New Three–Term CG-Method for Unconstrained Optimization

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Received on: 29/06/2011
Accepted on: 14/12/2011

ABSTRACT

In this paper, we proposed a new three-term nonlinear Conjugate Gradient (CG) method for solving unconstrained optimization problems. The new three-term method generates decent direction with an inexact line search under Wolfe conditions and the descent property of the new method is proved. Numerical results on some well-known test function with various dimensions showed that the new method is an efficient.

Keywords: Optimization, three term CG unconstrained optimization methods.

1. Introduction.

In this paper, we deal with conjugate gradient methods for solving the following unconstrained optimization problem:

Minimize \( f(x) \) \hspace{1cm} (1)

where \( f: \mathbb{R}^n \rightarrow \mathbb{R} \) is smooth and its gradient \( g(x) = \nabla f(x) \) is available. Conjugate gradient methods are very efficient for solving large-scale unconstrained optimization problems (1). For solving this problem, starting from initial guess \( x_0 \in \mathbb{R}^n \), a nonlinear conjugate gradient methods generates a sequence \( \{x_k\} \) as:

\[ x_{k+1} = x_k + \alpha_k d_k \quad \text{for} \quad k = 1, 2, \ldots \] \hspace{1cm} (2)

where step size \( \alpha_k \) is positive, which is computed by carrying out some line search, and the direction \( d_k \) is generated as:

\[ d_k = \begin{cases} -g_k & \text{for} \quad k = 1 \\ -g_k + \beta_k d_{k-1} & \text{for} \quad k \geq 2 \end{cases} \] \hspace{1cm} (3)

In (3) \( \beta_k \) is known as conjugate gradient parameter. The search direction, assumed to be a descent one which is play the main role in these methods. On the other hand, the step size \( \alpha_k \) guarantees the global convergence in some cases and is crucial in efficiency. Plenty of conjugate gradient methods are known, and an excellent survey of these methods, with special attention on their convergence, is given by Hager and Zhang [5]. Different conjugate gradient algorithms correspond to different choices for
the scalar $\beta_k$. The line search in the conjugate gradient algorithms often is based on
standard Wolfe conditions. The standard Wolfe conditions [9,10] are
\[
 f(x_k + \alpha_k d_k) - f(x_k) \leq \delta \alpha_k g_k^T d_k, \quad \cdots (4)
\]
\[
 g_{k+1}^T d_k \geq \sigma g_k^T d_k, \quad \cdots (5)
\]
where $d_k$ is a decent direction and $0 < \delta < \sigma < 1$. For some conjugate gradient
algorithms, stronger Wolfe conditions defined by:
\[
 f(x_k + \alpha_k d_k) - f(x_k) \leq \delta \alpha_k g_k^T d_k, \quad \cdots (6)
\]
\[
 |g(x_k + \alpha_k d_k)^T d_k| \leq -\sigma g_k^T d_k \quad \cdots (7)
\]
are needed to ensure convergence and to enhance stability. It has been shown [9] that
for FR scheme, the strong Wolfe conditions may not yield a direction of decent unless
$\sigma \leq 1/2$. In typical implementations of the Wolfe conditions, it is most efficient to
choose $\sigma$ close to one.

It is known that choices of $\beta_k$ affect numerical performance of the method, and
hence many researchers studied choices of $\beta_k$. Well-known formulas for $\beta_k$ are the
Hestenes-Stiefel (HS) [6], Fletcher-Reeves (FR) [4], Conjugate-Decent(CD) [3] and
Dai-Yuan (DY) [2] formulas, which are respectively given by
\[
\beta^\text{HS}_k = \frac{g_k^T y_{k-1}}{d_{k-1}^T y_{k-1}}, \quad \beta^\text{FR}_k = \frac{\|g_k\|^2}{\|g_{k-1}\|^2}, \quad \beta^\text{CD}_k = -\frac{\|g_k\|^2}{d_{k-1}^T g_{k-1}}, \quad \beta^\text{DY}_k = \frac{\|g_k\|^2}{d_{k-1}^T y_{k-1}} \quad \cdots (8)
\]
Where $\|\cdot\|$ means the Euclidean norm and, $y_{k-1} = g_k - g_{k-1}$.

Note that these formulas for $\beta_k$ are equivalent each other if the objective function is
a strictly convex quadratic function and $\alpha_k$ is the one dimensional minimizer.

