A new modified conjugate gradient coefficient for solving system of linear equations

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Abstract. Conjugate gradient (CG) method is an evolution of computational method in solving unconstrained optimization problems. This approach is easy to implement due to its simplicity and has been proven to be effective in solving real-life application. Although this field has received copious amount of attentions in recent years, some of the new approaches of CG algorithm cannot surpass the efficiency of the previous versions. Therefore, in this paper, a new CG coefficient which retains the sufficient descent and global convergence properties of the original CG methods is proposed. This new CG is tested on a set of test functions under exact line search. Its performance is then compared to that of some of the well-known previous CG methods based on number of iterations and CPU time. The results show that the new CG algorithm has the best efficiency amongst all the methods tested. This paper also includes an application of the new CG algorithm for solving large system of linear equations.

1. Introduction

In mathematical term, the method of solving models and finding the best alternatives is known as optimization. The unconstrained optimization function is stated by

\[ \min_{x \in \mathbb{R}^n} f(x), \]  

where \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) as a continuously differentiable function and its gradient at point \( x_k \) denoted as \( g_k \).

The iterative method used to solve (1.1) is formed by

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

where \( \alpha_k > 0 \) is the stepsize, \( x_k \) is the iterative point and \( d_k \) is the search direction. In this paper, the exact line search is used to calculate the stepsize which is given by

\[ f(x_k + \alpha_k d_k) = \min_{\alpha \geq 0} f(x_k + \alpha d_k). \]  

For CG method, basic known search direction is described by

\[ d_k = \begin{cases} 
- g_k & \text{if } k = 0 \\
- g_k + \beta_k d_{k-1} & \text{if } k \geq 1 
\end{cases} \]  

where \( \beta_k \) is a positive constant.
where $g_k = \nabla f(x_k)$, while the scalar parameter $\beta_k$ is the conjugate gradient coefficient. There are few common $\beta_k$ used in this research,

$$
\beta_k^{FR} = \frac{g_k^T g_k}{\|g_k\|^2}, \quad \beta_k^{HS} = \frac{g_k^T (g_k - g_{k-1})}{d_{k-1}^T (g_k - g_{k-1})}, \quad \beta_k^{NPRP} = \frac{(g_k^T g_k) \left\| g_k \right\| \left\| g_{k-1} \right\|}{\left\| g_{k-1} \right\|^2},
$$

where $g_{k-1} = \nabla f(x_{k-1})$ and $\|\|$ indicates the Euclidian norm of vectors. The above methods are known as Fletcher-Reeves (FR) [1], Hestenes-Stiefel (HS) [2] and NPRP [3]. Further reading on new methods can be referred to [4, 5, 6, 7, 8].

The structure of this paper is arranged as follows. The new CG is proposed in Section 2. In section 3, we presented the sufficient descent condition and global convergence analysis of general CG method. Numerical results and performance profile corresponding to the new conjugate gradient are reported in the section 4. Implementation of new method and conclusion are presented in section 5 and 6 respectively.

2. New CG method

In this section, we present a new conjugate gradient coefficient, $\beta_k^{NHMR*}$ method. We propose these methods similar to that of WYL method. The equation of this new CG coefficient is as follows:

$$
\beta_k^{NHMR*} = \max \left\{ 0, -\frac{g_k^T (g_k - \frac{\left\| g_k \right\|}{\left\| g_{k-1} \right\|} g_{k-1})}{g_k^T (g_k - d_{k-1})} \right\}.
$$

The following is the NHMR* algorithm.

**Step 1**: Initialization. Given $x_0$, set $k = 0$.

**Step 2**: Compute $\beta_k$ based on (2.1).

**Step 3**: Compute $d_k$ based on (1.4). If $g_k = 0$, then stop.

**Step 4**: Compute $\alpha_k$ based on (1.3).

**Step 5**: Update the new point based on (1.2).

**Step 6**: Convergence test and stopping criteria. If $f(x_{k+1}) < f(x_k)$ and $\|g_k\| < \varepsilon$ then stop. Otherwise go to Step 1 with $k = k + 1$.

3. Convergent analysis

In order to support of our method, the convergence properties of $\beta_k^{NHMR*}$ will be studied. An algorithm must satisfy the sufficient descent condition and the global convergence properties. In this case, the global convergence properties are already established in the previous paper [4], so we will just focus on the sufficient descent condition.

