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Two-versions of descent conjugate gradient methods for large-scale unconstrained optimization

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ABSTRACT

The conjugate gradient methods are noted to be exceedingly valuable for solving large-scale unconstrained optimization problems since it needn't the storage of matrices. Mostly the parameter conjugate is the focus for conjugate gradient methods. The current paper proposes new methods of parameter of conjugate gradient type to solve problems of large-scale unconstrained optimization. A Hessian approximation in a diagonal matrix form on the basis of second and third-order Taylor series expansion was employed in this study. The sufficient descent property for the proposed algorithm are proved. The new method was converged globally. This new algorithm is found to be competitive to the algorithm of fletcher-reeves (FR) in a number of numerical experiments.

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1. INTRODUCTION

The problem of unconstrained optimization is generally formulated as:

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

where $f \rightleftarrows\rightleftarrows: R^n \to R^1$ is a function that is continuously differentiable. Numerous famous techniques are found for solving (1); however, the conjugate gradient (CG) techniques are the mainly characterized ones. Newton technique is famous if the gradient matrix is non negative definite, for more details see [1]. These CG-techniques are in the variety of iterations known by:

$$x_0 \in R^n, x_{k+1} = x_k + \lambda_k S_k \tag{2}$$

where λ_k is the step length , as a rule obtained by the Wolfe line search:

$$f(x_k) - f(x_k + \lambda_k S_k) \geq -\alpha \lambda_k \eta_k^T S_k \tag{3}$$

$$g(x_k + \lambda_k S_k)^T S_k \geq \sigma \eta_k^T S_k \tag{4}$$

where $0 < \alpha < \sigma < 1$. The iterative searcher directions S_k CG-technique are calculated as:

$$d_0 = -g_0, d_{k+1} = -g_{k+1} + \beta_k d_k \quad (5)$$

at this point β_k is a scalar given as the parameter of conjugate gradient, η_{k+1} denotes gradient of $f(x_{k+1})$ at the points x_{k+1}, $s_k = x_{k+1} - x_k$ and $y_k = \eta_{k+1} - \eta_k$. The next sufficient descent state (6):

$$\eta_{k+1}^T S_{k+1} \leq -c\|\eta_{k+1}\|^2 \quad (6)$$

A lot used for analyzing the worldwide CG-technique convergence in mixture with inexact techniques of line search [2]. In the technique of quasi-Newton (QN), the direction of search is calculated using an approximation of the Hessian matrix inverse. In meticulous (5) is changed by:

$$S_{k+1} = -B_{k+1}^{-1}\eta_{k+1} \quad (7)$$

where by the Hessian matrix $B_{k+1} = G_{k+1} = \nabla^2 f(x_{k+1})$ is updated during the iterations. More details can be found in [3], [4]. In modern years, a diversity of CG-formulas was known, majorly, differences are in the parameter β_k, the work by discussed details on some CG-techniqus with special emphasis on their worldwide convergence. Furthermore, the design of CG-techniques had been studied by many of researchers for archetype refer to [5]-[10].

In this paper, the new proposed method is solved by second and third-order Taylor-series. The subsequent sections of study are organized in this way: the second section presents the outlines of the new algorithm and the deriving a new formula. Some interesting the convergence analysis of the new algorithm presented in the third section. Results of the current numerical experiments are presented in the fourth section by using the test problems found in [11]. Finally, the fifth section presents some obvious findings.

2. A NEW CONJUGATE GRADIENT METHOD

This section develops a new CG-method on the basis of approximating the Hessian with a symmetric positive-definite matrix. Now, the second and third-order Taylor-series approximation is employed to f at the point x_k can be written as by following the same approaches as in [12] as:

$$f(x_k) = f(x_{k+1}) - \eta_{k+1}^T r_k + \frac{1}{2} r_k^T G_{k+1} r_k, f_k = f_{k+1} - \eta_{k+1}^T r_k + \frac{1}{2} r_k^T G_{k+1} r_k + \frac{1}{6} r_k^T T_{k+1} r_k \quad (8)$$

