

A Nonlinear Conjugate Gradient Algorithm with An Optimal Property and An Improved Wolfe Line Search*

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Abstract

In this paper, we seek the conjugate gradient direction closest to the direction of the scaled memoryless BFGS method and propose a family of conjugate gradient methods for unconstrained optimization. An improved Wolfe line search is also proposed, which can avoid a numerical drawback of the Wolfe line search and guarantee the global convergence of the conjugate gradient method under mild conditions. To accelerate the algorithm, we develop an adaptive strategy to choose the initial stepsize and introduce dynamic restarts along negative gradients based on how the function is close to some quadratic function during some previous iterations. Numerical experiments with the CUTER collection show that the proposed algorithm is promising.

Key words: conjugate gradient method, memoryless BFGS method, unconstrained optimization, global convergence, Wolfe line search.

1 Introduction

Consider the unconstrained optimization problem

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

where f is smooth and its gradient g is available. More exactly, we assume that f satisfies

Assumption 1.1. (i) f is bounded below; namely, $f(x) > -\infty$ for all $x \in \mathcal{R}^n$; (ii) f is differentiable and its gradient g is Lipschitz continuous; namely, there exists a constant $L > 0$ such that

$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\| \quad \text{for any } x, y \in \mathcal{R}^n, \quad (1.2)$$

where $\|\cdot\|$ stands for the Euclidean norm.

Conjugate gradient methods are very useful for solving (1.1), especially if its dimension n is large. They are of the form

$$x_{k+1} = x_k + \alpha_k d_k, \quad (1.3)$$

*This work was partially supported by the NSFC grant 10831006 and the CAS grant kjcx-yw-s7.

where the stepsize $\alpha_k > 0$ is obtained by some line search. The next search direction d_{k+1} ($k \geq 1$) is generated by

$$d_{k+1} = -g_{k+1} + \beta_k d_k, \quad (1.4)$$

where $g_{k+1} = -\nabla f(x_{k+1})$ and $d_1 = -g_1$. The scalar $\beta_k \in \mathcal{R}$ is so chosen that (1.3)-(1.4) reduces to the linear conjugate gradient method if f is a strictly convex quadratic function and if α_k is the exact one-dimensional minimizer. For general nonlinear functions, different choices of β_k lead to different conjugate gradient methods. Well-known formulae for β_k are called the Fletcher-Reeves (FR), Hestenes-Stiefel (HS), Polak-Ribière-Polyak (PRP) and Dai-Yuan (DY) formulae (see [14]; [20]; [29], [30] and [8], respectively), and are given by

$$\begin{aligned} \beta_k^{FR} &= \frac{\|g_{k+1}\|^2}{\|g_k\|^2}, & \beta_k^{HS} &= \frac{g_{k+1}^T y_k}{d_k^T y_k}, \\ \beta_k^{PRP} &= \frac{g_{k+1}^T y_k}{\|g_k\|^2}, & \beta_k^{DY} &= \frac{\|g_{k+1}\|^2}{d_k^T y_k}, \end{aligned}$$

where $y_k = g_{k+1} - g_k$.

Recent efforts have been made to relate the nonlinear conjugate gradient method to modified conjugacy conditions. Specifically, Dai and Liao [7] considered the following conjugacy condition

$$d_{k+1}^T y_k = -t g_{k+1}^T s_k, \quad (1.5)$$

where $s_k = \alpha_k d_k = x_{k+1} - x_k$ and t is some parameter, and derived a new formula for β_k

$$\beta_k^{DL}(t) = \frac{g_{k+1}^T y_k}{d_k^T y_k} - t \frac{g_{k+1}^T s_k}{d_k^T y_k}. \quad (1.6)$$

If f is a convex quadratic function and $g_{k+1}^T s_k \neq 0$, it was shown in [7] that a one-dimensional minimizer along the corresponding direction of (1.6) with a small $t > 0$ will lead to a bigger descent than that brought with $t = 0$. Due to the existence of the parameter t , it would be more suitable to call the methods (1.3), (1.4) and (1.6) by Dai-Liao family of conjugate gradient methods (one can see [4] and the references therein for more families of conjugate gradient methods). Further, Dai and Liao [7] considered the following truncated form of (1.6),

$$\beta_k^{DL+}(t) = \max \left\{ \frac{g_{k+1}^T y_k}{d_k^T y_k}, 0 \right\} - t \frac{g_{k+1}^T s_k}{d_k^T y_k}. \quad (1.7)$$

Despite of possible negative values of β_k^{DL+} , we still use the sign $+$ to symbolize *truncation* in order to remember the truncation introduced by Powell [33] and analyzed by Gilbert and Nocedal [15] for the PRP method (they considered $\beta_k^{PRP+} = \max\{\beta_k^{PRP}, 0\}$).

Hager and Zhang [17] paid attention to the self-scaling memoryless BFGS method by Perry [28] and Shanno [34] and proposed the formula

$$\beta_k^N = \frac{g_{k+1}^T y_k}{d_k^T y_k} - 2 \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k}, \quad (1.8)$$

which can be regarded as (1.6) with $t = \frac{2\|y_k\|^2}{s_k^T y_k}$. Interestingly enough, they were able to establish for their method the sufficient descent condition

$$-g_k^T d_k \geq \frac{7}{8} \|g_k\|^2, \quad \forall k \geq 1, \quad (1.9)$$

provided that $d_k^T y_k \neq 0$. To establish global convergence for general nonlinear functions, they considered the following truncated form

$$\bar{\beta}_k^N = \max \left\{ \beta_k^N, \frac{-1}{\|d_k\| \min\{\eta, \|g_k\|\}} \right\}, \quad (1.10)$$

where $\eta > 0$ is a constant. A fortran code, called `cg_descent`, was also built based on the formula (1.10) and the so-called approximate Wolfe line search (see [18]). In a survey paper [19], the authors introduced a parameter θ_k in (1.8), yielding

$$\beta_k^{HZ}(\theta_k) = \frac{g_{k+1}^T y_k}{d_k^T y_k} - \theta_k \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} \quad (1.11)$$

(see the relation (7.1) in [19]). Due to the existence of the parameter θ_k , it would be more convenient to call the methods (1.3), (1.4) and (1.11) by Hager-Zhang family of conjugate gradient methods. It is obvious that β_k^N is corresponding to $\beta_k^{HZ}(\theta_k)$ with $\theta_k \equiv 2$. No any other special choices of θ_k were suggested and tested in [19].

More recent advances can be found in Yabe and Takano [39] and Li *et al.* [21], who studied conjugate gradient methods based on two variants of the conjugacy condition (1.5); namely, by replacing y_k with more efficient vectors. Some generalizations of the Hager-Zhang family (1.11) were provided by Yu *et al.* [40, 41]. The works by Cheng and Liu [3] and Zhang *et al.* [42] investigated new conjugate gradient methods that can ensure the sufficient descent property, namely, $-g_k^T d_k \geq c\|g_k\|^2$ for some constant $c > 0$ and all $k \geq 1$. More recent reviews on nonlinear conjugate gradient methods can be found in Dai [5] and Hager and Zhang [19].

One main contribution of this paper is to seek the conjugate gradient direction that is closest to the direction of the scaled memoryless BFGS method, providing the following family of conjugate gradient methods for unconstrained optimization

$$\beta_k(\tau_k) = \frac{g_{k+1}^T y_k}{d_k^T y_k} - \left(\tau_k + \frac{\|y_k\|^2}{s_k^T y_k} - \frac{s_k^T y_k}{\|s_k\|^2} \right) \frac{g_{k+1}^T s_k}{d_k^T y_k}, \quad (1.12)$$

where τ_k is a parameter corresponding to the scaling parameter in the scaled memoryless BFGS method. Among many others, four different choices of τ_k are analyzed and tested with the following truncation,

$$\beta_k^+(\tau_k) = \max \left\{ \beta_k(\tau_k), \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \right\}, \quad (1.13)$$

where $\eta \in [0, 1)$ is some parameter. We found that the most efficient choice is corresponding to

$$\tau_k = \frac{s_k^T y_k}{\|s_k\|^2}, \quad (1.14)$$

which was dated back to Oren and Luenberger [25, 26]. Surprisingly enough, in this case, substituting (1.14) into (1.12) gives the following very simple formula,

$$\beta_k = \frac{g_{k+1}^T y_k}{d_k^T y_k} - \frac{\|y_k\|^2}{s_k^T y_k} \frac{g_{k+1}^T s_k}{d_k^T y_k}, \quad (1.15)$$

which is corresponding to the Dai-Liao family of methods (1.6) with $t = \frac{\|y_k\|^2}{s_k^T y_k}$. It is also a special member of the Hager-Zhang family of methods (1.11) with $\theta_k \equiv 1$. More efficient choices of τ_k in (2.12) still remains under investigation.

The rest of this paper is organized as follows. In the next section, we will seek the conjugate gradient direction that is closest to the direction of the scaled memoryless BFGS method and propose a family of conjugate gradient methods for unconstrained optimization. In Section 3, we discuss how to choose the stepsize α_k in (1.3). This is also an important issue in nonlinear conjugate gradient methods. Specifically, we will provide an adaptive strategy for the choice of the initial stepsize (see Algorithm 3.1) and develop an improved Wolfe line search (see (3.8) and (3.6), or Algorithm 3.2). In Section 4, we will present our conjugate gradient algorithm, Algorithm 4.1, which is combined with dynamic restarts. Meanwhile, global convergence results of the algorithm with or without restarts are established under the improved Wolfe line search. In Section 5, we compare the Dolan-Moré [11] performance profile of the new algorithm with `cg_descent` by Hager and Zhang [18] and test the efficiency of the new restart technique using the unconstrained optimization problems from the CUTer collection. Conclusions and discussions are made in the last section.