3.1. Sufficient descent condition of NHMR* method

The following theorem prove that the new CG coefficient NHMR* possess sufficient descent condition with exact line search.

**Theorem 1.** Consider NHMR* method with (1.4) where NHMR* satisfies condition $g_k^T d_k \leq -C\|g_k\|^2$ for all $k > 0$.
Proof. If \( k = 0 \), then clearly we can get \( g_0^T d_0 = -C \| g_0 \|^2 \). Hence, condition \( g_k^T d_k \leq -C \| g_k \|^2 \) holds true. Next, we will show that for \( k = 0 \) condition \( g_k^T d_k \leq -C \| g_k \|^2 \), will holds true.

Multiply (1.4) by \( g_k^T \), then

\[
g_k^T d_k = g_k^T (-g_k + \beta_k d_{k-1}) = -\| g_k \|^2 + \beta_k g_k^T d_{k-1}.
\]

For exact line search, \( g_k^T d_{k-1} = 0 \).

\[
g_k^T d_k = -\| g_k \|^2,
\]

which implies \( d_k \) is sufficient descent direction. Hence, \( g_k^T d_k \leq -C \| g_k \|^2 \) holds true. The proof is complete.

4. Numerical results and discussion

In this section, NHMR* is compared to other methods such as FR, HS and NPRP. Then the performances of these methods are evaluated based on the comparison of the iteration numbers and Central Processing Unit (CPU) per time to reach the minimum point. All these problems are executed with four different initial points, starting from a point which is closer to the solution point till to the point further away from the solution point. We considered \( \varepsilon = 10^{-6} \) and all these methods terminate when the stopping criteria \( \| g_k \| \leq 10^{-6} \) and \( k = 10000 \) are fulfilled [9]. All the problems stated below are computed by Matlab programme using exact line search. We compare our method by using standard test problems by Molga and Smutnicki [10] and Andrei [11].

**Table 1.** A list of test problems.

| No. | Problems                  | Dimensions              | Initial points                      |
|-----|---------------------------|-------------------------|--------------------------------------|
| 1   | Booth                     | 2                       | (1,1), (5,5), (10,10), (15,15)       |
| 2   | Six hump                  | 2                       | (1,1), (5,5), (10,10), (15,15)       |
| 3   | Three hump                | 2                       | (1,1), (5,5), (10,10), (15,15)       |
| 4   | Extended white & holst    | 2, 500, 1000, 5000, 10000 | (2,2,…,2), (5,5,…,5), (10,10,…,10), (12,12,…,12) |
| 5   | Extended rosenbrock       | 2, 500, 1000, 5000, 10000 | (2,2,…,2), (5,5,…,5), (10,10,…,10), (15,15,…,15) |
| 6   | Extended beale            | 2, 500, 1000, 5000, 10000 | (-1,-1,…-1), (0.50,0.50,…0.50), (1,1,…,1), (2,2,…,2) |
| 7   | Extended himmelblau       | 2, 500, 1000, 5000, 10000 | (1,1,…,1), (5,5,…,5), (10,10,…,10), (15,15,…,15) |
| 8   | Diagonal 2                | 2, 1000, 5000           | (1,1,…,1), (0.50,0.50,…0.50), (0.25,0.25,…0.25), (0.20,0.20,…,0.20) |
| 9   | Extended DENSCHNB         | 2, 500, 1000, 5000, 10000 | (1,1,…,1), (5,5,…,5), (10,10,…,10), (15,15,…,15) |
| 10  | Shallow                   | 2, 500, 1000, 5000, 10000 | (-2,-2,…,-2), (2,2,…,2), (5,5,…,5), (10,10,…,10) |
| 11  | Extended quadratic penalty QP2 | 2, 1000, 5000, 10000 | (2,2,…,2), (5,5,…,5), (10,10,…,10), (15,15,…,15) |
The results are compiled in two graphs of performance profile based on Dolan and More [12] to show the performance of NHMR* method relative to other CG methods. The right side represents the test problems that are successfully solved by each method while the left side of the figure represents the method which is fastest in solving test problems.

