Solving Unconstrained Optimization Problem Using Hybrid CG Method with Exact Line Search

Nurul 'Aini*, Ain Aqiela Azamuddin

Faculty of Computer and Mathematical Sciences, Universiti Teknologi MARA Johor, Segamat, Johor, Malaysia

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Abstract: The conjugate gradient (CG) method is a one of the common approaches for solving unconstrained optimization problems, notably known for its suitability for large scale problems. Many recent studies show that this method is also useful for problems of smaller scale. One of the methods used for improving the performance of CG method is hybrid approach, where a CG method is combined with another method. In this study, the ARM CG method is combined with the SMR CG method and tested under exact line search. The resulting hybrid algorithm is globally convergent under exact line search and shown to perform well numerically in comparison to other tested CG methods.

Keywords: Conjugate gradient method, exact line search, hybrid conjugate gradient method, unconstrained optimization

I. Introduction

The unconstrained optimization problem is formulated by

$$\min_{x \in R^n} f(x), \tag{1}$$

such that $f : R^n \to R$ is a function, continuously differentiable with gradient at point x_k denoted as g_k. Iterative method is commonly used as

$$x_{k+1} = x_k + \alpha_k d_k, \qquad k = 0,1,2,... \tag{2}$$

with $\alpha_k > 0$ denotes the step size, x_k is the iteration point and d_k is the search direction. In this study, the exact line search is used to determine the step size which is given as follows:

$$f(x_k + \alpha_k d_k) = \min_{\alpha \geq 0} f(x_k + \alpha d_k) \tag{3}$$

The exact line search determines the optimal step size for each iterative step that gives the best possible reduction of the objective function. However, it is often argued to be very slow and even fail if the initial point chosen is far from the solution point [1]. As a result, the inexact line search methods such as strong Wolfe and Armijo line search are usually preferred as they are more practical and easier to implement [2,3]. In recent years, the development of faster processors has helped overcome the traditional slowness of exact line search [4,5]. In addition, several studies also suggested that the exact line search has stronger convergence properties with fewer iterations in some cases and simpler analysis structure [6,7]. This makes exact line search to be still a viable approach for solving unconstrained optimization problems alongside various other inexact approaches.

The conjugate gradient (CG) algorithm is widely regarded as one of the most effective methods for solving unconstrained optimization problems, particularly in large-scale settings where memory and computational efficiency are critical. The CG methods are iterative and require relatively low storage, making them well-suited for large optimization tasks. These made CG methods a popular choice in fields such as machine learning, data fitting, engineering design, and scientific computing. The search direction of CG method is given by

$$d_k = \begin{cases} -g_k, & k = 0 \\ -g_k + \beta_k d_{k-1}, & k \geq 1 \end{cases}, \tag{4}$$

where the β_k is known as the CG coefficient. The types of CG method can be classified based on the design of their CG coefficient. Some notable examples are the classical CG methods such as the Fletcher-Reeves (FR) [8], and Polak-Ribiere-Polyak (PRP) [9] methods. These methods are usually used as the base for development of current CG methods. The Polak–Ribière–Polyak (PRP) method is one of the most effective CG techniques, largely because it often solves optimization problems using fewer iterations than classical methods like Fletcher–Reeves (FR). However, Powell [10] later showed that despite its practical efficiency, the PRP method is not guaranteed to be globally convergent. The findings highlighted the importance of ensuring that the CG coefficient remains positive. Then, various improvements have been proposed to the modify the CG formula to maintain a positive CG coefficient [11-13]. This study proposes a hybrid CG method with improved performance in solving unconstrained optimization problems under exact line search.

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II. Methodology

The ARM-SMR method proposed by Aini et al. [14] is a hybrid CG method that combines the CG coefficient of ARM and SMR methods. This hybrid method incorporates the properties of ARM method while eliminating its drawback of generating negative CG coefficient as the presence of these negative CG coefficients could cause the method to sometimes fail to converge [10]. When tested with strong Wolfe line search, the ARM-SMR method showed the most efficient results in comparison to the other CG methods it was compared with, i.e, ARM, AMR and FR methods [14]. While most of the recent studies generally favour inexact line search over exact line search, there are still cases where exact line search is preferred, such as when there is need for method with stronger convergence properties [6]. In this section, the ARM-SMR method is presented under exact line search. The hybrid method is defined as