2. Three-Term CG-Methods:

The first three-term nonlinear CG-method was presented by Nazareth [8], in which the
search direction is determined by:
\[
d_{k-1} = -y_k + \frac{y_k^T y_k}{y_k^T d_k} d_k + \frac{y_{k-1}^T y_k}{y_{k-1}^T d_{k-1}} d_{k-1} \quad \cdots (9)
\]

The main property of $d_k$ is that, for convex quadratic function, it remains conjugate
even without ELS.

Zhang et al. [11] proposed the modified FR method (ZFR) which is defined by:
\[
d_k = -\theta_k g_k + \beta^\text{FR} d_{k-1}, \quad \cdots (10)
\]
where $\theta_k = d_{k-1}^T y_{k-1} / \|g_{k-1}\|^2$. Since this search direction satisfies $g_k^T d_k \leq -\|g_k\|^2$ for
all $k$, It can be written by the three-term form:
\[
d_k = -g_k + \beta^\text{FR} d_{k-1} - \theta_k^{(3)} g_k, \quad \cdots (11)
\]
where $\theta_k^{(3)} = g_k^T d_{k-1} / \|g_{k-1}\|^2$.

They also proposed the modified PR method (ZPR) [12] and the modified HS
method (ZHS) [13], which are respectively given by:
\[
d_k = -g_k + \beta^\text{PR} d_{k-1} - \theta_k^{(2)} y_{k-1}, \quad \cdots (12)
\]
\[
d_k = -g_k + \beta^\text{HS} d_{k-1} - \theta_k^{(3)} y_{k-1}, \quad \cdots (13)
\]
where $\theta_k^{(2)} = g_k^T d_{k-1} / \|g_{k-1}\|^2$ and $\theta_k^{(3)} = g_k^T d_{k-1} / d_{k-1}^T y_{k-1}$.

These three-term conjugate gradient methods which always satisfy the sufficient
descent condition:
for a positive constant c, independently of line searches.

3. New Three-term CG-Method.

Miras and Hassan [7] proposed a seven-parameter family defined by:

$$
\beta_k^\text{seven} = \frac{(1 - \lambda_k - \delta_k - \gamma_k - \varphi_k - \psi_k) \beta_k^T g_k + \lambda_k \beta_k^T g_k}{d_k^T v_k} + \delta_k g_k^T y_k + \gamma_k g_k^T g_k - \varphi_k g_k^T d_k + \psi_k p^T g_k \ldots(14)
$$

where

$$
p = (y_k - 2d_k g_k) \lambda_k \mu_k \in [0,1] \omega_k \in [0,1 - \mu_k] \delta_k \in [0,1 - \lambda_k] \text{ and } \gamma_k \in [0,1 - \delta_k] \varphi_k \in [0,1 - \gamma_k, \psi_k \in [0,1 - \varphi_k] \text{ parameters. (i.e. } \lambda_k, \delta_k, \gamma_k, \varphi_k \text{ and } \psi_k \text{ are impossible to be equal to one at the same time; the same thing is also correct for } \mu_k \text{ and } \omega_k).
$$

The seven-parameter family contains already existing twelve well-known formulas for $\beta_k$, so there were 27=128 cases, 12 cases were succeeded, 116 cases were failed.

In the present work, we derived a new three term conjugate gradient method from this family. We choose one of the failed cases that is when $(\lambda, \delta, \gamma, \varphi, \psi, \mu, \omega)$ are equal to $(0,1,0,0,1,0,1)$ respectively, so $\beta^\text{seven}$ yield to:

$$
\beta_k = -\frac{g_k^T (y_k - \alpha_k d_k) + g_k^T y_k + p^T g_k}{d_k^T y_k} \ldots(15a)
$$

where $p = (y_k - 2d_k g_k)$ using (ILS) eq.(15a) became:

$$
\beta_k = \frac{\alpha_k d_k^T g_k + 1}{d_k^T y_k} \left( y_k - 2d_k g_k \right) g_k \ldots(15b)
$$

Now we know that:

$$
d_{k+1} = -g_{k+1} + \beta_k d_k
$$

We see $Q_{k+1}$ is not symmetric, to symmetrize $Q_{k+1}$ we add and subtract the term

$$
\frac{y_k d_k^T}{d_k^T y_k}
$$

to get:

$$
Q_{k+1}^* = I - d_k^T y_k - \frac{y_k d_k^T}{d_k^T y_k} + \frac{y_k d_k^T}{d_k^T y_k} - \frac{\alpha_k d_k^T y_k}{d_k^T y_k} + \frac{2\|y_k\|^2 d_k^T}{(d_k^T y_k)^2} - \frac{2\|y_k\|^2 d_k^T}{(d_k^T y_k)^2}
$$