![Performance profile relative to number of iteration.](image1)

![Performance profile relative to CPU time.](image2)

5. Implementation of new method

In this section, we apply the following theorem to generate the equations for solving systems of linear equations,

\[ Ax = b, \]

where \( A \) is a given \( m \times m \) real matrix and \( b \) is given real \( m \) vector. The CG method is most effective for cases in which the symmetric part of the matrix corresponds to easily solvable systems of linear equations. These matrices are formed from positive-definite symmetric matrices in order to make them work.

**Theorem 2.** Suppose that vector \( x \) that minimizes \( \| Ax - b \|^2 \) is given by the solution to the equation \( A^T A x = A^T b \); that is \( x = (A^T A)^{-1} A^T b \).
First, we derive equations from above matrices by using Theorem 2. Then, the equations are computed by Matlab programme using different initial points to show that our new proposed methods are capable of solving large-scale systems of linear equations. Table 3 displayed the result of each method in terms of number of iteration and CPU time. Meanwhile, Table 4 shows CPU time per iterations for each method. In case of ‘Fail’, there is no available number of iterations and CPU time to be justified.

Table 2. A list of matrices.

| Matrix | \( A \) | \( b \) |
|--------|--------|--------|
| 5\( \times \)5 | \[
\begin{bmatrix}
5 & -2 & 3 & -2 & -2 \\
-2 & 5 & -2 & 3 & -2 \\
3 & -2 & 5 & -2 & -2 \\
-2 & 3 & -2 & 5 & -2 \\
-2 & 3 & -2 & -2 & 2
\end{bmatrix}
\] | 7 |
| 15\( \times \)15 | \[
\begin{bmatrix}
6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 \\
-2 & 6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 \\
3 & -2 & 6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 \\
-2 & 3 & -2 & 6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 \\
3 & -2 & 3 & -2 & 6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 \\
-2 & 3 & -2 & 3 & -2 & 6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 \\
3 & -2 & 3 & -2 & 6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 \\
-2 & 3 & -2 & 3 & -2 & 6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 \\
3 & -2 & 3 & -2 & 6 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3 & -2 & 3
\end{bmatrix}
\] | 7 |

Table 3. Result of each method in terms of number iteration and CPU time.

| Matrix | Initial points | FR | HS | NPRP | NHMR* |
|--------|----------------|----|----|------|-------|
|        | NI  | CPU  | NI  | CPU  | NI  | CPU  | NI  | CPU  |
| 5\( \times \)5 | 5   | 40   | 1.6491 | 79   | 0.8968 | Fail | Fail | 2157 | 79.0731 |
|      | 50  | 40   | 1.7426 | 109  | 1.1999 | Fail | Fail | 1818 | 64.5793 |
|      | 100 | 42   | 1.7206 | 56   | 0.6565 | Fail | Fail | 2055 | 73.6911 |
|      | 500 | 37   | 1.5449 | 79   | 0.8773 | Fail | Fail | 2744 | 98.6436 |
| 15\( \times \)15 | 5   | 259  | 12.731 | Fail | Fail | 814  | 29.4603 | 1451 | 66.0296 |
Based on Table 4, NHMR*’s performance is more efficient than FR and NPRP but still cannot surpass HS. Other than that, the best approximation method is also chosen based on the smallest sum of error. The sums of error given by FR and HS are 0.00000103 and 0.00000251, respectively. However, both methods failed at certain initial points as shown in Table 3. On the other hand, NPRP has the largest sum of error among all methods which is 0.84311896. Overall, NHMR* manage to solve all given matrices and also have small sum of error, 0.00000901. Hence, NHMR* can be defined as the best approximation method for solving large-scale systems of linear equations.

### 6. Conclusion

The new CG, NHMR* has been proven to be the best method when compared to other standard CG methods, such as NPRP, FR and HS. It also manages to solve all of the tested linear problems while retaining small sum of error. Hence, the NHMR* method is promising for further study. This study can be extended under strong Wolfe line search to prove its ability in solving unconstrained optimization problems.

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| Method  | CPU time per iterations |
|---------|-------------------------|
| FR      | 0.0455                  |
| HS      | 0.0139                  |
| NPRP    | 0.0424                  |
| NHMR*   | 0.0392                  |

**Table 4.** CPU time per iterations.