

A MODIFIED PROJECTED CONJUGATE GRADIENT ALGORITHM FOR UNCONSTRAINED OPTIMIZATION PROBLEMS

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Abstract

We propose a modified projected Polak–Ribière–Polyak (PRP) conjugate gradient method, where a modified conjugacy condition and a method which generates sufficient descent directions are incorporated into the construction of a suitable conjugacy parameter. It is shown that the proposed method is a modification of the PRP method and generates sufficient descent directions at each iteration. With an Armijo-type line search, the theory of global convergence is established under two weak assumptions. Numerical experiments are employed to test the efficiency of the algorithm in solving some benchmark test problems available in the literature. The numerical results obtained indicate that the algorithm outperforms an existing similar algorithm in requiring fewer function evaluations and fewer iterations to find optimal solutions with the same tolerance.

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1. Introduction

Since unconstrained optimization problems are fundamental optimization models in the fields of industrial engineering, management sciences and applied mathematics, it is important to design efficient algorithms to find optimal solutions of these problems, especially for large-scale problems. In this paper, we consider the following unconstrained optimization problem:

$$\min f(x), \quad x \in \mathbb{R}^n, \quad (1.1)$$

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is continuously differentiable. Let $g(x)$ denote the gradient of f at x , and x_0 an arbitrary initial approximate solution of (1.1). The well-known conjugate

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gradient method allows an iterative process to generate a solution sequence

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

where α_k is a step length obtained by line search and d_k is a direction determined by

$$d_k = \begin{cases} -g_k & \text{if } k = 0 \\ -g_k + \beta_k d_{k-1} & \text{if } k > 0, \end{cases} \quad (1.2)$$

where β_k is a parameter and g_k is an abbreviation of $g(x_k)$.

In (1.2), a different choice of the parameter β_k gives a class of conjugate gradient methods [3–7, 9, 10, 12, 13]. Amongst the popular conjugate gradient methods, it is noted that the Polak–Ribière–Polyak (PRP) method outperforms the others in numerical behaviour [4]. In this case, the parameter β_k is chosen as

$$\beta_k^{\text{PRP}} \triangleq \frac{g_k^T y_{k-1}}{\|g_{k-1}\|^2},$$

where $y_{k-1} = g_k - g_{k-1}$ and $\|\cdot\|$ is the Euclidean norm of a vector [9].

Zhang et al. [14] present a three-term PRP conjugate gradient method (MPRP). The search direction is determined by

$$d_k = \begin{cases} -g_k & \text{if } k = 0 \\ -g_k + \beta_k^{\text{PRP}} d_{k-1} - \theta_k y_{k-1} & \text{if } k > 0, \end{cases} \quad (1.3)$$

where

$$\theta_k = \frac{g_k^T d_{k-1}}{\|g_{k-1}\|^2}.$$

An attractive feature of this MPRP method is that for each k , independent of the line search used, d_k given by (1.3) satisfies

$$d_k^T g_k = -\|g_k\|^2. \quad (1.4)$$

As a result, d_k is always a sufficient descent direction of f at x_k . The MPRP method reduces to the standard PRP method if the line search is exact. Furthermore, under suitable conditions, the MPRP method proves to be globally convergent with a modified Armijo-type line search.

Recently, An et al. [1] provided another approach to construct a sufficient descent direction, where

$$d_k = -g_k + \lambda_k \left(I - \frac{g_k g_k^T}{\|g_k\|^2} \right) \bar{d}_k. \quad (1.5)$$

The second term in (1.5) is a projection of \bar{d}_k onto the orthogonal complementary subspace of the gradient. With any line search, the direction d_k obtained by (1.5) satisfies (1.4). If λ_k is chosen as a conjugate parameter in the Fletcher–Reeves

method [3] and \bar{d}_k is replaced by d_{k-1} , then the method (1.5) turns out to be the same as in the paper by Zhang et al. [15].