Use the Lipschitz condition for the third term to the numerator and denominator to get:

$$
Q_{k+1}^* = I - d_k^T y_k + \frac{y_k d_k^T}{d_k^T y_k} + \frac{2\|y_k\|^2 d_k^T}{(d_k^T y_k)^2}
$$

31
\[ Q_{k+1}^* = I - \frac{d_k y_k^T + y_k d_k^T}{d_k^T y_k} + \left( \frac{1}{d_k^T y_k} - \frac{\alpha_k}{d_k^T d_k} + \frac{2 \|y_k\|^2}{(d_k^T y_k)^2} \right) d_k d_k^T \]

Hence, \( Q_{k+1}^* \) is symmetric, but not satisfy QN condition i.e. \( Q_{k+1}^* y_k \neq v_k \), to forces \( Q_{k+1}^* \) to satisfy QN condition we can write it as:

\[ Q_{k+1}^* = I - \frac{d_k y_k^T + y_k d_k^T}{d_k^T y_k} + \frac{d_k d_k^T}{d_k^T d_k} \frac{d_k^T y_k}{d_k^T y_k} + \frac{2 \|y_k\|^2}{(d_k^T y_k)^2} + \left( 2\alpha_k - \frac{d_k^T y_k}{d_k^T d_k} - \frac{y_k^T y_k}{d_k^T y_k} \right) d_k d_k^T \]

Therefore, a direct computation shows \( Q_{k+1}^* y_k = v_k \) hence \( Q_{k+1}^* \) is symmetric and satisfy QN condition, it remains to show that \( Q^* \) is positive definite or equivalent the search directions generated by:

\[ d_{k+1} = -Q^* g_{k+1} \]

are decent directions for all \( k \). Now, our direction can be written as:

\[ d_{k+1} = -(I - \frac{d_k y_k^T + y_k d_k^T}{d_k^T y_k} + \frac{d_k d_k^T}{d_k^T d_k} \frac{d_k^T y_k}{d_k^T y_k} + \frac{2 \|y_k\|^2}{(d_k^T y_k)^2} + \left( 2\alpha_k - \frac{d_k^T y_k}{d_k^T d_k} - \frac{y_k^T y_k}{d_k^T y_k} \right) d_k d_k^T ) g_{k+1} \]

We call eq. (16) a new three-term conjugate gradient method. So we can write the direction of the new three-term method as follows:

\[ d_{k+1} = \begin{cases} -g_{k+1} & \text{for } k = 0 \\ -g_{k+1} + \frac{d_k^T g_{k+1}}{d_k^T y_k} y_k + \frac{1}{d_k^T y_k} (y_k^T g_{k+1} - s_k^T g_{k+1} - \|y_k\|^2 d_k^T g_{k+1}) d_k & \text{for } k \geq 1 \end{cases} \]

Note: Abbo has proposed formula which is nearly similar to (17). For more details See [1].

3.1 New Algorithm

Step 2. if \( \|g_k\| < 0 \), then stop.

Step 3. Compute \( d_k \) using (17).

Step 4. Find the step length \( \alpha_k \) satisfying (6) (7) set \( x_{k+1} = x_k + \alpha_k d_k \).

Step 5. Set \( k = k + 1 \), go to step 2.

4. Descent Property of the New Algorithm

The search directions generated by (17) are descent for all \( k \) if the step size satisfies Wolfe conditions.

Proof: Let \( d_k = -g_k \), for \( k \geq 1 \) assume \( d_k g_k < 0 \), then for \( k = k + 1 \) we have:

\[ d_{k+1} = -g_{k+1} + \frac{d_k^T g_{k+1} y_k}{d_k^T y_k} + \frac{1}{d_k^T y_k} (y_k^T g_{k+1} - \alpha_k d_k^T g_{k+1} - \|y_k\|^2 d_k^T g_{k+1}) d_k \]

\[ d_{k+1} = \frac{1}{d_k^T y_k} \left( -(d_k^T y_k)^2 g_{k+1} + (d_k y_k)^2 y_k + d_k^T y_k y_k^T g_{k+1} - \alpha_k d_k^T g_{k+1} - \|y_k\|^2 d_k^T g_{k+1} \right) d_k \]