2 A New Family of Conjugate Gradient Methods

The aim of this section is to derive a new family of conjugate gradient methods from the self-scaling memoryless BFGS method by Perry [28] and Shanno [34], which defines the search direction by

$$d_{k+1} = -H_{k+1} g_{k+1}, \quad (2.1)$$

where

$$H_{k+1} = \frac{1}{\tau_k} \left(I - \frac{s_k y_k^T + y_k s_k^T}{s_k^T y_k} \right) + \left(1 + \frac{1}{\tau_k} \frac{\|y_k\|^2}{s_k^T y_k} \right) \frac{s_k s_k^T}{s_k^T y_k}, \quad (2.2)$$

where τ_k is a scaling parameter. The approximation matrix H_{k+1} can be regarded to obtain from a scaled identity matrix $\frac{1}{\tau_k} I$ by the BFGS updating formula. Substituting (2.2) into (2.1) leads to the search direction with a multiplier difference

$$d_{k+1}^{PS} = -g_{k+1} + \left[\frac{g_{k+1}^T y_k}{s_k^T y_k} - \left(\tau_k + \frac{\|y_k\|^2}{s_k^T y_k} \right) \frac{g_{k+1}^T s_k}{s_k^T y_k} \right] s_k + \frac{g_{k+1}^T s_k}{s_k^T y_k} y_k. \quad (2.3)$$

Noting that $s_k = \alpha_k d_k$, the simple deletion of the last term in (2.3) leads to the conjugate gradient method

$$d_{k+1}^D = -g_{k+1} + \beta_k^D(\tau_k) d_k, \quad (2.4)$$

where

$$\beta_k^D(\tau_k) = \frac{g_{k+1}^T y_k}{d_k^T y_k} - \left(\tau_k + \frac{\|y_k\|^2}{s_k^T y_k} \right) \frac{g_{k+1}^T s_k}{d_k^T y_k}. \quad (2.5)$$

Particularly, if τ_k is chosen to be the value suggested by Oren and Spedicato [26],

$$\tau_k^H = \frac{\|y_k\|^2}{s_k^T y_k}, \quad (2.6)$$

the formula (2.5) reduces to (1.8), which is provided by Hager and Zhang [17].

We are interested in more efficient conjugate gradient variants arising from (2.3) based on the following two observations. Firstly, there are more efficient ways to choose the scaling parameter

τ_k . Oren and Luenberger [25, 26] proposed the scaling parameter $\frac{s_k^T y_k}{s_k^T B_k s_k}$ with $B_k = H_k^{-1}$ for the Broyden's family of quasi-Newton methods. If H_k is the identity matrix, this choice reduces to

$$\tau_k^B = \frac{s_k^T y_k}{\|s_k\|^2}. \quad (2.7)$$

Al-Baali [1] suggested to choose

$$\bar{\tau}_k^H = \min \left\{ 1, \frac{\|y_k\|^2}{s_k^T y_k} \right\} \quad \text{and} \quad \bar{\tau}_k^B = \min \left\{ 1, \frac{s_k^T y_k}{\|s_k\|^2} \right\}. \quad (2.8)$$

For more choices on scalar τ_k , we refer readers to [1, 25, 26, 27] and the references therein.

Secondly, there is a more reasonable way to deal with the last term in (2.3) instead of simple deletion. Specifically, denoting the one-dimensional manifold

$$\mathcal{S}_{k+1} = \{-g_{k+1} + \beta d_k : \beta \in \mathcal{R}\}, \quad (2.9)$$

we can choose the vector in \mathcal{S}_{k+1} closest to d_{k+1}^{ML} in (2.3) as the next search direction; namely,

$$d_{k+1}^P = \arg \min \{ \|d - d_{k+1}^{ML}\|_2 : d \in \mathcal{S}_{k+1} \}. \quad (2.10)$$

Noting that the value $\zeta = \frac{d_k^T y_k}{\|d_k\|^2}$ minimizes $\|y_k - \zeta d_k\|$ for $\zeta \in \mathcal{R}$, we can deduce that the search direction in (2.10) is equivalent to

$$d_{k+1}^P = -g_{k+1} + \beta_k(\tau_k) d_k, \quad (2.11)$$

where

$$\beta_k(\tau_k) = \frac{g_{k+1}^T y_k}{d_k^T y_k} - \left(\tau_k + \frac{\|y_k\|^2}{s_k^T y_k} - \frac{s_k^T y_k}{\|s_k\|^2} \right) \frac{g_{k+1}^T s_k}{d_k^T y_k}. \quad (2.12)$$

If $d_k^T g_{k+1} = 0$, the second term in (2.12) is missing and reduces to the HS or PRP formula. Therefore we have obtained a family of conjugate gradient methods (1.3), (2.11) and (2.12), where the parameter τ_k is corresponding to the scaling parameter in the self-scaling memoryless BFGS method.

It is interesting to note that the formula (2.12) is corresponding to (1.6) if we adaptively choose t to be

$$t_k = \tau_k + \frac{\|y_k\|^2}{s_k^T y_k} - \frac{s_k^T y_k}{\|s_k\|^2}. \quad (2.13)$$

To establish a basic property for the family of conjugate gradient methods (1.3), (2.11) and (2.12), we define

$$p_k = \frac{\|d_k\|^2 \|y_k\|^2}{(d_k^T y_k)^2} \quad \text{and} \quad \gamma_k = \tau_k \frac{\|s_k\|^2}{s_k^T y_k}. \quad (2.14)$$

Lemma 2.1. *For the family of conjugate gradient methods (1.3), (2.11) and (2.12), if $d_k^T y_k \neq 0$, we always have that*

$$-d_{k+1}^T g_{k+1} \geq \min \left(\gamma_k, \frac{3}{4} \right) \|g_{k+1}\|^2. \quad (2.15)$$

Proof. Noting that $s_k = \alpha_k d_k$, we can write the search direction d_{k+1} in the form

$$d_{k+1}^P = -H_{k+1}^P g_{k+1}, \quad (2.16)$$

where

$$H_{k+1}^P = I - \frac{d_k z_k^T}{d_k^T y_k}, \quad z_k = y_k - p_k s_k. \quad (2.17)$$

To proceed our analysis, we symmetrize H_{k+1}^P and define

$$\bar{H}_{k+1}^P = \frac{1}{2} \left[H_{k+1}^P + (H_{k+1}^P)^T \right] = I - \frac{d_k z_k^T + z_k d_k^T}{2 d_k^T y_k}. \quad (2.18)$$

For any vectors $u, v \in \mathcal{R}^n$, notice that

$$(uv^T + vu^T) \left(u \pm \frac{\|u\|}{\|v\|} v \right) = (u^T v \pm \|u\| \|v\|) \left(u \pm \frac{\|u\|}{\|v\|} v \right). \quad (2.19)$$

By this, it is not difficult to see that the minimal eigenvalue of \bar{H}_{k+1}^P is

$$\lambda_{\min} = \min \left\{ 1, 1 - \frac{1}{2} \left(\frac{d_k^T z_k}{d_k^T y_k} + \frac{\|d_k\| \|z_k\|}{|d_k^T y_k|} \right) \right\}. \quad (2.20)$$

With the definitions of p_k and γ_k , we can rewrite (2.20) as

$$\lambda_{\min} = \min \left\{ 1, \frac{1}{2} \left(p_k + \gamma_k - \sqrt{p_k^2 + (2\gamma_k - 3) p_k + (\gamma_k^2 - 4\gamma_k + 3)} \right) \right\}. \quad (2.21)$$

Now we consider the second term in the braces of (2.21). It is easy to verify that if $\gamma_k \leq \frac{3}{4}$, it is monotonically increasing for $p_k \in [1, +\infty)$ and hence reaches its minimum, that is γ_k , at $p_k = 1$; if $\gamma_k > \frac{3}{4}$, it is monotonically decreasing for $p_k \in [1, +\infty)$ and hence is always greater than its limit $\frac{3}{4}$ as p_k tends to $+\infty$. Thus we always have

$$-g_{k+1}^T d_{k+1} = g_{k+1}^T \bar{H}_{k+1}^P g_{k+1} \geq \lambda_{\min} \|g_{k+1}\|^2 \geq \min \left(\gamma_k, \frac{3}{4} \right) \|g_{k+1}\|^2, \quad (2.22)$$

which completes our proof. \square

Lemma 2.2. *Assume that f satisfies Assumption 1.1. Consider the family of conjugate gradient methods (1.3), (2.11) and (2.12). If τ_k is chosen to be any of τ_k^B , τ_k^H , $\bar{\tau}_k^B$ and $\bar{\tau}_k^H$ and if $d_k^T y_k \neq 0$, we have that*

$$-g_{k+1}^T d_{k+1} \geq c \|g_{k+1}\|^2 \quad \text{for some positive constant } c > 0. \quad (2.23)$$

Proof. (i) If $\tau_k = \tau_k^B$, we have by (2.14) that $\gamma_k = 1$, which with Lemma 2.1 implies the truth of (2.23) with $c = \frac{3}{4}$; (ii) If $\tau_k = \tau_k^H$, then $\gamma_k = p_k$. By (2.21) and the fact that $p_k \geq 1$, we see that

$$\lambda_{\min} = \min \left\{ 1, p_k - \sqrt{p_k^2 - \frac{7}{4} p_k + \frac{3}{4}} \right\} > \min \left\{ 1, p_k - \sqrt{p_k^2 - \frac{7}{4} p_k + \frac{49}{64}} \right\} = \frac{7}{8}. \quad (2.24)$$

