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A new Non-monotone Spectral Conjugate Gradient method for Unconstrained Optimization

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Abstract

In this paper, we combine spectral Conjugate Gradient method which combines the conjugate gradient direction with spectral step-length effectively with a non-monotone line search technique and we obtain a new algorithm. besides, in this spectral Conjugate Gradient method the spectral step-length is applied to the entire Conjugate Gradient direction rather than the negative gradient direction, The global convergent properties of the algorithm are proved under some appropriate conditions.

Mathematics Subject Classification: xxxxx

Keywords: Spectral conjugate Gradient method, nonmonotone line search, global convergence, unconstrained optimization

1 Introduction

Consider the following unconstrained optimization problem:

$$\min f(x),\ x \in R^n \tag{1}$$

Where $f : R^n \to R$ is a twice continuously differentiable function. Throughout this paper, we use the following notation:$\|\cdot\|$ is the Euclidean norm. $g(x) = \nabla f(x) \in R^n$ and $H(x) \in R^{n*n}$ are the gradient and Hessian matrix of f evaluated at the point of x, respectively. $f_k = f(x_k)$, $g_k = g(x_k)$,$H_k = \nabla^2 f(x_k)$ and B_k is a symmetric matrix which is eitherH_k or an approximation of H_k.

Unconstrained optimization problem is an important research topic in mathematical programming fields. There are some methods for solving unconstrained optimization problem, such as feasible direction algorithm, gradient-type methods, Newton-type and so on. It is well-known that conjugate gradient method is a good method for solving the unconstrained optimization problem in management and engineering. It has the following formula for solving problem (1):

$$x_{k+1} = x_k + \alpha_k d_k$$

$$d_k = \begin{cases} -g_k, & k = 0, \\ -g_k + \beta_k d_{k-1}, & k \geq 1. \end{cases}$$

where d_k is a search direction, β_k is a scalar, $g_k = \nabla f(x_k)$, α_k is a positive step-size along the search direction.

In many literatures(refer to [1-3]), the main thing is to choose the scalar β_k, which leads to many different conjugate gradient methods according to the different β_k. A well-known conjugate gradient method was proposed by Fletcher and Reeves[1], and some other choices as followed:

$$\beta_k^{HS} = \frac{g_k^T y_{k-1}}{d_{k-1}^T y_{k-1}}, \beta_k^{FR} = \frac{\|g_k\|^2}{\|g_{k-1}\|^2},$$

$$\beta_k^{PRP} = \frac{g_k^T y_{k-1}}{\|g_{k-1}\|^2}, \beta_k^{CD} = -\frac{\|g_k\|^2}{d_{k-1}^T g_{k-1}},$$

$$\beta_k^{LS} = -\frac{g_k^T y_{k-1}}{d_{k-1}^T y_{k-1}}, \beta_k^{DY} = \frac{\|g_k\|^2}{d_{k-1}^T y_{k-1}},$$

where $\| \cdot \|$ denotes Euclidean norm,$y_{k-1} = g_k - g_{k-1}$.

Raydan introduced the spectral gradient method (SGM) for potentially large-scale unconstrained optimization[4]. The main feature of this method is that only gradient directions are used at each line search whereas a non-monotone strategy guarantees global convergence. The idea of nonmonotone technique can be traced back to Grippo et al. in 1988 [5], thanks its excellent numerical exhibition, many non-monotone techniques have been developed in recent years, for example, non-monotone line search approaches, and non-monotone trust region methods.

In this paper, we combined a new nonmonotone techniques with the spectral conjugate gradient method to obtain a more efficient algorithm, in this spectral Conjugate Gradient method the parameter β_k is chosen from Yasushi-Narushima and HiroshiYabe [6], in addition, We will apply spectral step-length to the entire Conjugate Gradient direction instead of the negative gradient direction, and take advantage of a new non-monotone line search technique[7] by Zhang and W.Hager to obtain the next iteration point.