\[ \therefore d_{k+1}^T g_{k+1} = \frac{1}{d_k^T y_k} \left( -(d_k^T y_k)^2 g_{k+1} + (d_k y_k)^2 y_k + d_k^T y_k y_k^T g_{k+1} - \alpha_k d_k^T g_{k+1} - \|y_k\|^2 d_k^T g_{k+1} \right) \]

\[ + (d_k^T y_k)^2 (y_k^T g_{k+1} - \alpha_k d_k^T g_{k+1}) (d_k^T g_{k+1}) - \alpha_k d_k^T y_k (d_k^T g_{k+1})^2 - y_k^T y_k (d_k^T g_{k+1})^2 \]
New Three–Term CG-Method for Unconstrained Optimization

\[ \therefore d_{k+1}^T g_{k+1} = \frac{1}{(d_k^T y_k)^2} \left\{ -(d_k^T y_k)^2 g_{k+1}^T g_{k+1} + 2(d_k^T y_k)(d_k^T g_{k+1}) (y_k^T g_{k+1}) \right\} \]

\[ \therefore - (d_k^T y_k)(d_k^T g_{k+1})^2 - (y_k^T y_k)(d_k^T g_{k+1})^2 \]

Now

\[ (d_k^T y_k)(d_k^T g_{k+1}) (y_k^T g_{k+1}) = (d_k^T y_k)(d_k^T g_{k+1})^T (y_k^T g_{k+1}) \]

Let \( u=(d_k^T y_k)g_{k+1} \), \( v=(d_k^T g_{k+1})y_k \) then

\[ u^T v \leq \frac{1}{2} [u^T u + v^T v] \]

substitute in (18) we get

\[ \therefore d_{k+1}^T g_{k+1} \leq \frac{1}{(d_k^T y_k)^2} \left\{ -(d_k^T y_k)^2 g_{k+1}^T g_{k+1} + 2 \left( \frac{1}{2} \right) (d_k^T y_k)^2 g_{k+1}^T g_{k+1} + (d_k^T g_{k+1})^2 (y_k^T y_k) \right\} \]

\[ \therefore \alpha_k (d_k^T y_k)(d_k^T g_{k+1})^2 - (y_k^T y_k) \]

\[ \therefore d_{k+1}^T g_{k+1} \leq \frac{1}{(d_k^T y_k)^2} \left\{ -\alpha_k (d_k^T y_k)(d_k^T g_{k+1})^2 \right\} \]

\[ \therefore d_{k+1}^T g_{k+1} \leq \frac{1}{(d_k^T y_k)^2} \left\{ -\alpha_k (d_k^T g_{k+1}) \right\} \]

By Wolfe condition \( d_k^T y_k > 0 \), then \( d_{k+1} \) descent for all \( k \).

5. Numerical Result

Tables (1), (2), (3) and (4) are comparing between new algorithm and Zhang, Zhou and Li three–term conjugate gradient methods. The comparison involves some well-known test function with different dimensions(500, 1000, 5000, 10000). The program is written in double precision using Fortran(2000). The comparative Performance of the algorithm is evaluated by considering both the total number of function evaluations which is normally assumed to be the most costly factor in each iteration and the total number of iterations. The actual convergence criterion was \( \| g_k \| \leq 10^{-6} \). All these algorithms are implemented with the standard Wolfe line search conditions with \( \rho = 0.001 \), \( \sigma = 0.9 \). The results indicate that the new algorithm is more efficient.

Table(1) Numerical Comparisons between the New Method and Zhang, Zhou and Li Methods (N=500)

| TEST FUNCTION | New Method NOF(NOI) | ZFR NOF(NOI) | ZPR NOF(NOI) | ZHS NOF(NOI) |
|---------------|---------------------|--------------|--------------|--------------|
| 1-POWELL3     | 63(31)              | fail         | 42(20)       | 48 (22)      |
| 2-WOOD        | 70(31)              | 62(27)       | 67 (30)      | 63(28)       |
| 3-CUBIC       | 44(16)              | 45(16)       | 45(16)       | 44(16)       |
| 4-SHALLOW     | 25 (10)             | 25(10)       | 25 (10)      | 25 (10)      |
| 5-SUM         | 117(24)             | 139(24)      | 136(25)      | 107(20)      |
| 6-BELL        | 27(11)              | 27 (11)      | 27 (11)      | 29 (12)      |
| 7-ROSEN       | 38 (16)             | 76 (30)      | 76 (30)      | 76 (30)      |
| 8-RECIPE      | 18 (6)              | 18 (6)       | 18 (6)       | 18 (6)       |
| 9-HELCIAL     | 71 (32)             | 81 (39)      | 68 (32)      | 66 (31)      |
| 10-CANTREL    | 287 (33)            | 418 (49)     | 345 (39)     | 564(59)      |
Table(2) Numerical Comparisons between the New Method and Zhang, Zhou and Li Methods (N=1000)