So (2.23) holds with $c = \frac{7}{8}$; (iii) By the Lipschitz condition (1.2) and the definitions of y_k and s_k , we have that

$$\|y_k\| \leq L \|s_k\|. \quad (2.25)$$

If $\frac{s_k^T y_k}{\|s_k\|^2} < 1$, we have $\tau_k = \frac{s_k^T y_k}{\|s_k\|^2}$ and hence $\gamma_k = 1$. Otherwise, if $\frac{s_k^T y_k}{\|s_k\|^2} \geq 1$, we must have from this, the Cauchy-Schwartz inequality and (2.25) that

$$\gamma_k = \frac{\|s_k\|^2}{s_k^T y_k} \geq \frac{\|s_k\|}{\|y_k\|} \geq \frac{1}{L}. \quad (2.26)$$

Consequently, we always have $\gamma_k \geq \min(1, \frac{1}{L})$. By Lemma 2.1, (2.23) holds with $c = \min(\frac{3}{4}, \frac{1}{L})$; (iv) If $\frac{\|y_k\|^2}{s_k^T y_k} < 1$, we have that $\gamma_k = p_k \geq 1$. Otherwise, if $\frac{\|y_k\|^2}{s_k^T y_k} \geq 1$, we know that $s_k^T y_k > 0$ and the inequality (2.26) is still valid. Thus we also have $\gamma_k \geq \min(1, \frac{1}{L})$. By Lemma 2.1, (2.23) holds with $c = \min(\frac{3}{4}, \frac{1}{L})$. \square

To generalize Lemma 2.2, we consider the convex combination of τ_k^H and τ_k^B

$$\tau_k = \nu \frac{\|y_k\|^2}{s_k^T y_k} + (1 - \nu) \frac{s_k^T y_k}{\|s_k\|^2}, \quad (2.27)$$

where $\nu \in [0, 1]$. This formed interval of τ_k is corresponding to the subclass of the self-scaled variable metric (SSVM) methods with the scaling parameter in $\left[\frac{s_k^T y_k}{y_k^T H_k y_k}, \frac{s_k^T H_k^{-1} s_k}{s_k^T y_k} \right]$ (assuming $s_k^T y_k > 0$). This subclass was proposed in [24] and it forms the basis for the SSVM algorithms in [25], [26] and [27]. Specially, [27] studied on this subclass of SSVM algorithms with some additional optimal property.

Lemma 2.3. *Assume that f satisfies Assumption 1.1. Consider the subfamily of conjugate gradient methods (1.3), (2.11) and (2.12), where τ_k is of the form (2.27) with $\nu \in [0, 1]$. If $d_k^T y_k \neq 0$, we have that $-g_{k+1}^T d_{k+1} \geq \frac{3}{4} \|g_{k+1}\|^2$.*

Proof. Since, by (2.12), $\beta_k(\tau_k)$ is linear with τ_k , it is easy see that d_{k+1} and hence $-g_{k+1}^T d_{k+1}$ is also linear with τ_k . By items (i) and (ii) of the proof to Lemma 2.2, we know that (2.23) holds with $c = \frac{3}{4}$ for both τ_k^H and τ_k^B . Thus the statement is true for their convex combination. \square

Powell [32] constructed a counter-example showing that the PRP method with exact line search may not converge for general nonlinear functions. Since for any τ_k , $\beta_k(\tau_k) = \beta_k^{PRP}$ if $g_{k+1}^T d_k = 0$, Powell's example can also be used to show the method (1.3) and (2.11) with $\beta_k(\tau_k)$ given by (2.12) need not converge for general functions. Therefore similarly to Gilbert and Nocedal [15], who proved the global convergence of the PRP method for general functions by restricting $\beta_k \geq 0$, we replace (2.12) by

$$\beta_k^+(\tau_k) = \max \left\{ \beta_k(\tau_k), \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \right\}, \quad (2.28)$$

where $\eta \in [0, 1)$ is some parameter and its suggested value is 0.5 in our practical computations. This way of truncation comes from the observation that, while projecting the d_{k+1}^{PS} in (2.3) into

the one-dimensional manifold (2.9), its last term provides the contribution $\frac{g_{k+1}^T d_k}{\|d_k\|^2} d_k$. Further, the following downhill direction

$$-g_{k+1} + \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} d_k \quad (2.29)$$

seems to be a better restart direction than $-g_{k+1}$ since it includes some curvature information achieved along the previous search direction.

Lemma 2.4. *Assume that f satisfies Assumption 1.1. Consider the family of conjugate gradient methods (1.3), (2.11) and (2.12), where $\beta_k(\tau_k)$ is replaced with the $\beta_k^+(\tau_k)$ in (2.28) and τ_k is chosen to be any of τ_k^B , τ_k^H , $\bar{\tau}_k^B$ and $\bar{\tau}_k^H$. If $d_k^T y_k \neq 0$, we have that*

$$-g_{k+1}^T d_{k+1} \geq \bar{c} \|g_{k+1}\|^2 \quad \text{for some positive constant } \bar{c} > 0. \quad (2.30)$$

Proof. By Lemma 2.2, we only need to consider the case that

$$\beta_k^+(\tau_k) = \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \quad \text{with } 0 \leq \eta < 1.$$

In this case, it is obvious that

$$-d_{k+1}^T g_{k+1} = \|g_{k+1}\|^2 - \eta \frac{(g_{k+1}^T d_k)^2}{\|d_k\|^2} \geq (1 - \eta) \|g_{k+1}\|^2.$$

This, with Lemma 2.2, indicates that (2.30) holds with $\bar{c} = \min(c, (1 - \eta))$. \square

Remark 1. In the above, we have proposed a family of conjugate gradient methods (1.3), (2.11) and (2.12). Its proposition is natural; namely, by projecting the self-scaling memoryless BFGS direction by Perry [28] and Shanno [34] into the one-dimensional manifold (2.9). Four choices for the parameter τ_k are presented and analyzed. The numerical experiments in Section 5 will suggest that the τ_k^B in (2.7) is the most efficient one. If we substitute this special choice into (2.12) and (2.28), we can obtain a relatively simple formula for β_k and its truncation form. They are

$$\beta_k = \frac{g_{k+1}^T y_k}{d_k^T y_k} - \frac{\|y_k\|^2}{s_k^T y_k} \frac{g_{k+1}^T s_k}{d_k^T y_k} \quad (2.31)$$

and

$$\beta_k^+ = \max \left\{ \frac{g_{k+1}^T y_k}{d_k^T y_k} - \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T s_k}{d_k^T y_k}, \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \right\}, \quad (2.32)$$

where $\eta \in [0, 1)$. We see that the formula (2.31) is corresponding to the Dai-Liao family of methods (1.6) with $t = \frac{\|y_k\|^2}{s_k^T y_k}$. (2.31) also differs (1.8) only with a constant coefficient in the second term and corresponds with the Hager-Zhang family of methods (1.11) with $\theta_k \equiv 1$.

Remark 2. The interval of τ_k formed in (2.27) with $\nu \in [0, 1]$ gives a subfamily of conjugate gradient methods with

$$\frac{g_{k+1}^T y_k}{d_k^T y_k} - \theta_k \frac{\|y_k\|^2}{s_k^T y_k} \frac{g_{k+1}^T s_k}{d_k^T y_k}, \quad (2.33)$$

where

$$\theta_k \in \left[1, 2 - \frac{(s_k^T y_k)^2}{\|s_k\|^2 \|y_k\|^2} \right]. \quad (2.34)$$

Surprisingly, this subfamily has (2.31) as its special member but excludes the Hager-Zhang choice (1.8). This, to some extent, explains the efficiency of the formula (2.31) over (1.8) in our numerical experiments.

Remark 3. Powell [32]'s counter-example was extended in [6] to show that, for any small constant $\varepsilon > 0$, the modified PRP method with $\beta_k = \max\{\beta_k^{PRP}, -\varepsilon\}$ need not converge for general functions. This implies to some extent that the restriction $\beta_k \geq 0$ is essential in ensuring the global convergence of the PRP method. However, Gilbert and Nocedal [15] showed that, for the PRP method using exact line searches, it is possible that $\beta_k^{PRP} < -\beta_k^{FR} < 0$ for a strongly convex function, although it is known that the original PRP method converges globally in this case. There have been several strategies that allow negative values of β_k and guarantee global convergence of the conjugate gradient method for general functions. For example, Dai and Liao [7] considered the truncation in (1.7) and Hager and Zhang suggested the truncation in (1.10). The restriction (2.28) provides another possibility and proves very useful in our convergence analysis and practical calculations.

3 An Improved Wolfe Line Search with An Adaptive Strategy

As is known, the search direction and the line search are two important factors of a line search algorithm. The purpose of this section is to develop an improved Wolfe line search, which allows a small increase on the objective function value and can avoid a numerical drawback of the Wolfe line search. As shown in the next section, this improved Wolfe line search guarantees the global convergence of the conjugate gradient method. An adaptive strategy is also designed to choose the initial stepsize.