The rest of this paper is organized as follow. in section 2, we introduce the spectral conjugate gradient methods, non-monotone line search and the new algorithm is proposed, in section 3, the global convergences of the algorithm are established.

2 A new Non-monotone Spectral Conjugate Gradient Algorithm

2.1 Spectral Conjugate Gradient

In this subsection, we will give a new spectral conjugate gradient. assume that $f : R^n \to R$ has continuous partial derivatives. The problem considered in this paper is formulation (1)

The iteration formulation for (2) is as follows:

$$x_{k+1} = x_k + \alpha_k d_k$$

where d_k is a search direction and α_k is a step length chosen to induce the value of $f(x)$, the direction is generated by

$$d_k = -\theta_k g_k + \beta_k d_k,$$

where g_k denotes $\nabla f(x_k)$ and $d_k = -\theta_0 g_0$ and θ_k is a arbitrary parameter

$$\beta_k = \frac{(\theta_k y_{k-1} + s_{k-1})^T g_k}{d_{k-1}^T y_{k-1}},$$

where $s_k = x_{k+1} - x_k = \alpha_k d_k$ and $y_k = g_{k+1} - g_k$.

In general, we denote θ_k as

$$\theta_k = \frac{s_{k-1}^T s_{k-1}}{s_{k-1}^T g_{k-1}}([8])$$

we give the conjugate gradient direction proposed by Yu, where the parameter chosen from Yasushi Narushima and Hiroshi Yabe [6]

Set d_k^1

$$d_k^1 = -g_k + \beta_k d_{k-1},$$

Where

$$\beta^{RY} = \begin{cases} 0, & g_k^T d_{k-1} \leq 0 \\ \frac{\|g_k\|^2}{g_k^T d_{k-1} + \|g_k^T\| \|d_{k-1}\|}, & otherwise. \end{cases}$$

and, we define spectral conjugate gradient as follow:

$$d_k = \theta_k d_k^1, \tag{2}$$

The definition of parameter θ_k will be given in the following algorithm 2.1.

2.2 Nonmonotone line search

After the direction is determined d_k, In this subsection, the next task is to find a step size α_k along the search direction. The ideal line search rule is the exact one which satisfies:

$$f(x_k + \alpha_k d_k) = \min_{\alpha > 0} f(x_k + \alpha d_k)$$

in fact, the exact step size is difficult or even impossible to seek in practical computation, and thus many researchers constructed some inexact line search rule, such as Armijo rule, Goldtein rule, Wolfe rule and non-montone line search[9].

In 1982, Chamberlain et al. in [10] proposed a watchdog technique for constrained optimization, in which some standard line search conditions were relaxed to overcome the Marotos effect. Motivated by this idea, Grippo, Lampariello and Lucidi in [9] presented a non-monotone Armijo type line search technique for the Newton method. The traditional line search rules require the function value descent monotonically at each iteration. It may considerably slow the rate of convergence in the intermediate stages of the minimization process, especially in the presence of the narrow curved valley. However the non-monotone line search rules are effective or even powerful at some iteration, especially when the iterates are trapped in a narrow curved valley of objective functions.

The earliest non-monotone line search framework was developed by Grippo, Lampariello and Lucidi in[9] for Newton's methods. before introduce the new non-monotone technique, we describe the non-monotone Armijo rule. α_k is a stepsize with $\alpha_k \geq 0$ and d_k is a search direction satisfied $g_k^T d_k \leq 0$, Let $a > 0$, $\gamma \in (0,1)$, $\beta \in (0,1)$and let M be a nonnegative integer. For each k , let $m(k)$ satisfies

$$m(0) = 0, 0 \leq m(k) \leq \min[m(k-1)+1, M], for\ k \geq 1,$$

Let $\alpha_k = \beta^{p^k} a$ and p^k be the smallest nonnegative integer p such that

$$f(x_k + \alpha_k) \leq \max_{0 \leq j \leq m(k)} [f(x_{k-j})] + \gamma \beta^{p^k} a g_k^T d_k.$$