| TEST FUNCTION | New Method NOF(NOI) | ZFR NOF(NOI) | ZPR OF(NOI) | ZHS NOF(NOI) |
|---------------|---------------------|--------------|-------------|--------------|
| 1-POWELL3     | 63(31)              | fail         | 42(20)      | 48 (22)      |
| 2-WOOD        | 70(31)              | 62 (27)      | 67 (30)     | 63 (28)      |
| 3-CUBIC       | 44(16)              | 45(16)       | 45 (16)     | 44 (16)      |
| 4-SHALLOW     | 25 (10)             | 25 (10)      | 25 (10)     | 25 (10)      |
| 5-SUM         | 119(21)             | 105(26)      | 105(26)     | 121(24)      |
| 6-BELL        | 27(11)              | 29 (12)      | 27 (11)     | 29 (12)      |
| 7-ROSEN       | 38 (16)             | 76 (30)      | 76 (30)     | 76 (30)      |
| 8-RECIP       | 18 (6)              | 18 (6)       | 18 (6)      | 18 (6)       |
| 9-HELICAL     | 71 (32)             | 81 (39)      | 68 (32)     | 66 (31)      |
| 10-CANTREL    | 287 (33)            | 433 (50)     | 345 (39)    | 564(59)      |

Table(3) Numerical Comparisons between the New Method and Zhang, Zhou and Li Methods(N=5000)

| TEST FUNCTION | New Method NOF(NOI) | ZFR NOF(NOI) | ZPR OF(NOI) | ZHS NOF(NOI) |
|---------------|---------------------|--------------|-------------|--------------|
| 1-POWELL3     | 63(31)              | fail         | 42(20)      | 48 (22)      |
| 2-WOOD        | 70(31)              | 62 (27)      | 67 (30)     | 63 (28)      |
| 3-CUBIC       | 44(16)              | 45(16)       | 45 (16)     | 44 (16)      |
| 4-SHALLOW     | 25 (10)             | 25 (10)      | 25 (10)     | 25 (10)      |
| 5-SUM         | 190(31)             | 149(33)      | 149(33)     | 170(33)      |
| 6-BELL        | 27(11)              | 29 (12)      | 27 (11)     | 29 (12)      |
| 7-ROSEN       | 38 (16)             | 76 (30)      | 76 (30)     | 76 (30)      |
| 8-RECIP       | 18 (6)              | 18 (6)       | 18 (6)      | 18 (6)       |
| 9-HELICAL     | 71 (32)             | 81 (39)      | 68 (32)     | 66 (31)      |
| 10-CANTREL    | 287 (33)            | 522 (55)     | 451 (45)    | 617(62)      |

Table(4) Numerical Comparisons between the New Method and Zhang, Zhou and Li Methods(N=10000)

| TEST FUNCTION | New Method NOF(NOI) | ZFR NOF(NOI) | ZPR OF(NOI) | ZHS NOF(NOI) |
|---------------|---------------------|--------------|-------------|--------------|
| 1-POWELL3     | 63(31)              | fail         | 42(20)      | 48 (22)      |
| 2-WOOD        | 70(31)              | 62 (27)      | 67 (30)     | 63 (28)      |
| 3-CUBIC       | 44(16)              | 45(16)       | 45 (16)     | 44 (16)      |
| 4-SHALLOW     | 25 (10)             | 25 (10)      | 25 (10)     | 25 (10)      |
| 5-SUM         | 190(31)             | 149(33)      | 149(33)     | 170(33)      |
| 6-BELL        | 27(11)              | 29 (12)      | 27 (11)     | 29 (12)      |
| 7-ROSEN       | 38 (16)             | 76 (30)      | 76 (30)     | 76 (30)      |
| 8-RECIP       | 18 (6)              | 18 (6)       | 18 (6)      | 18 (6)       |
| 9-HELICAL     | 71 (32)             | 81 (39)      | 68 (32)     | 66 (31)      |
| 10-CANTREL    | 287 (33)            | 522 (55)     | 451 (45)    | 617(62)      |
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