( \beta_k \) used in [13] is not applicable to exact line search. We pick out 17 standard test problems from [4], [16] and [20]. The capabilities of each method under exact line search are measured in terms of number of iterations and CPU time taken to solve the test problems. We set the algorithm to stop when \( \|g_k\| \leq 10^{-6} \) or when the number of iterations exceeds 10,000. The codes are written in Matlab r2012a subroutine programming and all the tests are performed by using a portable PC with CPU processor Intel(R) Core (TM) i3 and 6GB RAM memory. The list of functions used and their dimensions are displayed in Table I.

| No. | Function                  | Variables | Initial points                                                                 |
|-----|---------------------------|-----------|-------------------------------------------------------------------------------|
| 1   | Six Hump                  | 2         | (3.3), (13.13), (37.37)                                                      |
| 2   | Zettl                     | 2         | (6.6), (14.14), (64.64)                                                      |
| 3   | Dixon and Price           | 2, 4      | (12, 12), (23,23), (69, 69)                                                   |
| 4   | Raydan 1                  | 2, 4      | (7.7), (12,12), (22,22)                                                      |
| 5   | Raydan 2                  | 2, 4      | (6.6), (11,11), (18, 18)                                                     |
| 6   | Powell                    | 4,8       | (3.5, 3.5, ..., 3.5), (15, 15, ..., 15), (40, 40, ..., 40)                    |
| 7   | ARWHEAD                   | 2, 4, 10, 100 | (3.3), (23,23), (81,81)                                      |
| 8   | Extended White and Holst  | 2, 4, 10, 100, 500, 1000 | (-1, -1.5), (5.6), (11,2,11)                                                         |
| 9   | Extended Rosenbrock       | 2, 4, 10, 100, 500, 1000 | (-10, -10), (18,18), (68,68),                                                  |
| 10  | Extended Beale            | 2, 4, 10, 100, 500, 1000 | (-1.3, -1.3), (2,2), (11,11),                                              |
| 11  | Extended Strait           | 2, 4, 10, 100, 500, 1000 | (4.4), (11,11), (38,38),                                                   |
| 12  | Himmelblau                | 2, 4, 10, 100, 500, 1000 | (17.8,17.8), (40,40), (115,106)                                               |
| 13  | DENSCHNB                  | 2, 4, 10, 100, 500, 1000 | (5.5), (25,25), (225,225),                                                  |
| 14  | Generalized Quartic       | 2, 4, 10, 100, 500, 1000 | (11,11), (28,28), (87, 80),                                                  |
| 15  | FLETCHR                   | 2, 4, 10, 100, 500, 1000 | (7.7,7.7), (15, -13), (40 40)                                              |
| 16  | Extended Tridiagonal 1    | 2, 4, 10, 100, 500, 1000 | (13,13), (24.7, 24.7), (60,60)                                               |
| 17  | Generalized Quartic 2     | 2, 4, 10, 100, 500, 1000 | (4,4), (-19,-19),(70,-70)                                                     |
The results obtained from the numerical tests are graphed in the form of performance profile suggested by [6] for easier analysis. Figures 1 and 2 below show the performance of BFGS, BFGS-SD and BFGS-ARM method based on number of iterations and CPU time respectively.

**Figure 1.** Performance profile based on the number of iterations

**Figure 2.** Performance profile based on CPU time

From both figures, it is apparent that the proposed hybrid algorithm performs efficiently in comparison to BFGS and BFGS-SD methods. While it may not be obvious in the graph, BFGS-ARM managed to solve up until 99.09% of the tests presented which is slightly more than BFGS-SD at 98.64%. On the other hand, BFGS solved only 97.29% of the test problems which is lesser than the amount solved by both of the tested hybrid BFGS solvers. Additionally, the curve of BFGS-ARM method in both figures
are at the top left position, thus implying that the solver uses the least number of iterations and CPU time.

5. Conclusions
In this paper, we have proposed a new hybrid BFGS method which we call BFGS-ARM method. The hybrid search direction of the proposed method fulfills the sufficient descent condition under exact line search. In addition, the convergence analysis on the new algorithm proved that the BFGS-ARM method converges globally. The efficiency of BFGS-ARM is assessed by performing numerical test on a set of 17 unconstrained optimization test problems. According to the results obtained, the proposed hybrid algorithm performs better than some BFGS-based method both in number of iterations and time taken for solving each test functions. All these suggest that BFGS-ARM has better overall performance than the other tested methods.

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