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A new conjugate gradient method for acceleration of gradient descent algorithms

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ABSTRACT. An accelerated of the steepest descent method for solving unconstrained optimization problems is presented. which propose a fundamentally different conjugate gradient method, in which the well-known parameter β_k is computed by an new formula. Under common assumptions, by using a modified Wolfe line search, descent property and global convergence results were established for the new method. Experimental results provide evidence that our proposed method is in general superior to the classical steepest descent method and has a potential to significantly enhance the computational efficiency and robustness of the training process.

Mathematics Subject Classification (2020). 65K05, 90C25, 90C26, 90C27, 90C30.

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1. Introduction

Consider the 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. The line search method usually takes the following iterative formula

$$x_{k+1} = x_k + \alpha_k d_k, \quad (1.2)$$

for (1.1), where x_k is the current iterate point, $\alpha_k > 0$ is a steplength and d_k is a search direction. Different choices of d_k and α_k will determine different line search methods [10, 18, 13]. We denote $f(x_k)$ by f_k , $\nabla f(x_k)$ by g_k , and $\nabla f(x_{k+1})$ by g_{k+1} , respectively. $\|\cdot\|$ denotes the Euclidian norm of vectors and define $y_k = g_{k+1} - g_k$.

We all know that a method is called steepest descent method if we take $d_k = -g_k$ as a search direction at every iteration, which has wide applications in solving large-scale minimization problems [24, 25, 15]. One drawback of the method is often yielding zigzag phenomena in solving practical problems, which makes the algorithm converge to an optimal solution very slowly, or even fail to converge [21, 20].

If we take $d_k = -H_k g_k$ as a search direction at each iteration in the algorithm, where H_k is an $n \times n$ matrix approximating $[\nabla^2 f(x_k)]^{-1}$, then the corresponding method is called the Newton-like method [21, 20, 27] such as the Newton method, the quasi-Newton method, variable metric method, etc. Many papers have proposed this method for optimization problems [8, 9, 5].

However, the Newton-like method needs to store and compute matrix H_k at each iteration and thus adds to the cost of storage and computation. Accordingly, this method is not suitable to solve large-scale optimization problems in many cases.

The steepest descent method is one of the simplest and the most fundamental minimization methods for unconstrained optimization. Since it uses the negative gradient as its descent direction, it is also called the gradient method.

For many problems, the steepest descent method is very slow. Although the method usually works well in the early steps, as a stationnary point is approached, it descends very slowly with zigzagging phenomena. There are some ways to overcome these difficulties of zigzagging by defleting the gradient. Rather then moving along $d_k = -\nabla f(x_k) = -g_k$, we can move along

$$d_k = -D_k \nabla f(x_k),$$

or along

$$d_k = -g_k + h_k, \quad (1.3)$$

where D_k is an appropriate matrix and h_k is an appropriate vector.

Due to its simplicity and its very low memory requirement, the conjugate gradient method is a powerful line search method for solving the large-scale optimization problems. In fact, the CG method is not among the fastest or most robust optimization algorithms for nonlinear problems available today, but it remains very popular for engineers and mathematicians who are interested in solving large problems [12, 3, 11, 6, 28, 26]. The conjugate gradient method is designed to solve unconstrained optimization problem (1.1). More explicitly, the conjugate

gradient method is an algorithm for finding the nearest local minimum of a function of variables which presupposes that the gradient of the function can be computed. We consider only the case where the method is implemented without regular restarts. The iterative formula of the conjugate gradient method is given by (1.2), where α_k is a steplength which is computed by carrying out a line search, and d_k is the search direction defined by

$$d_{k+1} = \begin{cases} -g_k & \text{si } k = 1 \\ -g_{k+1} + \beta_k d_k & \text{si } k \geq 2 \end{cases} \quad (1.4)$$

where β_k is a scalar, and g_k denotes $g(x_k)$. Some well known formulas for β_k are given as follows:

$$\begin{aligned} \beta_k^{HS} &= \frac{g_{k+1}^T y_k}{d_k^T y_k}, \beta_k^{FR} = \frac{\|g_{k+1}\|^2}{\|g_k\|^2}, \beta_k^{PRP} = \frac{g_{k+1}^T y_k}{\|g_k\|^2}, \beta_k^{CD} = -\frac{\|g_{k+1}\|^2}{d_k^T g_k} \\ \beta_k^{LS} &= -\frac{g_{k+1}^T y_k}{d_k^T g_k}, \beta_k^{DY} = \frac{\|g_{k+1}\|^2}{d_k^T y_k}, \beta_k^{HZ} = \left(y_k - 2d_k \frac{\|y_k\|^2}{d_k^T y_k} \right)^T \frac{g_{k+1}}{d_k^T y_k} \end{aligned}$$

The above corresponding methods are known as Hestenes–Stiefel (HS) method [16], the Fletcher–Reeves (FR) method [14], the Polak–Ribière–Polyak (PR) method (see [23, 4]), the Conjugate Descent method (CD) [14], the Liu–Storey (LS) method [19], the Dai–Yuan (DY) method [12], and Hager and Zhang (HZ) method [17], respectively.