If the search is the nonmonotone Goldstein line search, so α_k should satisfied the following condition:

$$f(x_k + \alpha_k) \leq \max_{0 \leq j \leq m(k)} [f(x_{k-j})] + \mu_1 \lambda_k g_k^T d_k,$$

$$f(x_k + \alpha_k) \leq \max_{0 \leq j \leq m(k)} [f(x_{k-j})] + \mu_2 \lambda_k g_k^T d_k,$$

where $0 < \mu_1 \leq \mu_2 < 1$

If the search is the nonmonotone wolfe line search, so α_k should satisfied the following condition:

$$f(x_k + \alpha_k) \leq \max_{0 \leq j \leq m(k)} [f(x_{k-j})] + \gamma_1 \alpha_k g_k^T d_k,$$

$$g(x_k + \alpha_k d_k)^T d_k \geq \gamma_2 g_k^T d_k,$$

where $0 < \gamma_1 \leq \gamma_2 < 1$

the nonmonotone line search methods have been studied by many authors Toint (1996); Dai (2002); Zhang and Hager (2004); Shi and Shen (2006); Yu and Pu (2008); Hadi Nosratipour (2013). Theoretical analysis and numerical results show that the nonmonotone algorithms are very efficient.

Although these nonmonotone technique work well in many case, there are some drawbacks, First, a good function value generated in any iteration is essentially discard due to the max. Second, in some case, the numerical performance is very dependent on the choice of M [9.4.11] now we give a new nonmonotone line search proposed by Zhang and W.Hager as follows: [7]

Initialization : Choose starting guess x_0, and parameter $0 \leq \eta_{min} \leq \eta_{max} \leq 1$, $0 < \delta < 1 < \rho$ and $\mu > 0$. Set $C_0 = f(x_0)$, $Q_0 = 1$, and $k = 0$.

Convergence test : If $\|\nabla f(x_k)\|$ sufficiently small, then stop.

Line search update : Set $x_{k+1} = x_k + \alpha_k d_k$ Where α_k satisfies the non-monotone Armijo condition:$\alpha_k = \bar{\alpha}_k \rho^{h_k}$.

$$f(x_k + \alpha_k d_k) \leq C_k + \delta \alpha_k \nabla f(x_k) d_k,$$

Where $\bar{\alpha}_k > 0$ is the trial step, and h_k is the largest integer such that Line search update holds and $\alpha_k \leq \mu$.

Cost update : Choose $\eta_k \in [\eta_{min}, \eta_{max}]$, and set

$$Q_{k+1} = \eta_k Q_k + 1, C_{k+1} = (\eta_k Q_k C_k + f(k+1))/Q_{k+1}$$

Replace k by $k + 1$ and return to the convergence test.

Observe that C_k is a convex combination of C_k and $f(x_{k+1})$.Since $C_0 = f(x_0)$,it follows that C_k is a convex combination of the function values $f(x_0)$, $f(x_1)$,$f(x_2)$,$\cdots$,$f(x_k)$.The choice of η_k controls the degree of nonmonotonicity. If $\eta_k = 0$ for each k, then the line is the usual monotone Armijo line search. If $\eta_k = 1$ for each k, then $C_k = A_k$, where

$$A_k = \frac{1}{k+1} \sum_{i=0}^{k} f_i, f_i = f(x_i),$$

is the average function value. the scheme with $C_k = A_k$ was suggested to us by Yu-hong Dai. In [12], the possibility of comparing the current function value with an average was analyzed.

2.3 Algorithm model

Now, we state the algorithm which combine spectral Conjugate Gradient method which combines the conjugate gradient direction with spectral step-length effectively with a non-monotone line search technique. In this algorithm we can obtain the best convergence result by choosing varying η_k dynamically, using values closer to 1 when the iterates were far from the optimum, and using values closer to 0 when the iterates were near an optimum.