Based on a modified conjugacy condition,

$$d_k^T y_{k-1} = -t g_k^T s_{k-1} = -t \alpha_{k-1} g_k^T d_{k-1}, \quad (1.6)$$

where $s_{k-1} = x_k - x_{k-1}$ and $t \in [0, +\infty)$ is a constant scalar, Dai and Liao [2] present a new choice of conjugacy parameter, namely

$$\beta_k^{\text{DL}} \triangleq \frac{g_k^T (y_{k-1} - t s_{k-1})}{d_{k-1}^T y_{k-1}}. \quad (1.7)$$

It is easy to see that (1.7) can be viewed as a modification of the following Hestenes–Stiefel method [5]:

$$\beta_k^{\text{HS}} \triangleq \frac{g_k^T y_{k-1}}{d_{k-1}^T y_{k-1}}.$$

REMARK 1.1. With exact line search, owing to $g_k^T d_{k-1} = 0$, the modified conjugacy condition (1.6) reduces to the ordinary conjugacy condition $d_k^T y_{k-1} = 0$. However, in the case of inexact line search, (1.6) is not the ordinary conjugacy condition unless $t = 0$.

Motivated by the above observations, we present a new projected PRP conjugate gradient method, where the modified conjugacy condition (1.6) and the method (1.5) which generates sufficient descent directions are employed to construct a suitable conjugacy parameter β_k . It is shown that the proposed method is a modification of the PRP method and satisfies the sufficient descent condition (1.4) at each iteration. Under two mild assumptions, we establish the theory of global convergence of the proposed method with an Armijo-type line search. Numerical experiments are employed to test the efficiency of the algorithm in solving some benchmark test problems available in the literature.

The rest of the paper is organized as follows. On the basis of a suitable choice for the conjugacy parameter, the modified projected PRP conjugate gradient algorithm is developed in Section 2. Global convergence of the algorithm is established in Section 3. Numerical efficiency of the developed algorithm is reported in Section 4.

2. A modified projected PRP conjugate gradient algorithm

In this section we design a modified projected PRP conjugate gradient algorithm with sufficient descent search direction at each iteration. We begin with the determination of the search direction. If in (1.5) we take $\lambda_k = \beta_k^{\text{DL}}$ and $\bar{d}_k = d_{k-1}$, then for any $k \geq 0$, the search direction at the current iterate point x_k is given by

$$d_k = \begin{cases} -g_k & \text{if } k = 0 \\ -g_k + \frac{g_k^T (y_{k-1} - t s_{k-1})}{d_{k-1}^T y_{k-1}} \left(I - \frac{g_k g_k^T}{\|g_k\|^2} \right) d_{k-1} & \text{if } k > 0. \end{cases} \quad (2.1)$$

It is easy to prove the following result.

PROPOSITION 2.1. *Let d_k be defined by equation (2.1). Then for any $k \geq 0$, d_k satisfies condition (1.4).*

From Proposition 2.1, it follows that

$$d_{k-1}^T y_{k-1} = g_k^T d_{k-1} - g_{k-1}^T d_{k-1} = g_k^T d_{k-1} + \|g_{k-1}\|^2. \tag{2.2}$$

In the case of exact line search, the first term on the right-hand side of (2.2) is zero, that is, $g_k^T d_{k-1} = 0$. Similar to the idea in the paper by Dai and Liao [2], if the line search is inexact we introduce a parameter $t \in [0, 1)$ such that (2.2) is modified as

$$d_{k-1}^T y_{k-1} = \|g_{k-1}\|^2 + t g_k^T d_{k-1}. \tag{2.3}$$

With $d_{k-1}^T y_{k-1}$ being replaced by the right-hand side of (2.3), the search direction (2.1) is transformed into

$$\begin{aligned} d_k &= -g_k + \frac{g_k^T (y_{k-1} - t s_{k-1})}{\|g_{k-1}\|^2 + t g_k^T d_{k-1}} \left(I - \frac{g_k g_k^T}{\|g_k\|^2} \right) d_{k-1} \\ &= -g_k + \frac{g_k^T (y_{k-1} - t s_{k-1})}{\|g_{k-1}\|^2 + t g_k^T d_{k-1}} d_{k-1} - \frac{g_k^T (y_{k-1} - t s_{k-1})}{\|g_{k-1}\|^2 + t g_k^T d_{k-1}} \frac{g_k^T d_{k-1}}{\|g_k\|^2} g_k. \end{aligned} \tag{2.4}$$