For convenience, we denote the one-dimensional line search function to be

$$\phi_k(\alpha) = f(x_k + \alpha d_k), \quad \alpha \geq 0. \quad (3.1)$$

When the algorithm goes on the k -th iteration, we look back at the line search function ϕ_{k-1} at the $(k-1)$ -th iteration. We have at least four function or derivative values of ϕ_{k-1} , which are $\phi_{k-1}(0) = f_{k-1}$, $\phi'_{k-1}(0) = g_{k-1}^T d_{k-1}$, $\phi_{k-1}(\alpha_{k-1}) = f_k$ and $\phi'_{k-1}(\alpha_{k-1}) = g_k^T d_{k-1}$, no matter how the stepsize α_{k-1} is found. By the four values, we can define a quantity indicating how ϕ_{k-1} is close to a quadratic function. The basic idea is to do a quadratic interpolation to get q_{k-1} by imposing the three conditions

$$q_{k-1}(0) = \phi_{k-1}(0), \quad q'_{k-1}(0) = \phi'_{k-1}(0), \quad q'_{k-1}(\alpha_{k-1}) = \phi'_{k-1}(\alpha_{k-1}) \quad (3.2)$$

(later, we will use another denotation to express the interpolation function, for example, q_{k-1} is also denoted by $q(\phi_{k-1}(0), \phi'_{k-1}(0), \phi'_{k-1}(\alpha_{k-1}))$). If the value of this interpolation function at α_{k-1} , namely, $q_{k-1}(\alpha_{k-1})$, is close to the real function value $\phi_{k-1}(\alpha_{k-1})$, we think that ϕ_{k-1} tends to be some quadratic function. More exactly, similarly to the ratio used for adjusting the radius in trust region methods, we define the quantity

$$r_{k-1} = \frac{\phi_{k-1}(0) - \phi_{k-1}(\alpha_{k-1})}{q_{k-1}(0) - q_{k-1}(\alpha_{k-1})}. \quad (3.3)$$

Further, noticing that $\phi_{k-1}(0) = q_{k-1}(0) = f_{k-1}$, $\phi_{k-1}(\alpha_{k-1}) = f_k$ and by direct calculations, $q_{k-1}(\alpha_{k-1}) = f_{k-1} + \frac{1}{2} \alpha_{k-1} (g_{k-1}^T d_{k-1} + g_k^T d_{k-1})$, the quantity r_{k-1} can be simplified as

$$r_{k-1} = \frac{2(f_k - f_{k-1})}{\alpha_{k-1} (g_{k-1}^T d_{k-1} + g_k^T d_{k-1})}. \quad (3.4)$$

If r_{k-1} is close to 1, we think that ϕ_{k-1} is close to some quadratic function and otherwise, not. A successful use of this quantity r_{k-1} in designing gradient descent algorithms can be found in [10]. In the nonlinear conjugate gradient field, since it is general that the function is nonlinear at the initial stage and tends to be quadratic when the iterate is close to some solution point, we believe that the quantity r_{k-1} must be very useful in designing nonlinear conjugate gradient algorithms. As will be seen in Algorithms 3.1 and 4.1, it will be used not only in choosing the initial stepsize but in choosing the search direction.

The choice of the initial stepsize is important for a line search. For Newton-like methods, the choice $\alpha_k^{(0)} = 1$ is essential in giving rapid convergence rate. For conjugate gradient methods, it is important to use the current information about the problem to make an initial guess [23]. There have been quite a few ways to choose the initial stepsize in the conjugate gradient method, for example, see [12, 35, 23, 17]. However, it does not reach a consensus which one is the best. In the following, we propose an adaptive way for the choice of the initial stepsize based on to which extent the function is close to some quadratic function during some previous iterations.

Algorithm 3.1. (An adaptive strategy for choosing the initial stepsize)

Step 0. Given positive parameters ϵ_α , ϵ_f , ψ_1 and ψ_2 ;

Step 1. If $|r_{k-1} - 1| \leq \epsilon_\alpha$ and $\left| \frac{\phi_k(\psi_1 \alpha_{k-1}) - \phi_k(0)}{\phi_k(0)} \right| \leq \epsilon_f$,
set $\alpha_k^{(0)} = \operatorname{argmin} q(\phi_k(0), \phi'_k(0), \phi_k(\psi_1 \alpha_{k-1}))$;

Step 2. Otherwise, set $\alpha_k^{(0)} = \psi_2 \alpha_{k-1}$.

In the above algorithm, the condition $\left| \frac{\phi_k(\psi_1 \alpha_{k-1}) - \phi_k(0)}{\phi_k(0)} \right| \leq \epsilon_f$ is used to guarantee that the points $x_k + \psi_1 \alpha_{k-1} d_k$ and x_k are not far away from each other and $q(\phi_k(0), \phi'_k(0), \phi_k(\psi_1 \alpha_{k-1}))$ denotes the interpolation function by the three values $\phi_k(0)$, $\phi'_k(0)$ and $\phi_k(\psi_1 \alpha_{k-1})$. The basic idea of Algorithm 3.1 is that, if the function is roughly close to some quadratic function and if the points $x_k + \psi_1 \alpha_{k-1} d_k$ and x_k are close to each other, then we would like to do an interpolation and take the minimizer of the interpolation function as a new initial stepsize. This has the cost of an extra function evaluation in computing $\phi_k(\psi_1 \alpha_{k-1})$, but it is worthwhile. Otherwise, we choose the initial stepsize as a multiple of the previous stepsize α_{k-1} . In this case, a larger initial stepsize is preferable, as $\psi_2 = 5$ in our numerical experiments of Section 5.

Next, we introduce new line search conditions, which can avoid a numerical drawback of the Wolfe conditions and ensure the global convergence of the conjugate gradient algorithm.

To this aim, recall the Wolfe conditions

$$\phi_k(\alpha) \leq \phi_k(0) + \delta \alpha \phi'_k(0), \quad (3.5)$$

$$\phi'_k(\alpha) \geq \sigma \phi'_k(0), \quad (3.6)$$

where $0 < \delta < \sigma < 1$. The Wolfe conditions (3.5)-(3.6) can be dated back to [37, 38] and was used to analyze nonlinear conjugate gradient methods in [8, 9]. Theoretically, under Assumption 1.1 on f , if d_k is a descent direction, there must exist some stepsize $\alpha_k > 0$ satisfying (3.5)-(3.6).

In practical computations, however, the first Wolfe condition, (3.5), may never be satisfied due to the existence of the numerical errors. Assume that $\alpha_k^* > 0$ is the exact minimizer of $\phi_k(\alpha)$. If $\alpha_k^* d_k$ is too small, we have that $\phi_k(0) - \phi_k(\alpha^*) = O(\|\alpha_k^* d_k\|^2)$. Consequently, $\phi_k(\alpha^*)$ is about the same as $\phi_k(0)$ provided that $\|\alpha_k^* d_k\|$ is on the order of square root of machine precision. It turns out that in this case, it is possible that $\phi_k(\alpha) \geq \phi_k(0)$ for all $\alpha \geq 0$ in numerical sense and hence (3.5) is never satisfied in practical computations. This numerical drawback of the Wolfe conditions was carefully analyzed in [17] with a one-dimensional quadratic function. We have observed this possibility for Problem JENSMP from CUTer collection, which was originally introduced in [22] and has the form

$$f(x_1, x_2) = [4 - (e^{x_1} + e^{x_2})]^2 + [6 - (e^{2x_1} + e^{2x_2})]^2. \quad (3.7)$$

We used the conjugate gradient method (1.3), (2.11) and (2.28) with τ_k replaced by (2.7) and α_k calculated by the Wolfe line search. At the 16th iteration, we obtained

$$x_{16} = (2.5782521324e-01, 2.5782521393e-01)^T, \quad d_{16} = (9.2964892641e-06, -2.5552928578e-06)^T$$

with values

$$f_{16} = 1.24362182e+02, \quad g_{16}^T d_{16} = -9.2954234226e-11, \quad \|g_{16}\| = 1.5815277275e-05.$$

We found that even with 50 trial stepsizes ranging from $1.7e-26$ to $1.2e-5$, the algorithm failed to find a stepsize along the search along d_{16} such that the first Wolfe condition is satisfied. Figure 1 plots the overall graphs of function $\phi_k(\alpha) := f(x_{16} + \alpha d_{16})$ for $\alpha \in [0, 1]$ and $\alpha \in [0, 1.0e-11]$. In this example, we did have $\phi_k(\alpha) \geq \phi_k(0)$ numerically for all $\alpha \geq 0$ and hence a satisfactory stepsize is not possible to be found.

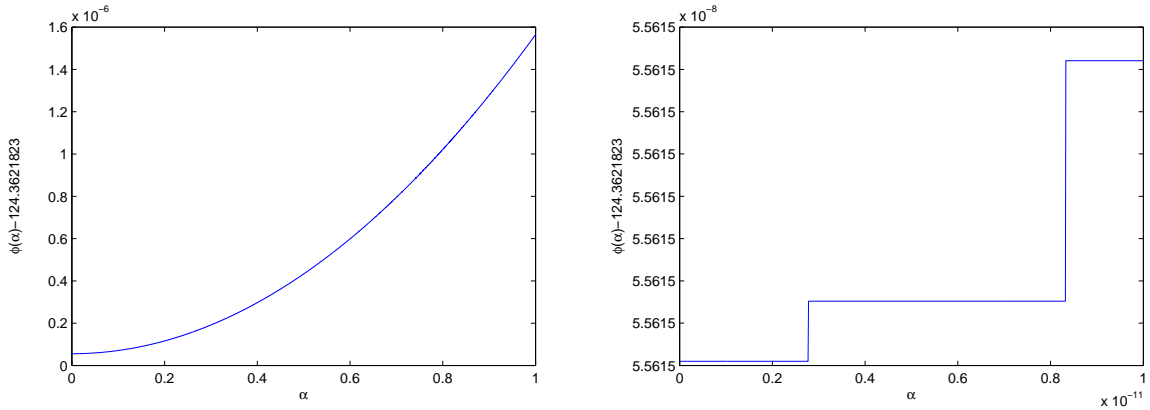


Figure 1: Graph of JENSMP along the search direction d_{16}

To avoid the above numerical drawback of the Wolfe line search, Hager and Zhang [17] suggested a combination of the original Wolfe conditions and the approximate Wolfe conditions that $\sigma \phi_k'(0) \leq \phi_k'(\alpha) \leq (2\delta - 1) \phi_k'(0)$. Their line search performed well in their numerical tests, but cannot guarantee the global convergence of the algorithm in theory. Given a constant parameter $\epsilon > 0$, a positive sequence $\{\eta_k\}$ satisfying $\sum_{k \geq 1} \eta_k < +\infty$ and again parameters δ and σ satisfying $0 < \delta < \sigma < 1$, we propose the following modified Wolfe condition

$$\phi_k(\alpha) \leq \phi_k(0) + \min \{ \epsilon |\phi_k'(0)|, \delta \alpha \phi_k'(0) + \eta_k \} \quad (3.8)$$

and call the line search satisfying (3.8) and (3.6) by *improved Wolfe line search*. The idea behind the condition (3.8) is that, it allows the stepsizes satisfying (3.5) and hence is an extension of the original Wolfe line search; meanwhile, if the trial point is close to x_k , in which case

$$\phi_k(\alpha) \leq \phi_k(0) + \epsilon |\phi_k'(0)|, \quad (3.9)$$

we switch to require

$$\phi_k(\alpha) \leq \phi_k(0) + \delta \alpha \phi_k'(0) + \eta_k \quad (3.10)$$

rather than (3.5). The extra positive term η_k in (3.10) or (3.8) allows a slight increase in the function value and hence is helpful in avoiding the numerical drawback of the first Wolfe line search condition (3.5). At the same time, the condition that the sequence $\{\eta_k\}$ is summable can guarantee the global convergence of the algorithm similarly to the Wolfe line search. Specifically, we set $\eta_k = \frac{1}{k^2}$ in our numerical experiments.