In the convergence analysis and implementation of conjugate gradient methods, one often requires the inexact line search such as the Wolfe conditions or the strong Wolfe conditions. The Wolfe line search is to find α_k such that

$$f(x_k + \alpha_k d_k) \leq f(x_k) + \delta \alpha_k g_k^T d_k \quad (1.5)$$

$$d_k^T g(x_k + \alpha_k d_k) \geq \sigma d_k^T g_k, \quad (1.6)$$

with $\delta < \sigma < 1$. The strong Wolfe line search is to find α_k such that

$$f(x_k + \alpha_k d_k) \leq f(x_k) + \delta \alpha_k g_k^T d_k \quad (1.7)$$

$$\left| d_k^T g(x_k + \alpha_k d_k) \right| \leq -\sigma d_k^T g_k, \quad (1.8)$$

where $\delta < \sigma < 1$ are constants.

The convergence behavior of the above formulas with some line search conditions has been studied by many authors for many years.

Al-Baali [1] has proved the global convergence of the FR method for nonconvex functions with the strong Wolfe line search if the parameter $\sigma < \frac{1}{2}$. The PRP method with exact line search may cycle without approaching any stationary point, see Powell's counter-example [22]. Although one would be satisfied with its global convergence properties, the FR method sometimes performs much worse than the PRP method in real computations. A similar case happen to the DY method and the HS method.

In next section, we will state the idea of the new method, then a new algorithm will be developed. Descent property and the global convergence will be established in Section 3. Section 4 is devoted to numerical experiments by implementing the algorithm to solve many large-scale benchmark test problems. The conclusions are presented in Section 5.

2. The new formula and the corresponding algorithm

In this section, we shall state the idea to propose a new conjugate gradient method and develop a new algorithm.

In this paper, based the modified strong Wolfe type line search, under some mild conditions, we give the Descent property and global convergence of the new β_k which is known as β_k^{BRB} , where *BRB* denotes **Belloufi, Rahali and Benzine**. Then we can define the following formulas β_k to compute the search directions in (1.4).

$$\beta_k^{BRB} = \frac{\|g_{k+1}\|^2}{\|d_k\|^2} \quad (2.1)$$

With the constructed search direction, we find a stepsize by the modified strong Wolfe line search strategy:

Modification of the strong Wolfe line search

The step length is computed by performing a line search along d_k . In practice, a relevant choice is to compute α_k according to the realization of the modified strong Wolfe conditions, namely

$$f(x_k + \alpha_k d_k) - f(x_k) \leq \delta \alpha_k g_k^T d_k \quad (2.2)$$

$$\left| g(x_k + \alpha_k d_k)^T d_k \right| \leq -\sigma g_k^T d_k \frac{\|d_k\|^2}{\|g_k\|^2} \quad (2.3)$$

The algorithm is given as follows:

algorithm Step 0: Given $x_1 \in \mathbb{R}^n$, set $d_1 = -g_1$, $k := 1$.

Step 1: If $\|g_k\| = 0$ then stop else go to Step 2.

Step 2: Set $x_{k+1} = x_k + \alpha_k d_k$ where d_k is defined by (1.4), (2.1) and α_k is defined by (2.2), (2.3).

Step 3: Set $k := k + 1$ and go to Step 1.

3. Descent property and global convergence

The following theorem indicates that, in the inexact case, the search direction d_k satisfies descent property.

Theorem 3.1. *If an α_k is calculated wich satisfies modified strong Wolfe line search (2.2) and (2.3) with $\sigma \in \left] 0, \frac{1}{2} \right]$, $\forall k$ then for the new conjugate gradient method, the inequality*

$$-\sum_{j=0}^{k-1} \sigma^j \leq \frac{g_k^T d_k}{\|g_k\|^2} \leq -2 + \sum_{j=0}^{k-1} \sigma^j \quad (3.1)$$

holds for all k , and hence the descent property

$$g_k^T d_k < 0, \forall k \quad (3.2)$$

holds, as long as $g_k \neq 0$.

Proof. The proof is by induction. For $k = 1$ Equations (3.1) and (3.2) is clearly satisfied.

Now we suppose that (3.1) and (3.2) hold for any $k \geq 1$.