For the sake of global convergence, we further modify (2.4) as

$$d_k = \begin{cases} -g_k & \text{if } k = 0 \\ -g_k + \theta_k^{(1)} d_{k-1} - \theta_k^{(1)} \theta_k^{(3)} g_k & \text{if } k > 0 \text{ and } y_{k-1}^T d_{k-1} \geq 0 \\ -g_k + \theta_k^{(2)} d_{k-1} - \theta_k^{(2)} \theta_k^{(3)} g_k & \text{if } k > 0 \text{ and } y_{k-1}^T d_{k-1} < 0, \end{cases} \tag{2.5}$$

where

$$\theta_k^{(1)} = \frac{g_k^T (y_{k-1} - t s_{k-1})}{\|g_{k-1}\|^2 + t g_k^T d_{k-1}}, \quad \theta_k^{(2)} = \frac{g_k^T (y_{k-1} - t s_{k-1})}{\|g_{k-1}\|^2}, \quad \theta_k^{(3)} = \frac{g_k^T d_{k-1}}{\|g_k\|^2},$$

and $t \in [0, 1)$ is a constant.

The following result is clear.

PROPOSITION 2.2. *Let d_k be defined by equation (2.5). Then for any $k \geq 0$, d_k satisfies condition (1.4).*

REMARK 2.3. If the line search is exact, then d_k defined by (2.5) is a search direction obtained in the standard PRP conjugate gradient method. Thus (2.5) is a modification of the PRP conjugate gradient method obtained by incorporating the advantages of the methods in the papers by An et al. [1] and Dai and Liao [2] into the choice of parameters.

Next we state the choice of step length along the direction d_k . We adopt the line search rule proposed by Zhang et al. [14]. We choose a step length $\alpha_k = \max\{\rho^j : j = 0, 1, 2, \dots\}$ such that the following inequality holds:

$$f(x_k + \alpha_k d_k) \leq f(x_k) - \delta \alpha_k^2 \|d_k\|^2, \quad (2.6)$$

where $\delta \in (0, 1)$ is a given constant scalar. In view of existing numerical results [10–12, 14], we choose an initial step length which is conducive to the improvement of numerical performance for the algorithm developed in this paper. Set

$$z_k := \frac{g(x_k + \varepsilon_0 d_k) - g(x_k)}{\varepsilon_0}, \quad t_k := \left| \frac{g_k^T d_k}{d_k^T z_k} \right|,$$

where $\varepsilon_0 > 0$ is a given small constant. For any $k \geq 0$, the initial step length at the k th iteration is given by

$$\alpha_k^{(0)} = \begin{cases} t_k & \text{if } |d_k^T z_k| > 0 \text{ and } f(x_k + t_k d_k) < f(x_k) - \delta \|t_k d_k\|^2 \\ 1 & \text{otherwise.} \end{cases} \quad (2.7)$$

Consequently, a modified line search rule is to find a step length

$$\alpha_k = \max\{\alpha_k^{(0)} \rho^j : j = 0, 1, 2, \dots\}$$

such that (2.6) holds.

Similar to the proof of Proposition 2.3 in the paper by Jiang et al. [6], we obtain the following result.

PROPOSITION 2.4. *Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a continuously differentiable function and d_k be defined by (2.5). Then there exists a nonnegative integer j_0 such that $\alpha_k = \alpha_k^{(0)} \rho^{j_0}$ satisfies inequality (2.6).*

With the above preparations, we are now in a position to develop a new projected PRP conjugate gradient algorithm.

ALGORITHM 2.5 (Modified projected PRP conjugate gradient algorithm).