Under Assumption 1.1 on f , if $g_k^T d_k < 0$, it is obvious that there must exist a suitable stepsize satisfying (3.8) and (3.6) since they are weaker than the Wolfe conditions. In the following, we describe a detailed procedure to implement the improved Wolfe line search, where a point x_k and a descent direction d_k are given.

Algorithm 3.2. (An Improved Wolfe Line Search)

Step 0. Determine $\alpha_k^{(0)}$ via Algorithm 3.1.

Set $a_0 = 0$, $\phi_a = f(x_k)$, $\phi'_a = g_k^T d_k$ and $b_0 = M$, where M is some big number.

Set $t_1 = 1.0$, $t_2 = 0.1$, $\rho > 1$ and $i = 0$.

Step 1. Evaluate $\phi_k(\alpha_k^{(i)})$ and test condition (3.8).

If (3.8) is satisfied, goto Step 2.

Set $b_i = \alpha_k^{(i)}$, $\phi_b = \phi_k(\alpha_k^{(i)})$, $\alpha^ = \operatorname{argmin} q(\phi_a, \phi'_a, \phi_b)$ and $t_1 = 0.1t_1$.*

Choose $\alpha_k^{(i+1)} := \min \{\max [\alpha^, a_i + t_1(b_i - a_i)], b_i - t_2(b_i - a_i)\}$.*

Set $i = i + 1$ and goto Step 1.

Step 2. Evaluate $\phi'(\alpha_k^{(i)})$ and test condition (3.6).

If (3.6) is satisfied, return $\alpha_k = \alpha_k^{(i)}$, stop.

Set $t_1 = 0.1$, $t_2 = 0.1t_2$. If $b_i = M$, goto Step 3.

Set $a_i = \alpha_k^{(i)}$, $\phi_a = \phi(\alpha_k^{(i)})$, $\phi'_a = \phi'(\alpha_k^{(i)})$ and $\alpha^ = \operatorname{argmin} q(\phi_a, \phi'_a, \phi_b)$.*

Choose $\alpha_k^{(i+1)} := \min \{\max [\alpha^, a_i + t_1(b_i - a_i)], b_i - t_2(b_i - a_i)\}$.*

Set $i = i + 1$, goto Step 1.

Step 3. Set $a_i = \alpha_k^{(i)}$, $\phi_a = \phi(\alpha_k^{(i)})$, $\phi'_a = \phi'(\alpha_k^{(i)})$ and $\alpha_k^{(i+1)} = \rho \alpha_k^{(i)}$.

Set $i = i + 1$, goto Step 1.

We can see that the above procedure is similar, but not identical, to the classical implementation of the Wolfe line search in Fletcher [13]. At first, we determine $\alpha_k^{(0)}$ via Algorithm 3.1 and initialize the interval $[a_0, b_0]$ as $[0, M]$, where M is some big number. Then in the current bracket $[a_i, b_i]$, we choose a new trial stepsize $\alpha_k^{(i+1)}$ to be the minimizer of the quadratic interpolation function $q(\phi_a, \phi'_a, \phi_b)$, but prevent it from being arbitrarily close to the extremes of the interval using the preset factors t_1 and t_2 . If $\alpha_k^{(i+1)}$ satisfies (3.8) and (3.6), the line search is terminated with $\alpha_k = \alpha_k^{(i+1)}$. If $\alpha_k^{(i+1)}$ only satisfies (3.8), we update $[a_i, b_i]$ as $[\alpha_k^{(i+1)}, b_i]$;

otherwise, we update $[a_i, b_i]$ as $[a_i, \alpha_k^{(i+1)}]$. We should note that in case of updating $[a_i, M]$, $\alpha_k^{(i+1)}$ is chosen to be a multiple of a_i , namely, ρa_i with $\rho > 1$ since M is preset to a very big number and the interpolation in the interval $[a_i, M]$ is likely not to be reliable. On the whole, the procedure will generate a sequence of intervals $[a_i, b_i]$ with properties $[a_{i+1}, b_{i+1}] \subset [a_i, b_i]$ for all i , $|b_i - a_i| \rightarrow 0$ and

$$\phi_k(a_i) \leq \phi_k(0) + \min\{\epsilon |\phi_k(0)|, \delta a_i \phi'(0) + \eta_k\} \quad \text{but} \quad \phi'_k(a_i) < \sigma \phi'_k(0), \quad (3.11)$$

$$\phi_k(b_i) > \phi_k(0) + \min\{\epsilon |\phi_k(0)|, \delta b_i \phi'(0) + \eta_k\}, \quad (3.12)$$

until a satisfactory stepsize is successfully found.

For the improved Wolfe line search, we can establish the Zoutendijk condition (3.13) (see [43]) all the same.

Lemma 3.3. *Assume that f satisfies Assumption 1.1. Consider the iterative method of the form (1.3) where the direction d_k satisfies $g_k^T d_k < 0$ and the stepsize α_k satisfies (3.8) and (3.6). Then we have that*

$$\sum_{k \geq 1} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty. \quad (3.13)$$

Proof. It follows from the Lipschitz condition (1.2) and the line search condition (3.6) that

$$L\alpha_k \|d_k\|^2 \geq (g_{k+1} - g_k)^T d_k \geq (\sigma - 1)g_k^T d_k.$$

Thus we have

$$\alpha_k \geq \frac{\sigma - 1}{L} \frac{g_k^T d_k}{\|d_k\|^2}. \quad (3.14)$$

It follows from (3.8) that

$$f_{k+1} \leq f_k + \min\{\epsilon |f_k|, \delta \alpha_k g_k^T d_k + \eta_k\} \leq f_k + \delta \alpha_k g_k^T d_k + \eta_k, \quad (3.15)$$

which with (3.14) implies that

$$f_k - f_{k+1} + \eta_k \geq c \frac{(g_k^T d_k)^2}{\|d_k\|^2}, \quad (3.16)$$

where $c = \delta(1 - \sigma)/L$. Summing (3.16) over k and noting that $\sum_{k \geq 1} \eta_k < +\infty$ and that f is bounded below, we see that (3.13) holds. \square

4 Algorithm and Convergence Analysis

In this section, we give the whole scheme of our new conjugate gradient algorithms with the improved Wolfe line search. A restart technique, which makes good use of the quantity r_k in (3.4), is also incorporated to accelerate the algorithm.

More exactly, if there are continuously many iterations such that r_k is close 1, we restart the algorithm with the steepest descent direction. In this case, we think that the algorithm is very likely to enter some region where the objective function is close to some quadratic function and

hence a restart along $-g_k$ is worthwhile provided that not all values of r_k are around one since the last restart.

In addition, if the number of the total iterations since the last restart reaches some threshold, $MaxRestart$, we also restart the algorithm. In our experiment, we choose this threshold to be $6n$ to avoid frequent restarts for small nonlinear functions. For large-scale problems, this restarting criterion is generally not active.

The following is a detailed description of our algorithm.

Algorithm 4.1. (A Nonlinear Conjugate Gradient Algorithm)

Step 0. Given $x_1 \in \mathcal{R}^n$, $\varepsilon > 0$, $\epsilon_r > 0$ and positive integers $MaxRestart$, $MinQuad$.

Step 1. Set $k := 1$. If $\|g_1\| \leq \varepsilon$, stop.

Let $d_1 = -g_1$ and set $IterRestart := 0$ and $IterQuad := 0$.

Step 2. Compute a stepsize $\alpha_k > 0$ via Algorithm 3.2.

Step 3. Let $x_{k+1} = x_k + \alpha_k d_k$. If $\|g_{k+1}\| \leq \varepsilon$, stop.

$IterRestart := IterRestart + 1$.

Compute r_k by (3.4). If $|r_k - 1| \leq \epsilon_r$, $IterQuad := IterQuad + 1$; else, $IterQuad := 0$.

Step 4. If $IterRestart = MaxRestart$ or ($IterQuad = MinQuad$ and $IterQuad \neq IterRestart$), let $d_{k+1} = -g_{k+1}$ and set $IterRestart := 0$, $IterQuad := 0$, $k := k + 1$, goto Step 2.

Step 5. Compute β_k by (2.28) and d_{k+1} by (1.4). $k := k + 1$, goto Step 2.