It follows from the definition (1.4) and (2.1) of d_{k+1} that

$$\frac{g_{k+1}^T d_{k+1}}{\|g_{k+1}\|^2} = -1 + \frac{g_{k+1}^T d_k}{\|d_k\|^2} \quad (3.3)$$

and hence from (2.3) and (3.2) that

$$-1 + \sigma \frac{g_k^T d_k}{\|g_k\|^2} \leq \frac{g_{k+1}^T d_{k+1}}{\|g_{k+1}\|^2} \leq -1 - \sigma \frac{g_k^T d_k}{\|g_k\|^2} \quad (3.4)$$

Also, by induction assumption (3.1), we have

$$\begin{aligned} -\sum_{j=0}^k \sigma^j &= -1 - \sigma \sum_{j=0}^{k-1} \sigma^j \leq \frac{g_{k+1}^T d_{k+1}}{\|g_{k+1}\|^2} \\ &\leq -1 + \sigma \sum_{j=0}^{k-1} \sigma^j = -2 + \sum_{j=0}^k \sigma^j \end{aligned}$$

Then, (3.1) holds for $k + 1$.

Since

$$g_{k+1}^T d_{k+1} \leq \|g_{k+1}\|^2 \left(-2 + \sum_{j=0}^k \sigma^j \right) \quad (3.5)$$

and

$$\sum_{j=0}^k \sigma^j < \sum_{j=0}^{\infty} \sigma^j = \frac{1}{1 - \sigma} \quad (3.6)$$

where $\sigma \in \left] 0, \frac{1}{2} \right]$, it follows from $1 - \sigma > \frac{1}{2}$ that $-2 + \sum_{j=0}^k \sigma^j < 0$. Hence, from (3.5), we obtain

$g_{k+1}^T d_{k+1} < 0$. We complete the proof by induction.

In order to establish the global convergence of the proposed method, we assume that the following assumption always holds, i.e. Assumption 3.1 :

Assumption 3.1 :

Let f be twice continuously differentiable, and the level set $L = \{x \in \mathbb{R}^n \mid f(x) \leq f(x_1)\}$ be bounded

Theorem 3.2. Suppose that x_1 is a starting point for which Assumption 3.1 holds. Consider the New method (1.4) and (2.1). If the steplength α_k is computed by the modified strong Wolfe line search (2.2) and (2.3) with $\delta < \sigma < \frac{1}{2}$ and if

$$\frac{1}{\|d_{k-1}\|^4} \leq \frac{1}{\|g_{k-1}\|^4} \quad (3.7)$$

then the method is globally convergent, i.e.,

$$\liminf_{k \rightarrow \infty} \|g_k\| = 0 \quad (3.8)$$

Proof. It is shown in theorem 1 that the descent property (3.2) holds for $\sigma \in \left]0, \frac{1}{2}\right]$, so from (2.3), (3.1), and (3.6) it follows that

$$\left|g_k^T d_{k-1}\right| \leq -\sigma g_{k-1}^T d_{k-1} \frac{\|d_{k-1}\|^2}{\|g_{k-1}\|^2} \leq \|d_{k-1}\|^2 \sigma \sum_{j=0}^{k-2} \sigma^j = \|d_{k-1}\|^2 \sum_{j=0}^{k-1} \sigma^j \leq \frac{\sigma}{1-\sigma} \|d_{k-1}\|^2 \quad (3.9)$$

Thus from the definition of d_k and using (2.1) and (3.9) we deduce that

$$\begin{aligned} \|d_k\|^2 &= \|g_k\|^2 - 2\beta_{k-1} g_k^T d_{k-1} + \beta_{k-1}^2 \|d_{k-1}\|^2 \\ &\leq \|g_k\|^2 + \frac{2\sigma}{1-\sigma} \beta_k \|d_{k-1}\|^2 + \beta_{k-1}^2 \|d_{k-1}\|^2 \\ &= \left(\frac{1+\sigma}{1-\sigma}\right) \|g_k\|^2 + \frac{\|g_k\|^4}{\|d_{k-1}\|^4} \|d_{k-1}\|^2 \\ &\leq \left(\frac{1+\sigma}{1-\sigma}\right) \|g_k\|^2 + \frac{\|g_k\|^4}{\|g_{k-1}\|^4} \|d_{k-1}\|^2 \end{aligned} \quad (3.10)$$

where we used the facts that

$$\frac{1}{\|d_{k-1}\|^4} \leq \frac{1}{\|g_{k-1}\|^4}$$

By applying this relation repeatedly, it follows that

$$\|d_k\|^2 \leq \left(\frac{1+\sigma}{1-\sigma}\right) \|g_k\|^4 \sum_{j=1}^k \frac{1}{\|g_j\|^2} \quad (3.11)$$