$$\beta_k^{ARM-SMR} = \begin{cases} \beta_k^{ARM}, & \text{if} \quad m_k \|g_k\|^2 < \left|g_k^T g_{k-1}\right| \\ \beta_k^{SMR}, & \text{otherwise} \end{cases}. \tag{5}$$

where $\beta_k^{ARM} = \dfrac{m_k \|g_k\|^2 - \left|g_k^T g_{k-1}\right|}{m_k g_{k-1}^T d_{k-1}}$, $m_k = \dfrac{\|d_{k-1} + g_k\|}{\|d_{k-1}\|}$ and $\beta_k^{SMR} = \max\left\{0, \dfrac{\|g_k\|^2 - \left|g_k^T g_{k-1}\right|}{g_{k-1}^T d_{k-1}}\right\}$. The proposed hybrid approach combines the ARM method with the SMR method by Mohamed et al. [15], which ensures the CG coefficient remains positive. In the hybrid method, the SMR method is used as a fallback whenever the ARM method generates a negative CG coefficient.

The resulting hybrid CG method, referred as the ARM-SMR method, is implemented according to following algorithm.

Algorithm 1: Hybrid ARM-SMR Method

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

Step 2 : If $\|g_k\| \leq 10^{-6}$ or $k = 10000$, then stop.

Step 3 : Calculate d_k by using (4) and (7).

Step 4: Determine the stepsize α_k by using (3).

Step 5: Compute the new iterative point x_k using (2).

Step 6: Set $k := k+1$ and return to Step 2.

Consider the following assumptions for objective function:

1. The function *f(x)* is bounded below on the level set $Q = \{x \mid f(x_0) \geq f(x)\}$, where x_0 is the initial point.

2. In some neighbourhood *W* of *Q* where the function *f(x)* is continuously differentiable and its gradient is Lipschitz continuous; then the condition $\|h(x) - h(z)\| \leq L\|x - y\|$ is satisfied for all $x, z \in W$, $L > 0$.

The proposed method is said to converge provided it meets the conditions for sufficient descent and global convergence. These conditions ensure that a descent direction is produced at each iteration, ultimately leading the algorithm to a solution. The sufficient descent condition holds when

$$g_k^T d_k \leq -c\|g_k\|^2, \quad \text{where } k > 0 \text{ and } c > 0$$

Next, it must also satisfies the global convergence property that is based on the following condition:

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

The analysis of the convergence properties of ARM-SMR method are discussed based on two cases, that is, when $\beta_k^{ARM} \geq 0$ and when $\beta_k^{ARM} < 0$. This can be further explained as follows.

Case 1: $\beta_k^{ARM} \geq 0$. In this case, the CG method will apply β_k^{ARM} in the calculation. Refer proof in [13].

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Case 2: $\beta_k^{ARM} < 0$. In this case, the CG method will use β_k^{SMR}. Refer proof in [14].

III. Numerical Result And Discussion

This section presents the numerical results obtained from evaluating the proposed ARM-SMR method in comparison with several well-established conjugate gradient (CG) methods under exact line search. For benchmarking purposes, the methods selected include the FR, ARM and SMR methods. The FR method is included as they are one of the earliest CG method which had served as a foundation for the development of many modern CG algorithms. The performance of each method is tested on a set of standard unconstrained optimization problems taken from [16], with problem dimensions ranging from 2 to 1000 variables to test their applicability for small to large scale problems. All methods employ the exact line search for stepsize calculation. Numerical experiments are carried out using MATLAB 2021.

The stopping criteria are defined as reaching a gradient norm below a pre-specified tolerance or exceeding 10,000 iterations. Next, the performance of the CG methods are evaluated based on the number of iterations and CPU time required to reach convergence. To provide a comprehensive comparison, performance profiles are constructed following the approach of Dolan and Moré [17], which offers a robust framework for assessing the relative efficiency of optimization algorithms across a diverse test set. The complete list of test functions used is provided in Table 1.

Table 1: List of test functions

No.	Test Problems	No. of Variables
1	Three hump	2
2	Six Hump	2
3	Zettl	2
4	Trecanni	2
5	Colville	4
6	Dixon and Price	2,4
7	Hager	2,10
8	Shalow	2, 100, 1000
9	Extended Himmelblau	2, 100, 1000
10	Extended Strait	2, 100, 1000
11	Qing	2, 100, 1000
12	FLETCHR	2, 100, 1000

Figures 1 and 2 illustrate the performance of the four tested CG methods, measured in terms of iteration count and CPU time, respectively. The left side of the figure shows the percentage of test problems for which a solver achieves the lowest iteration count or CPU time. The right side of the figure reflects the overall success rate of each method. Therefore, the solver positioned furthest to the top-right of the plot can be considered the most effective overall, demonstrating both high efficiency and consistent performance across the test set.