Particularly, if the parameter τ_k in (2.28) is chosen to be τ_k^H in (2.6), τ_k^B in (2.7), $\bar{\tau}_k^H$ and $\bar{\tau}_k^B$ in (2.8), the above algorithm is called as Algorithms 4.1(a), 4.1(b), 4.1(c) and 4.1(d), respectively.

Now we analyze the global convergence properties of the above conjugate gradient algorithm. For convenience, assume that

$$g_k \neq 0, \quad \forall k \geq 1$$

throughout this section, for otherwise a stationary point has been found. Since a restart along the negative gradient is done in at least $MaxRestart$ iterations, there must be global convergence of Algorithm 4.1 for general functions. Actually, assuming that $d_{k_i} = -g_{k_i}$ for some infinite subsequence $\{k_i\}$, we have from Lemma 3.3 that $\lim_{i \rightarrow \infty} \|g_{k_i}\| = 0$. In the following, we consider the global convergence properties of Algorithm 4.1 without any restarts.

For uniformly convex functions, we have the following convergence result.

Theorem 4.2. Assume that f satisfies Assumption 1.1. Consider the search direction defined by (1.3), (2.11), (2.12), where τ_k is chosen to be any of τ_k^H , τ_k^B , $\bar{\tau}_k^H$ and $\bar{\tau}_k^B$, and where stepsize α_k is calculated by the line search satisfying (3.8) and (3.6). If, further, f is uniformly convex, namely, there exists a constant $\mu > 0$ such that

$$(\nabla f(x) - \nabla f(y))^T(x - y) \geq \mu \|x - y\|^2, \quad \forall x, y \in \mathcal{R}^n, \quad (4.1)$$

we have that

$$\lim_{k \rightarrow \infty} g_k = 0. \quad (4.2)$$

Proof. It follows from (1.2) and (4.1) that

$$\|y_k\| \leq L \|s_k\|, \quad (4.3)$$

$$d_k^T y_k \geq \mu \|d_k\| \|s_k\|. \quad (4.4)$$

By (4.1) and (4.3), it is easy to see that for any τ_k of τ_k^H , τ_k^B , $\bar{\tau}_k^H$ and $\bar{\tau}_k^B$, there exists a positive constant c_τ such that

$$|\tau_k| \leq c_\tau. \quad (4.5)$$

Write $\beta_{k+1}(\tau_k)$ as the special form of (1.6) with t replaced by p_k . It follows from (4.3), (4.4) and (4.5) that

$$|p_k| \leq \frac{L^2}{\mu} + L + c_\tau. \quad (4.6)$$

Consequently,

$$\begin{aligned} \|d_{k+1}\| &\leq \|g_{k+1}\| + \left| \frac{g_{k+1}^T y_k}{d_k^T y_k} - p_k \frac{g_{k+1}^T s_k}{d_k^T y_k} \right| \|d_k\| \\ &\leq \left(1 + \frac{L \|s_k\| \|d_k\|}{d_k^T y_k} + |p_k| \frac{\|s_k\| \|d_k\|}{d_k^T y_k} \right) \|g_{k+1}\| \\ &\leq \left(1 + \frac{L^2 + 2\mu L + \mu c_\tau}{\mu^2} \right) \|g_{k+1}\|. \end{aligned} \quad (4.7)$$

On the other hand, Lemmas 2.2 and 3.3 imply that

$$\sum_{k \geq 1} \frac{\|g_k\|^4}{\|d_k\|^2} < \infty. \quad (4.8)$$

By (4.7) and (4.8), we have that

$$\sum_{k \geq 1} \|g_k\|^2 < \infty,$$

which implies (4.2). □

Denote θ_k to be the angle between d_k and $-g_k$; namely,

$$\cos \theta_k = \frac{-g_k^T d_k}{\|g_k\| \|d_k\|}.$$

In the case that f is uniformly convex, we know from (2.23) and (4.7) that there must some positive constant c_θ such that

$$\cos \theta_k \geq c_\theta, \quad \forall k \geq 1.$$

For general nonlinear functions, similarly to [15] and [7], we can establish a weaker convergence result in the sense that

$$\liminf_{k \rightarrow \infty} \|g_k\| = 0. \quad (4.9)$$

To this aim, we proceed by contradiction and assuming that there exists $\gamma > 0$ such that

$$\|g_k\| \geq \gamma, \quad \forall k \geq 1. \quad (4.10)$$

Lemma 4.3. *Assume that f satisfies Assumption 1.1. Consider the family of conjugate gradient methods of the form (1.3), where d_{k+1} is given by (2.11) and (2.28) and stepsize α_k is calculated by the improved Wolfe line search satisfying (3.8) and (3.6). If (4.10) holds, then $d_k \neq 0$ and*

$$\sum_{k \geq 2} \|u_k - u_{k-1}\|^2 < \infty, \quad (4.11)$$

where $u_k = d_k / \|d_k\|$.

Proof. First, note that $d_k \neq 0$, for otherwise the sufficient descent condition (2.30) would imply $g_k = 0$. Therefore u_k is well defined. Now, divide formula (2.28) for β_k into two parts as follows

$$\beta_k^{(1)} = \max \left\{ \frac{g_{k+1}^T y_k}{d_k^T y_k} - \left(1 + \tau_k \frac{s_k^T y_k}{\|y_k\|^2} \right) \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} + (1 - \eta) \frac{g_{k+1}^T d_k}{\|d_k\|^2}, 0 \right\}, \quad (4.12)$$

$$\beta_k^{(2)} = \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \quad (4.13)$$

and define

$$w_k = \frac{-g_k + \beta_{k-1}^{(2)} d_{k-1}}{\|d_k\|} \quad \text{and} \quad \delta_k = \frac{\beta_{k-1}^{(1)} \|d_{k-1}\|}{\|d_k\|}. \quad (4.14)$$

By $d_k = -g_k + \beta_{k-1} d_{k-1}$, we have for $k \geq 2$,

$$u_k = w_k + \delta_k u_{k-1}. \quad (4.15)$$

Using the identity $\|u_k\| = \|u_{k-1}\| = 1$ and (4.15), we obtain

$$\|w_k\| = \|u_k - \delta_k u_{k-1}\| = \|\delta_k u_k - u_{k-1}\| \quad (4.16)$$

(the last equality can be verified by squaring both sides). Using the condition $\delta_k \geq 0$, the triangle inequality, and (4.16), we have

$$\begin{aligned} \|u_k - u_{k-1}\| &\leq \|(1 + \delta_k)u_k - (1 + \delta_k)u_{k-1}\| \\ &\leq \|u_k - \delta_k u_{k-1}\| + \|\delta_k u_k - u_{k-1}\| \\ &= 2\|w_k\|. \end{aligned} \quad (4.17)$$

By the definition of $\beta_k^{(2)}$ in (4.13), we see that

$$\| -g_k + \beta_{k-1}^{(2)} d_{k-1} \| \leq \|g_k\| + |\beta_{k-1}^{(2)}| \|d_{k-1}\| \leq (1 + \eta) \|g_k\|. \quad (4.18)$$

This bound for the numerator of w_k coupled with (4.17) gives

$$\|u_k - u_{k-1}\| \leq 2\|w_k\| \leq 2(1 + \eta) \frac{\|g_k\|}{\|d_k\|}. \quad (4.19)$$

The relation (4.10), the sufficient descent condition (2.30) and the Zoutendijk condition (3.13) indicate that

$$\sum_{k \geq 1} \frac{\|g_k\|^2}{\|d_k\|^2} \leq \frac{1}{\gamma^2} \sum_{k \geq 1} \frac{\|g_k\|^4}{\|d_k\|^2} \leq \frac{1}{\gamma^2 \bar{c}^2} \sum_{k \geq 1} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < +\infty. \quad (4.20)$$

Thus (4.11) follows from (4.19) and (4.20). \square

Now we give the following convergence theorem for general objective functions.

Theorem 4.4. *Assume that f satisfies Assumption 1.1. Consider the family of methods of the form (1.3), where d_{k+1} is given by (2.11) and (2.28) and stepsize α_k is calculated by the improved Wolfe line search satisfying (3.8) and (3.6). If the generated sequence $\{x_k\}$ is bounded, if τ_k is chosen as any of τ_k^H , τ_k^B , $\bar{\tau}_k^H$ and $\bar{\tau}_k^B$, the method converges in the sense that (4.9) holds.*

Proof. We proceed by contradiction and assume that (4.10) holds. By the continuity of ∇f and the boundedness of $\{x_k\}$, there exists some positive constant $\bar{\gamma}$ such that

$$\|x_k\| \leq \bar{\gamma}, \quad \|g_k\| \leq \bar{\gamma}, \quad \forall k \geq 1. \quad (4.21)$$

The line search condition (3.6) indicates that

$$g_{k+1}^T d_k \geq \sigma g_k^T d_k. \quad (4.22)$$

It follows from this, (2.30) and (4.10) that

$$d_k^T y_k \geq -(1 - \sigma) d_k^T g_k \geq \bar{c}(1 - \sigma) \gamma^2. \quad (4.23)$$

Also we have by (4.22) and $g_k^T d_k < 0$ that

$$\frac{\sigma}{\sigma - 1} \leq \frac{d_k^T g_{k+1}}{d_k^T y_k} \leq 1. \quad (4.24)$$

For any τ_k of τ_k^H , τ_k^B , $\bar{\tau}_k^H$ and $\bar{\tau}_k^B$, it is not difficult to know by (1.2) and (4.5) that there exists some positive constant \bar{c}_τ such that

$$|\tau_k s_k^T y_k| \leq \bar{c}_\tau \|s_k\|^2, \quad \forall k \geq 1. \quad (4.25)$$