Step 0. Choose $\varepsilon, \varepsilon_0, \rho, \delta \in (0, 1), t \in [0, 1)$. Choose an initial point $x_0 \in \mathbb{R}^n$. Set $k := 0$.

Step 1. If $\|g_k\| < \varepsilon$, the algorithm stops. Otherwise, go to Step 2.

Step 2. Compute d_k from (2.5).

Step 3. Find a step size α_k from (2.6) and (2.7).

Step 4. Set $x_{k+1} := x_k + \alpha_k d_k$. Set $k := k + 1$, and go to Step 1.

REMARK 2.6. From (2.5) and Propositions 2.2 and 2.4, we know that Algorithm 2.5, which we call MPPRP for short, is well defined.

REMARK 2.7. Let $\{x_k\}$ be the sequence of approximate solutions generated by Algorithm 2.5. Then from (2.6), it follows that the sequence $\{f(x_k)\}$ is decreasing as $k \rightarrow +\infty$, and

$$\sum_{k=0}^{\infty} \alpha_k^2 \|d_k\|^2 < \infty$$

if f is bounded from below. Therefore, we conclude that

$$\lim_{k \rightarrow \infty} \alpha_k \|d_k\| = 0. \quad (2.8)$$

3. Global convergence

In this section we study the global convergence of Algorithm 2.5. We state some blanket assumptions to prove global convergence for all variants of conjugate gradient methods.

ASSUMPTION 3.1. The level set $\Omega = \{x \in R^n : f(x) \leq f(x_0)\}$ is bounded.

ASSUMPTION 3.2. In some neighbourhood N of Ω , f is continuously differentiable and its gradient is Lipschitz continuous, namely, there exists a constant $L > 0$ such that

$$\|g(x) - g(y)\| \leq L\|x - y\| \quad \text{for all } x, y \in N. \quad (3.1)$$

REMARK 3.3. Since the sequence $\{f(x_k)\}$ generated by Algorithm 2.5 is decreasing, Assumption 3.1 implies that the sequence $\{x_k\}$ is contained in the closed and bounded level set Ω . Thus, there exists a convergent subsequence of $\{x_k\}$. Without loss of generality, we suppose that $\{x_k\}$ is convergent. On the other hand, from Assumption 3.2, there is a constant $\gamma_1 > 0$ such that

$$\|g(x)\| \leq \gamma_1 \quad \text{for all } x \in \Omega. \quad (3.2)$$

Before stating the main result of the paper, we prove the following lemma.

LEMMA 3.4. Under Assumptions 3.1 and 3.2, if there is a constant $\varepsilon > 0$ such that

$$\|g_k\| \geq \varepsilon \quad \text{for all } k, \quad (3.3)$$

then there exists a constant $M > 0$ such that

$$\|d_k\| \leq M \quad \text{for all } k. \quad (3.4)$$

PROOF. Since

$$tg_k^T d_{k-1} = t(g_k^T - g_{k-1}^T)d_{k-1} + tg_{k-1}^T d_{k-1} = ty_{k-1}^T d_{k-1} - t\|g_{k-1}\|^2,$$

we obtain $y_{k-1}^T d_{k-1} \geq 0$ from Step 2 of Algorithm 2.5. Thus

$$\|g_{k-1}\|^2 + tg_k^T d_{k-1} = (1-t)\|g_{k-1}\|^2 + ty_{k-1}^T d_{k-1} \geq (1-t)\varepsilon^2 > 0. \quad (3.5)$$

In view of (3.3), it follows from (3.5) that

$$\min\{\|g_{k-1}\|^2, \|g_{k-1}\|^2 + tg_k^T d_{k-1}\} \geq (1 - t)\varepsilon^2. \tag{3.6}$$