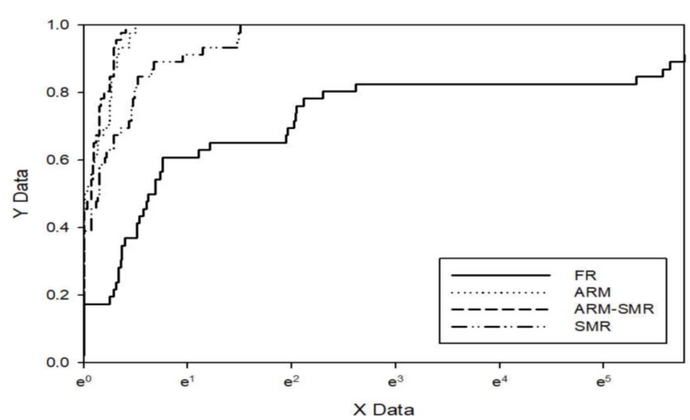

Figure 1: Performance profile based on number of iteration

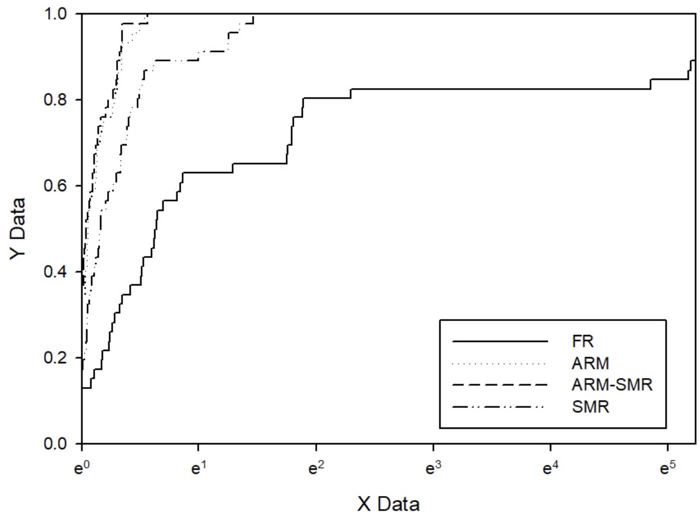

Figure 2: Performance profile based on CPU time

As shown in Figure 1, the proposed ARM-SMR method outperforms the other tested CG methods in terms of iteration count, consistently appearing at the top left and right regions of the performance profile—an indicator of both efficiency and robustness. The same result is shown in Figure 2, although the performance gap in CPU time between the best method (ARM-SMR) and second-best (ARM) is smaller. Compared to ARM-SMR, the original ARM method demonstrates slightly lower performance, with its curve positioned beneath that of ARM-SMR in both figures. This suggests that, for most test problems, ARM requires more iterations and CPU time to converge. The SMR method is the third best in overall efficiency, with its curve located below ARM and ARM-SMR methods. On the other hand, the FR method exhibits the lowest performance among all methods tested, with its performance profile appearing at the bottom in both figures. It also has the lowest success rate, solving 91.3% of the test problems, whereas the other methods—including the proposed ARM-SMR—successfully solved 100% of the test set.

Given its consistent placement at the top of the performance profiles and its perfect success rate, the ARM-SMR method demonstrates the most reliable and efficient overall performance, confirming its effectiveness as a hybrid CG approach for unconstrained optimization.

IV. Conclusion

This paper presents a modified CG method using hybrid approach where it combines the strengths of the ARM and SMR methods under exact line search. The hybrid, referred to as the ARM-SMR method, integrates the SMR strategy to address a known limitation of the ARM method—namely, the occurrence of negative CG coefficients that can hinder solver performance. By incorporating SMR when such values arise, the proposed algorithm ensures greater numerical stability and robustness. To evaluate its effectiveness, the ARM-SMR method was tested against the original ARM, SMR, and FR methods using a standard set of unconstrained optimization problems. The numerical results demonstrate that the ARM-SMR method consistently achieves superior performance in terms of iteration count, CPU time and problem-solving success rate. This result is consistent with the findings from [14], which indicates that ARM-SMR method is suitable for both exact and inexact line searches.

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