Now we write $\beta_k(\tau_k)$ in (2.12) as

$$\beta_k(\tau_k) = \frac{g_{k+1}^T y_k}{d_k^T y_k} - \left(1 - \frac{(d_k^T y_k)^2}{\|d_k\|^2 \|y_k\|^2}\right) \frac{\|y_k\|^2 g_{k+1}^T d_k}{d_k^T y_k d_k^T y_k} - \frac{\tau_k s_k^T y_k g_{k+1}^T d_k}{d_k^T y_k d_k^T y_k}. \quad (4.26)$$

Since by (4.21), $\|s_k\| = \|x_{k+1} - x_k\| \leq 2\bar{\gamma}$, we can show by this, (4.26), (4.21), (4.23), (4.25), $\|y_k\| \leq L\|s_k\|$ and $0 \leq (d_k^T y_k)^2 \leq \|d_k\|^2 \|y_k\|^2$ that

$$|\beta_k(\tau_k)| \leq c_\beta \|s_k\|, \quad \text{for some constant } c_\beta > 0 \text{ and all } k \geq 1. \quad (4.27)$$

Define $b = 2c_\beta \bar{\gamma}$ and $\lambda = \frac{1}{2c_\beta^2 \bar{\gamma}}$. It follows from (4.27) and (4.21) that for all k ,

$$|\beta_k| \leq b, \quad (4.28)$$

and

$$\|s_k\| \leq \lambda \implies |\beta_k| \leq \frac{1}{b}. \quad (4.29)$$

The relations (4.28) and (4.29) indicate that $\beta_k(\tau_k)$ in (2.12) has Property (*) in [15].

Now we look at the formula (2.28). By (4.10), (2.30) and (3.13), we clearly have that

$$\|d_k\| \rightarrow +\infty. \quad (4.30)$$

This means that $\beta_k(\tau_k)$ can only be less than the value $\beta_k^{(2)} = \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2}$ for finite times. Otherwise, we have that

$$\|d_{k+1}\| = \|g_{k+1} + \beta_k^{(2)} d_k\| \leq (1 + \eta) \|g_{k+1}\| \leq (1 + \eta) \bar{\gamma}$$

for infinite k 's and obtain a contradiction to (4.30). Consequently, we can assume that $\beta_k^+(\tau_k) = \beta_k(\tau_k)$ for all sufficiently large k . In this case, using Property (*) and the fact that $\|d_k\|^2$ is increasing at most linearly, we can show similarly to Lemma 4.2 in [15] that for any positive integers Δ and k_0 , there exists an integer $k \geq k_0$ such that the size of $\mathcal{K} = \{i : k \leq i \leq k + \Delta - 1, \|s_{i-1}\| > \lambda\}$ is greater than $\frac{\Delta}{2}$. Further, using this, Lemma 4.3 and the boundedness of $\{x_k\}$, we can obtain a contradiction similarly to the proof of Theorem 4.3 in [15]. The contradiction shows the truth of (4.9). \square

5 Numerical Experiments

In this section, we compare Algorithm 4.1 with the `cg_descent` method of Hager and Zhang in [17]. We also examine the performance of new conjugate gradient variants introduced in Section 2 using the same line search in the `cg_descent` method.

Algorithm 4.1 was implemented in C language and tested in Fedora 12 Linux environment. The computer used is a Lenovo X200 laptop with 2G RAM memory and Centrino2 processor. The following parameters were used in our implementation

$$\begin{aligned} \delta = 0.1, \quad \sigma = 0.9, \quad \alpha_1^{(0)} = 1, \quad \psi_1 = 1, \quad \psi_2 = 5, \quad \epsilon_\alpha = 10^{-3}, \quad \epsilon_f = 100, \\ \rho = 5, \quad \epsilon_r = 10^{-10}, \quad \eta = 0.5, \quad \text{MaxRestart} = 6n, \quad \text{MinQuad} = 3. \end{aligned}$$

where n is the problem dimension. We used the same termination criterion as in `cg_descent` method [17]; namely,

$$\|\nabla f(x_k)\|_\infty \leq \max\{10^{-6}, 10^{-12} \|\nabla f(x_1)\|_\infty\}. \quad (5.1)$$

The test problems are 155 unconstrained optimization problems drawn from CUTER [16] collection. For each comparison, however, we excluded those problems for which different solvers converge to different local minimizers. Besides it, we also eliminated those *easy* problems for which all the solvers can handle in less than ten iterations regardless of the problem dimension.

The performance profile by Dolan and Moré [11] is used to display the performance of the algorithms. Define \mathcal{P} as the whole set of n_p test problems and \mathcal{S} the set of the interested solvers. Let $l_{p,s}$ be the number of objective function evaluations required by solver s for problem p . Define the performance ratio as

$$r_{p,s} = \frac{l_{p,s}}{l_p^*},$$

where $l_p^* = \min\{l_{p,s} : s \in \mathcal{S}\}$. It is obvious that $r_{p,s} \geq 1$ for all p and s . If a solver fails to solve a problem, the ratio $r_{p,s}$ is assigned to be a large number M . The performance profile for each solver s is defined as the following cumulative distribution function for performance ratio $r_{p,s}$,

$$\rho_s(\tau) = \frac{\text{size}\{p \in \mathcal{P} : r_{p,s} \leq \tau\}}{n_p}.$$

Obviously, $\rho_s(1)$ represents the percentage of problems for which solver s is the best. See [11] for more details about the performance profile. The performance profile can also be used to

analyze the number of iterations, the number of gradient evaluations and the cpu time. Besides, to get a clear observation, we give the horizontal coordinate a log-scale in the following figures.

Figure 2 plots the performance profile with the four variants of the new algorithms; namely, Algorithms 4.1 (a), 4.1 (b), 4.1 (c) and 4.1 (d). After eliminating the problems for which the four variants converge to different local minimizers or all of them can solve in less than ten iterations, 113 problems are left. Observe that among the four algorithms, Algorithm 4.1 (b) occupies the first place, which is fastest for about 50% of the test problems; Algorithms 4.1 (c) and 4.1 (d) come second and Algorithm 4.1 (a) third. It indicates that the new choice β_k (2.28) with τ_k^B in (2.7) is more efficient than the one with τ_k^H in (2.6).

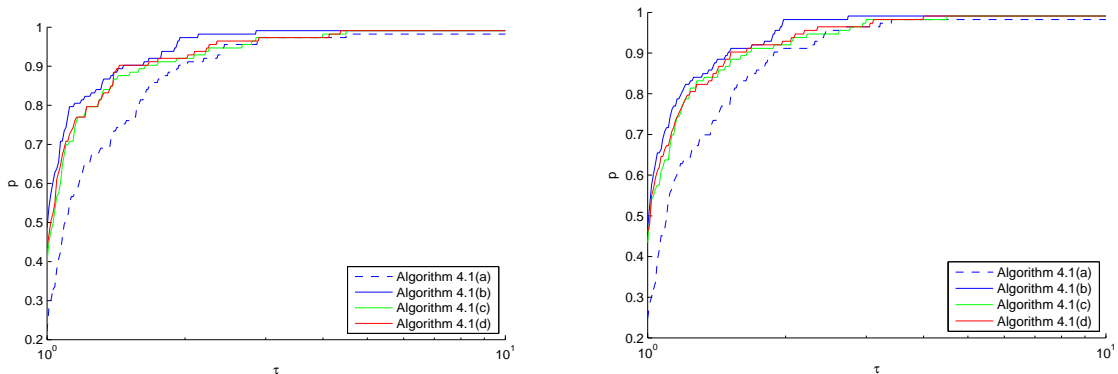


Figure 2: Performance profile of Algorithms 4.1 (a) (b) (c) and (d) based on the numbers of function evaluations (left) and gradient evaluations (right).

In Figure 3, we compare Algorithm 4.1 (b) with and without restarts to test the efficiency of the new restart technique. There are 148 problems left after the elimination process mentioned above. Figure 3 clearly shows that the new restart technique contributes to the efficiency of Algorithm 4.1 (b). Similar observations were also made for Algorithms 4.1 (a), (c) and (d).

In the following two experiments, we examine the effect of the new choice β_k and the effect of new line search algorithm, respectively. More exactly, in Figure 4, we compare cg_descent itself and a variant of cg_descent with β_k replaced by the new choice of β_k given by (2.28) and (2.7); in Figure 5, we compare cg_descent itself and Algorithm 4.1 (b), in which we use both the new line search algorithm and the new choice of β_k in (2.28) and (2.7). Figure 4 shows that compared with cg_descent itself, cg_descent with the new choice of β_k wins about 13.9% more problems in function evaluations and about 15.3% more problems in gradient evaluations. From Figure 5, Algorithm 4.1 (b) wins about 17.8% more problems in function evaluations and about 28.0% more problems in gradient evaluations. In a word, Figures 4 and 5 demonstrate that the superiority of Algorithm 4.1 (b) over cg_descent not only comes from the new choice of β_k , but also comes from the improved Wolfe line search.