From (3.1)–(3.3), (3.6) and the definition of d_k ,

$$\begin{aligned} \|d_k\| &\leq \|g_k\| + 2 \frac{\|g_k\| \|y_{k-1}\| + t\|g_k\| \|s_{k-1}\|}{\min\{\|g_{k-1}\|^2, \|g_{k-1}\|^2 - tg_k^T d_{k-1}\}} \|d_{k-1}\| \\ &\leq \gamma_1 + \frac{2\gamma_1\alpha_{k-1}(L + t)\|d_{k-1}\|}{(1 - t)\varepsilon^2} \|d_{k-1}\|. \end{aligned} \tag{3.7}$$

On the other hand, since $\alpha_k d_k \rightarrow 0$ as $k \rightarrow +\infty$, there exists a constant $r \in (0, 1)$ and a positive integer k_0 such that for each $k \geq k_0$, the following inequality holds:

$$\frac{2\gamma_1\alpha_{k-1}(L + t)\|d_{k-1}\|}{(1 - t)\varepsilon^2} \leq r. \tag{3.8}$$

Combining (3.7) and (3.8),

$$\begin{aligned} \|d_k\| &\leq \gamma_1 + r\|d_{k-1}\| \\ &\leq \gamma_1(1 + r + r^2 + \dots + r^{k-k_0-1}) + r^{k-k_0}\|d_{k_0}\| \\ &\leq \frac{\gamma_1}{1 - r} + \|d_{k_0}\|. \end{aligned} \tag{3.9}$$

Denote

$$M = \max\left\{\|d_1\|, \|d_2\|, \dots, \|d_{k_0}\|, \frac{\gamma_1}{1 - r} + \|d_{k_0}\|\right\}.$$

Then (3.4) is directly obtained from (3.9). □

Lemma 3.4 is used to prove the following main theorem.

THEOREM 3.5. *Let $\{g_k\}$ be the sequence generated by Algorithm 2.5. Under Assumptions 3.1 and 3.2,*

$$\liminf_{k \rightarrow \infty} \|g_k\| = 0.$$

PROOF. The proof is by contradiction. Assume that there exists a constant $\varepsilon > 0$ such that

$$\|g_k\| \geq \varepsilon \quad \text{for all } k. \tag{3.10}$$

If $\liminf_{k \rightarrow \infty} \alpha_k > 0$, we obtain from (1.4) and (2.8) that $\liminf_{k \rightarrow \infty} \|g_k\| = 0$. This contradicts (3.10). Suppose that $\liminf_{k \rightarrow \infty} \alpha_k = 0$. This says that there is an infinite index set K such that

$$\lim_{k \in K, k \rightarrow \infty} \alpha_k = 0.$$

Then, from Step 3 of Algorithm 2.5, it follows that for $k \in K$ large enough, $\rho^{-1}\alpha_k$ does not satisfy (2.6). This yields

$$f(x_k + \rho^{-1}\alpha_k d_k) - f(x_k) \geq -\delta\rho^{-2}\alpha_k^2\|d_k\|^2. \tag{3.11}$$

From Lemma 3.4, (3.1) and (1.4), there exists $h_k \in (0, 1)$ such that

$$\begin{aligned} f(x_k + \rho^{-1}\alpha_k d_k) - f(x_k) &= \rho^{-1}\alpha_k g(x_k + h_k \rho^{-1}\alpha_k d_k)^T d_k \\ &= \rho^{-1}\alpha_k g_k^T d_k + \rho^{-1}\alpha_k (g(x_k + h_k \rho^{-1}\alpha_k d_k) - g_k)^T d_k \\ &\leq \rho^{-1}\alpha_k g_k^T d_k + L\rho^{-2}\alpha_k^2 \|d_k\|^2, \end{aligned} \quad (3.12)$$

where $L > 0$ is the Lipschitz constant of g . Substituting the last inequality in (3.12) into (3.11), we conclude that for all $k \in K$ large enough, the following inequality holds:

$$\|g_k\|^2 \leq \rho^{-1}(L + \delta)\alpha_k \|d_k\|^2. \quad (3.13)$$

Since $\{d_k\}$ is bounded and $\lim_{k \in K, k \rightarrow \infty} \alpha_k = 0$, it follows from (3.13) that

$$\lim_{k \in K, k \rightarrow \infty} \|g_k\| = 0.$$

This also yields a contradiction. Thus, the desired conclusion is obtained. \square

4. Numerical experiments

In this section, we test the numerical efficiency of Algorithm 2.5 by applying it to solve some benchmark problems available in the literature. All test problems are from the paper by Moré et al. [8]. Their dimensions vary from 2 to 10 000. The numerical efficiency of the algorithm developed in this paper is compared with a similar algorithm available in the literature, the MPRP method presented by Zhang et al. [14], where an Armijo-type line search is employed.