Algorithm 2.1

Step0. Give starting guess x_1, and some constants, $0 \leq \eta_{min} \leq \eta_{max} \leq 1$,$0 < \beta < 1$, $0 < \delta < 1$, $\eta \in (\frac{1}{2}, 1)$ Set $C_1 = f(x_1)$, $Q_1 = 1$, and $k = 1$.

Step1. Compute g_k, and $\|g_k\| \leq \varepsilon$, STOP.

Step2. Compute d_k by (2).

Step3 Set trial step $\alpha_k = 1$.

Step4 Line search update:

$$f(x_k + \alpha_k d_k) \leq C_k + \delta \alpha_k \nabla f(x_k) d_k, \tag{3}$$

Where α_k satisfies the nonmonotone Armijo condition: $\alpha_k = \alpha_k \beta^{h_k}$. h_k is the smallest integer such that (3) holds.

Cost update: Choose $\eta_k \in [\eta_{min}, \eta_{max}]$, and set

$$Q_{k+1} = \eta_k Q_k + 1, C_{k+1} = (\eta_k Q_k C_k + f(k+1))/Q_{k+1} \tag{4}$$

Step5 Set $x_{k+1} = x_k + \alpha_k d_k$.

Step6. Set $k := k + 1$, and go to step 1 .

3 Convergence analysis

In this section, we discuss the global convergence property of algorithm with the new nonmonotone line search. In order to achieve the convergence of the algorithm, we give some Assumptions as follow:

Assumption 3.1

A: f(x) is bounded above on the level set $L = \{x | f(x) \leq f(x_0)\}$

B: In some neighborhood Ω of L, f is continuously differentiable, and its gradient $\nabla f(x)$ is Lipschitz continuous, namely, there exists a constant L such that

$$\|\nabla f(x) - \nabla f(x_k)\| \leq L\|x - x_k\|$$

Lemma 3.1 d_k is computed by (2), then we have

$$g_k^T d_k \leq -\frac{\theta_{min}}{2}\|g_k\|^2 \tag{5}$$

for any $k \geq 1$.

Proof: if $\beta_k = 0$ then $d_k = -\theta_k g_k$, since $\theta_k \geq \theta_{min} \geq 0$, so

$$g_k^T d_k = -\theta_k \|g_k\|^2 \leq -\frac{\theta_{min}}{2}\|g_k\|^2$$

if $\beta > 0$ by the definition of d_k , we have

$$\begin{aligned} g_k^T d_k =& \theta_k(-\|g_k\|^2 + \beta_k g_k^T d_{k-1}) \\ \leq& \theta_k(-\|g_k\|^2 + \frac{\|g_k\|^2}{2 g_k^T d_{k-1}} g_k^T d_{k-1}) \\ \leq& -\frac{\theta_k}{2}\|g_k\|^2 \\ \leq& -\frac{\theta_{min}}{2}\|g_k\|^2. \end{aligned}$$

Lemma 3.2 d_k is computed by (2),then for any $k \geq 1$ we have

$$\|d_k\| \leq 2\theta_{max}\|g_k\| \tag{6}$$

Proof: If $\beta_k = 0$, by the definition of $d_k = -\theta_k g_k$ we have $\|d_k\| = \theta_k\|g_k\|$, and then $\|d_k\| = 2\theta_k\|g_k\|$
If $\beta_k > 0$, by the definition of $d_k = \theta_k(-g_k + \frac{\|g_k\|^2}{g_k^T d_k + \|g_k\|\|d_k\|} d_{k-1})$, now $g_k^T d_{k-1} > 0$ so the angle between d_{k-1} and $-g_k$ is an obtuse angle.