6 Conclusions and Discussions

We have proposed a family of conjugate gradient methods, namely, (1.3), (1.4) and (1.12), for unconstrained optimization via seeking the conjugate gradient direction closest to the direction

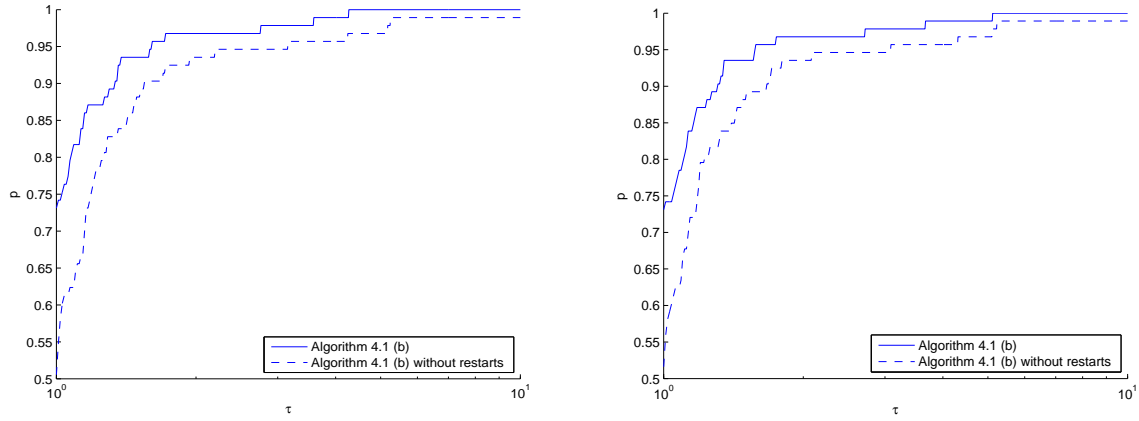


Figure 3: Performance profile of Algorithm 4.1(b) with and without the restart technique based on the numbers of function evaluations (left) and gradient evaluations (right).

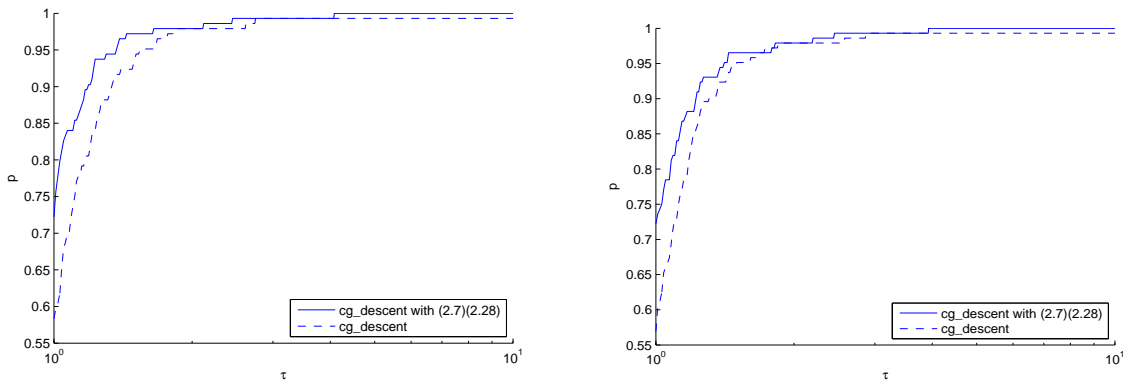


Figure 4: Performance profile of cg_descent and cg_descent with new β_k in (2.7) and (2.28) based on the numbers of function evaluations (left) and gradient evaluations (right).

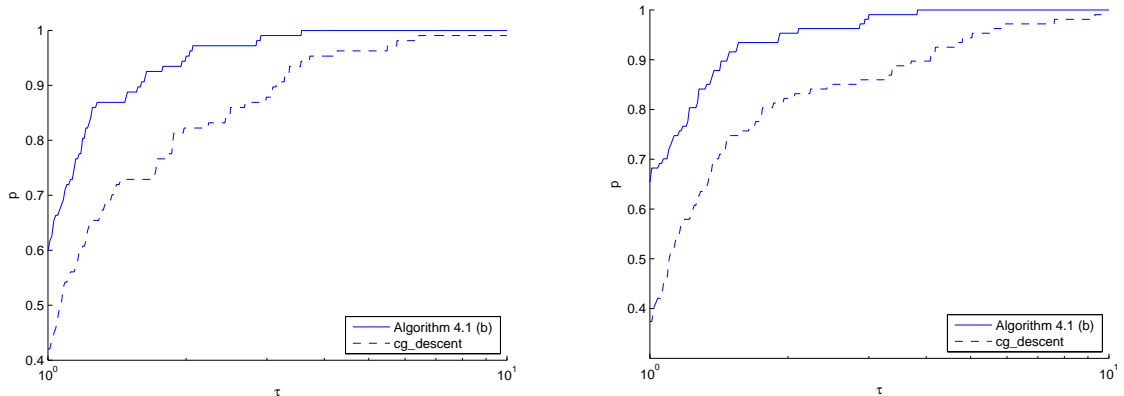


Figure 5: Performance profile of Algorithms 4.1(b) and cg_descent based on the numbers of function evaluations (left) and gradient evaluations (right).

of the scaled memoryless BFGS method. The sufficient descent condition is established for four special members of the family. An improved Wolfe line search has been introduced, which can avoid a numerical drawback of the Wolfe line search observed in [17] and guarantee the global convergence of the conjugate gradient method under mild conditions. Besides it, we have developed an adaptive strategy to choose the initial stepsize and a dynamic restart technique to accelerate the algorithm. The numerical results indicate that Algorithm 4.1 (b), that calculates β_k by (2.28) and (2.7) or equivalently by (2.32), performs much better than the cg_descent method by Hager and Zhang [18] for the test problems from the CUTEr collection.

To a great extent, both the new family (1.12) proposed in this paper and the Hager-Zhang family (1.11) could be regarded as subfamilies of the Dai-Liao family (1.6). Comparing the new family with the Hager-Zhang one, the parameter τ_k in (1.12) has a clear meaning; namely, it is corresponding to the self-scaling parameter in the scaled memoryless BFGS method. On the occasion of quasi-Newton methods, to improve the condition numbers of quasi-Newton matrices, this parameter τ_k (see [25, 26]) must be such that

$$\tau_k^B \leq \tau_k \leq \tau_k^H, \quad (6.1)$$

where τ_k^B and τ_k^H are given in (2.7) and (2.6), respectively. This suggested the following interval of the quantity t_k in (2.13),

$$t_k \in \left[\frac{\|y_k\|^2}{s_k^T y_k}, 2 \frac{\|y_k\|^2}{s_k^T y_k} - \frac{s_k^T y_k}{\|s_k\|^2} \right]. \quad (6.2)$$

In this case, the new family of methods (1.12) does not include the formula (1.8) by Hager and Zhang [17] if $s_k^T y_k > 0$ for all k . We wonder whether this suggested interval (6.2) of t_k is helpful in nonlinear conjugate gradient field. In addition, since many choices on the self-scaling parameter τ_k have been proposed in [1, 25, 26, 27] and the references therein, we wonder if there exist any other members of the new family (1.12) which are more efficient than (2.28). This still remains under investigation.

As seen from Figure 3, the proposed dynamic restart strategy indeed contributes to the efficiency of Algorithm 4.1 (b). This is mainly based on the quantity r_{k-1} defined by (3.4), which

reflects how the function is close to some quadratic function in some sense. Another useful quantity in designing dynamical restart strategy is

$$\xi_{k-1} = \frac{g_k^T g_{k-1}}{\|g_k\|^2}. \quad (6.3)$$

Specifically, Powell [31] introduced the restart criterion $|\xi_{k-1}| \geq 0.2$ for Beale [2]'s three-term conjugate gradient method and obtained satisfactory numerical results. Such a restart criterion was also used by Shanno and his collaborator [34, 36] in building the CONMIN software. Therefore there is still a broad room how to develop more efficient restart strategy in the design of nonlinear conjugate gradient algorithms.

To extend the idea of this paper, we may consider the self-scaling memoryless Broyden family of methods, whose search direction is parallel to

$$\begin{aligned} d_{k+1} = & -g_{k+1} + \left[\theta_k \frac{y_k^T y_k}{s_k^T y_k} \left(\frac{g_{k+1}^T y_k}{y_k^T y_k} - \frac{g_{k+1}^T s_k}{s_k^T y_k} \right) - \tau_k \frac{g_{k+1}^T s_k}{s_k^T y_k} \right] s_k \\ & + \left[\frac{g_{k+1}^T y_k}{y_k^T y_k} + \theta_k \left(\frac{g_{k+1}^T s_k}{s_k^T y_k} - \frac{g_{k+1}^T y_k}{y_k^T y_k} \right) \right] y_k, \end{aligned} \quad (6.4)$$

where τ_k is the scaling parameter again and θ_k is the parameter related to the Broyden's family. By projecting the above direction into the one-dimensional manifold \mathcal{S} in (2.9), we can obtain the two-parameter family of methods where $d_{k+1} = -g_{k+1} + \beta_k(\tau_k, \theta_k) d_k$ and

$$\beta_k(\tau_k, \theta_k) = \left[\theta_k \left(\frac{y_k^T y_k}{d_k^T y_k} - \frac{d_k^T y_k}{\|d_k\|^2} \right) + \frac{d_k^T y_k}{\|d_k\|^2} \right] \frac{g_{k+1}^T y_k}{y_k^T y_k} - \left[\theta_k \left(\frac{y_k^T y_k}{s_k^T y_k} - \frac{s_k^T y_k}{s_k^T s_k} \right) + \tau_k \right] \frac{g_{k+1}^T s_k}{d_k^T y_k}. \quad (6.5)$$

If the line search is exact, in which case $g_{k+1}^T s_k = 0$, the above formula reduces to

$$\beta_k(\tau_k, \theta_k) = \left[\theta_k + (1 - \theta_k) \frac{(d_k^T y_k)^2}{\|d_k\|^2 \|y_k\|^2} \right] \frac{g_{k+1}^T y_k}{d_k^T y_k}. \quad (6.6)$$

Thus we can see that, the above two-parameter family of methods reduce to the linear conjugate gradient method only when $\theta_k = 1$, provided that the vectors d_k and y_k are not always parallel. Nevertheless, we might consider some dynamical ways of choosing θ_k . This remains under investigation.

Acknowledgements. The authors are very grateful to the anonymous referees for their useful suggestions and comments, which improved the quality of this paper.

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