Now we prove (3.8) by contradiction. It assumes that (3.8) does not hold, then there exists a constant $\varepsilon > 0$ such that

$$\|g_k\| \geq \varepsilon > 0 \quad (3.12)$$

holds for all k sufficiently large. Since g_k is bounded above on the level set L , it follows from (3.11) that

$$\|d_k\|^2 \leq c_1 k \quad (3.13)$$

where c_1 is a positive constant. From (3.1) and (3.6), we have

$$\cos \theta_k \geq \left(\frac{1-2\sigma}{1-\sigma}\right) \frac{\|g_k\|}{\|d_k\|} \quad (3.14)$$

Since $\sigma < \frac{1}{2}$, substituting (3.13) and (3.12) into (3.14) gives

$$\sum_k \cos^2 \theta_k \geq \left(\frac{1-2\sigma}{1-\sigma}\right)^2 \sum_k \frac{\|g_k\|^2}{\|d_k\|^2} \geq c_2 \sum_k \frac{1}{k} \quad (3.15)$$

where c_2 is a positive constant. Therefore, the series $\sum_k \cos^2 \theta_k$ is divergent.

Let M be an upper bound of $\|\nabla^2 f(x)\|$ on the level set L , then

$$g_{k+1}^T d_k = \left(g_k + a_k \nabla^2 f(x)\right)^T d_k \leq g_k^T d_k + M a_k \|d_k\|^2$$

Thus by using (2.3) and (3.7) we obtain

$$a_k \geq -\frac{(1-\sigma)}{M \|d_k\|^2} g_k^T d_k \quad (3.16)$$

Substituting a_k of (3.16) into (2.2) gives

$$f_{k+1} \leq f_k - c_3 \|g_k\|^2 \cos^2 \theta_k,$$

where $c_3 = \frac{(1-\sigma)\delta}{M} > 0$. Since $f(x)$ is bounded below, $\sum_k \|g_k\|^2 \cos^2 \theta_k$ converges, which indicates that $\sum_k \cos^2 \theta_k$ converges by use of (3.12). This fact contradicts (3.15). We complete the proof.

4. Numerical results and discussions

In this section we report some numerical results obtained with a Fortran implementation of gradient algorithms and their accelerated variants. All codes are written in Fortran and compiled with f77 (default compiler settings) on a Workstation Intel(R) core(TM), i3@ 2.20GHz. We selected a number of 75 large-scale unconstrained optimization test functions in generalized or extended form [2]. For each test function we have considered ten numerical experiments with the number of variables $n = 1000, 2000, \dots, 10000$. In the following we present the numerical performance of CG and ACG codes corresponding to different formula for β_k computation. All algorithms implement the Wolfe line search conditions with $\rho = 0.0001$ and $\sigma = 0.9$, and the same stopping criterion $\|g_k\|_\infty \leq 10^{-10}$, where $\|\cdot\|_\infty$ is the maximum absolute component of a vector.

The comparisons of algorithms are given in the following context. Let f_i^{ALG1} and f_i^{ALG2} be the optimal value found by ALG1 and ALG2, for problem $i = 1, \dots, 750$, respectively. We say that, in the particular problem i , the performance of ALG1 was better than the performance of ALG2 if:

$$|f_i^{ALG1} - f_i^{ALG2}| < 10^{-3},$$

and the number of iterations, or the number of function-gradient evaluations, or the CPU time of ALG1 was less than the number of iterations, or the number of function-gradient evaluations, or the CPU time corresponding to ALG2, respectively.

We compare the New method CGBRB with the steepest descent method, the CG_DESCENT method, and PRP conjugate gradient method.

Figures 1–4 list the performance of the CGBRB, steepest descent, CG_DESCNET and PRP conjugate gradient methods. Relative to CPU time, the number of iterations and the number of gradient evaluations, respectively, which were evaluated using the profiles of Dolan and Moré [7].

Clearly, Figures 1–4 present that our proposed method CGBRB exhibits the best overall performance since it illustrates the highest probability of being the optimal solver, followed by the steepest descent, CG_DESCNET, and PRP conjugate gradient methods relative to all performance metrics.

FIGURE 1. Performance based on CPU time.

FIGURE 2. Performance based on the number of iterations.

FIGURE 3. Performance based on the number of function evaluations.

FIGURE 4. Performance based on the number of gradient evaluations.

5. Conclusion

We have presented a new conjugate gradient algorithm for solving unconstrained optimization problems. Under the modified strong Wolfe line search conditions we proved the descent property and global convergence of the algorithm. For the test problems, the comparison of the numerical results shows that the new algorithms is a good search direction at every iteration.

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