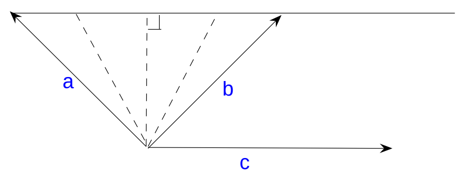

Figure 1: The relationship between d_{k-1} and $-g_k$

where $a = -\theta_k g_k$, $b = -d_k$, $c = \frac{\theta_k\|g_k\|^2}{g_k^T d_{k-1} + \|g_k\|\|d_{k-1}\|} d_{k-1}$. and $\|\cdot\|$ is the Euclidean norm, $\|d_k\|$is the norm of d_k, then

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

when $d_k \cdot d_{k-1} < 0$, $\|d_k\| \leq \theta_k\|g_k\|$, we have $\|d_k\| \leq 2\theta_{max}\|g_k\|$

when $d_k \cdot d_{k-1} > 0$,

$$\begin{aligned}\|d_k\| =& \| -\theta_k g_k + \frac{\|g_k\|^2}{g_k^T d_{k-1} + \|g_k\|\|d_{k-1}\|} d_{k-1}\| \\ \leq& \theta_k g_k + \| \frac{\theta_k \|g_k\|^2}{\|g_k\|\|d_{k-1}\|} d_{k-1}\| \\ =& \theta_k g_k + \frac{\theta_k \|g_k\|^2}{\|g_k\|\|d_{k-1}\|} \|d_{k-1}\| \\ =& 2\theta_k \|g_k\|.\end{aligned}$$

so we have $\|d_k\| \leq 2\theta_{max}\|g_k\|$, (6)holds end.

Lemma 3.3 If $\nabla f(x_k)d_k \leq 0$ for each k, then for the iterates generated by the algorithm (2.1), we have $f(x_k) \leq C_k \leq A_k$ for each k. Moreover, if $\nabla f(x_k)d_k < 0$ and $f(x_k)$ is bounded from below, then there exists α_k satisfying Armijo conditions of the line search update.

Proof: Defining $D_k : R \to R$ by

$$D_k(t) = \frac{tC_{k-1} + f_k}{t+1},$$

we have

$$D_k^{'}(t) = \frac{C_{k-1} - f_k}{(t+1)^2},$$

Since $\nabla f(x_k)d_k \leq 0$, it follows from (3) that $f_k \leq C_{k-1}$, which implies that $D_k^{'} \geq 0$ for all $t \geq 0$, Hence, D_k is nondecreasing, and $f_k = D_k(0) \leq D_k(k)$ for all $t \geq 0$. in particular, taking $t = \eta_{k-1}Q_{k-1}$ gives

$$f_k = D_k(0) \leq D_k(\eta_{k-1}Q_{k-1}) = C_k.$$

the upper bound $C_k \leq A_k$ is proved by induction. For $k = 0$ this holds by initialization $C_0 = f(x_0)$. Now assume that $C_j \leq A_j$ for all $0 \leq j < k$. by (4), the initialization $Q_0 = 1$, and the fact that $\eta_k \in [0, 1]$, we have

$$Q_{j+1} = 1 + \sum_{i=0}^{j} \prod_{m=0}^{i} \eta_{j-m} \leq j + 2. \tag{7}$$

Since D_k is monotone nondecreasing, (7) imply that

$$C_k = D_k(\eta_{k-1}Q_{k-1}) = D_k(Q_k - 1) \leq D_k(k). \tag{8}$$

By the induction step,

$$D_k(k) = \frac{kC_{k-1} + f_k}{k+1} \leq \frac{kA_{k-1} + f_k}{k+1} = A_k, \tag{9}$$

Relation (8) and (9),we have the upper bound of C_k.