To determine the effect of the parameter t on the numerical performance of our MPPRP algorithm, we implement Algorithm 2.5 with different values of t , namely 0, 0.2, 0.4, 0.6 and 0.8. All code was written in MATLAB R2009a, and implemented on a PC with 2.20 GHz CPU processor, 1.75 GB of RAM and the Windows XP operating system. The relevant algorithmic parameters are as follows. In MPPRP and MPRP,

$$\varepsilon = 10^{-6}, \quad \varepsilon_0 = 10^{-8}, \quad \delta = 10^{-4}, \quad \rho = 0.5.$$

The numerical results are reported in Table 1, where the ‘‘Fn.’’ column lists the test optimization problems from the paper by Moré et al. [8] (only the problem number is shown for simplicity); ‘‘Dim.’’ is the dimension of the problem; ‘‘MPRP’’ is the modified PRP conjugate gradient method from the paper by Zhang et al. [14]; $t = 0, 0.2, 0.4, 0.6, 0.8$ are values of t for the new algorithm proposed in this paper; and \cdot/\cdot is the number of iterations/the number of function evaluations. We see that:

- (i) The numerical performance of Algorithm 2.5 depends on the value of t . For some test problems such as P22, a suitable choice of t may greatly improve the efficiency of algorithm. This shows the importance of introducing the parameter t .
- (ii) Algorithm 2.5 outperforms the similar method proposed by Zhang et al. [14] by suitable choice of t . In 13 out of the 17 problems, Algorithm 2.5 required fewer iterations and fewer function evaluations to find optimal solutions than the MPRP method when $t = 0.4$.

TABLE 1. Numerical results of algorithms.

Fn.	Dim.	MPRP	$t = 0$	$t = 0.2$	$t = 0.4$	$t = 0.6$	$t = 0.8$
P1	2	31/82	30/72	34/95	29/71	33/77	30/78
P2	2	10/20	11/22	10/20	11/22	10/20	11/22
P4	2	17/87	16/120	16/58	13/26	13/26	17/34
P5	2	12/24	13/26	13/26	12/24	11/22	14/28
P14	4	349/779	140/338	162/393	140/328	177/438	200/488
P15	4	289/578	55/110	322/646	190/380	175/350	82/164
P24	4	127/268	131/272	99/207	83/172	582/1209	73/158
P28	6	25/50	22/44	23/46	23/46	22/44	22/44
P26	100	62/125	61/123	56/113	56/112	63/126	60/122
P26	1000	84/186	74/154	63/127	60/121	67/136	65/135
P22	100	3058/6116	3664/7328	1666/3353	3038/6076	3011/6022	1512/3039
P22	1000	4772/9544	5302/10604	4803/9612	4652/9304	4685/9370	2525/5056
P30	100	30/60	31/62	31/62	30/60	30/60	30/60
P30	1000	34/68	34/68	34/68	34/68	34/68	34/68
P21	100	31/80	29/70	34/95	29/71	31/73	30/77
P21	1000	32/83	29/70	34/95	29/71	31/73	32/81
P21	10000	35/88	29/70	34/95	30/73	31/73	32/81

5. Conclusion

We have presented a modified projected PRP conjugate gradient method for solving unconstrained minimization problems. Global convergence of the developed algorithm has been established with an Armijo-type line search. The algorithm outperforms a similar existing algorithm in that it requires fewer function evaluations and fewer iterations to find an optimal solution with the same tolerance.

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