In fact, when $\alpha_k = 0$, $f(x_k + \alpha_k d_k) = f(x_k)$ there must exist a sufficient small α_k

$$f(x_k + \alpha_k d_k) \leq f_k + \delta\alpha_k \nabla f(x_k)d_k,$$

because of $\nabla f(x_k)d_k \leq 0$ and $0 < \delta < 1$. what is more, $f(x_k) \leq C(x_k)$, So we have

$$f(x_k + \alpha_k d_k) \leq C_k + \delta\alpha_k \nabla f(x_k)d_k.$$

Lemma 3.4 As we are known, α_k is generated by step(4), so α_k satisfies (3), If assumption 3.1 holds, we have

$$\alpha_k \geq \frac{2\beta(1-\delta)|g_k^T d_k|}{L\|d_k\|^2}. \tag{10}$$

Proof: by algorithm 2.1 we have $\alpha_k \leq 1$, and $\alpha_k = \alpha_k \beta^{h_k}$, h_k is the smallest integer such that (3) holds. since we have

$$f(x_k + \frac{\alpha_k}{\beta}d_k) > C_k + \delta\frac{\alpha_k}{\beta}g_k^T d_k \geq f(x_k) + \delta\frac{\alpha_k}{\beta}g_k^T d_k \tag{11}$$

while ∇f is Lipschitz continuous,

$$\begin{aligned} f(x_k + \alpha d_k) - f(x_k) =& \alpha g_k^T d_k + \int_0^\alpha [\nabla f(x_k + td_k) - \nabla f(x_k)]d_k dt \\ \leq& \alpha g_k^T d_k + \int_0^\alpha tL\|d_k\|^2 dt \\ =& \alpha g_k^T d_k + \frac{1}{2}L\alpha^2\|d_k\|^2. \end{aligned}$$

Theorem 3.1 The iterates x_k generated by the algorithm 2.1, then we have the property that

$$\lim_{k\to\infty} \nabla f(x_k) = 0. \tag{12}$$

Hence, every convergent subsequence of the iterates approaches a point x^*, where $\nabla f(x^*) = 0$.

Proof: we first show that

$$f_{k+1} \leq C_k - \varphi\|g_k\|^2, \tag{13}$$

where

$$\varphi = \frac{\delta\beta(1-\delta)\theta_{min}^2}{8L\theta_{max}^2},$$

by step 4 we known $\alpha \leq 1$ and by (10)

$$\alpha_k \geq \frac{2\beta(1-\delta)|g_k^T d_k|}{L\|d_k\|^2}.$$

and by (3) we have

$$f_{k+1} \leq C_k - \frac{2\delta\beta(1-\delta)}{L}(\frac{g_k^T d_k}{\|d_k\|})^2$$

Finally, with lemma3.1 lemma3.2

$$f_{k+1} \leq C_k - (\frac{\delta\beta(1-\delta)\theta_{min}^2}{8L\theta_{max}})\|g_k\|^2$$

which implies (13) Combine the cost update (4) and upper bound (13)

$$\begin{aligned} C_{k+1} =& \frac{\eta_k Q_k C_k + f_{k+1}}{Q_{k+1}} \\ \leq& \frac{\eta_k Q_k C_k + C_k - \varphi\|g_k\|^2}{Q_{k+1}} \\ =& C_k - \frac{\varphi\|g_k\|^2}{Q_{k+1}} \end{aligned} \tag{14}$$

Since f is bounded from below and $f_k \leq C_k$ for all k, we can conclude that C_k is bounded from below. It follows from (14) that

$$\sum_{k=0}^{\infty} \frac{\|g_k\|^2}{Q_{k+1}} < \infty. \tag{15}$$

because of $\eta_{max} < 1$,then by (7) we have

$$Q_{k+1} = 1 + \sum_{j=0}^{k}\prod_{i=0}^{j}\eta_{k-i} \leq 1 + \sum_{j=0}^{k}\eta_{max}^{j+1} \leq \sum_{j=0}^{\infty}\eta_{max}^{j} = \frac{1}{1-\eta_{max}}.$$

Consequently, (15) implies $\lim_{k\to\infty}\|g_k\| = 0$.

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