where T_{k+1} is the tensor of f at the point x_{k+1}. Then, by using a $\eta_{k+1}^T S_k = 0$ in second -order Taylor-series, the next relation (9) is obtained:

$$r_k^T G_{k+1} r_k = 2(f(x_k) - f(x_{k+1})) \quad (9)$$

the relation (10) is obtained by third-order Taylor-series expressions:

$$r_k^T G_{k+1} r_k = y_k^T r_k + 6(f_k - f_{k+1}) + 3(\eta_{k+1} + \eta_k)^T r_k \quad (10)$$

the step size λ_k is determined by many algorithms. In exact line search the step length λ_k is selected as (11).

$$\lambda_k = -\frac{\eta_k^T s_k}{s_k^T G s_k} \quad (11)$$

From some algebra, the (12) is obtained:

$$r_k^T G_{k+1} r_k = f(x_k) - f(x_{k+1}) - \frac{\lambda_k \eta_k^T s_k}{2}, r_k^T G_{k+1} r_k = \frac{1}{2} y_k^T r_k + 3(f_k - f_{k+1}) + \frac{3}{2}\eta_{k+1}^T r_k + \eta_k^T r_k \quad (12)$$

by (12), the (13) is derived and denote by G_{k+1}^Q and as follows:

$$G_{k+1}^Q = \frac{f(x_k) - f(x_{k+1}) - \alpha_k \eta_k^T s_k/2}{r_k^T r_k} I_{n\times n}, G_{k+1}^C = \frac{\frac{1}{2} y_k^T r_k + 3(f_k - f_{k+1}) + \frac{3}{2}\eta_{k+1}^T r_k + \eta_k^T r_k}{r_k^T r_k} I_{n\times n} \quad (13)$$

then, it can be written as:

$$S_{k+1}^{Q}=-\left(\frac{r_k^T r_k}{f(x_k)-f(x_{k+1})-\frac{\lambda_k \eta_k^T S_k}{2}}\right)\eta_{k+1}, S_{k+1}^{C}=-\left(\frac{r_k^T r_k}{\frac{1}{2}y_k^T r_k+3(f_k-f_{k+1})+\frac{3}{2}\eta_{k+1}^T r_k+\eta_k^T r_k}\right)\eta_{k+1} \quad (14)$$

by use the conjugacy condition $S_{k+1}^T y_k=0$ due to the conjugacy of Newton directions with exact line searches.

$$\begin{aligned} S_{k+1}^T y_k &= -\left(\frac{r_k^T r_k}{f(x_k)-f(x_{k+1})-\lambda_k \eta_k^T S_k/2}\right)\eta_{k+1}^T y_k=0 \\ S_{k+1}^T y_k &= -\left(\frac{r_k^T r_k}{\frac{1}{2}y_k^T r_k+3(f_k-f_{k+1})+\frac{3}{2}\eta_{k+1}^T r_k+\eta_k^T r_k}\right)\eta_{k+1}^T y_k=0 \end{aligned} \quad (15)$$

Similarly, by using CG methods for quadratic functions with exact line searches, formula (16) is obtained:

$$S_{k+1}^T y_k=-\eta_{k+1}^T y_k+\beta_k S_k^T y_k=0 \quad (16)$$

from (15) and (16), the (17 a and b) is derived as follows:

$$\begin{aligned} &-\left(\frac{r_k^T r_k}{f(x_k)-f(x_{k+1})-\alpha_k \eta_k^T S_k/2}\right)\eta_{k+1}^T y_k=-\eta_{k+1}^T y_k+\beta_k S_k^T y_k \\ &-\left(\frac{r_k^T r_k}{1/2 y_k^T r_k+3(f_k-f_{k+1})+3/2\eta_{k+1}^T r_k+\eta_k^T r_k}\right)\eta_{k+1}^T y_k=-\eta_{k+1}^T y_k+\beta_k S_k^T y \end{aligned} \quad (17\text{ a})$$

from above equation, we get:

$$\begin{aligned} \beta_k S_k^T y_k &= -\left(\frac{r_k^T r_k}{f(x_k)-f(x_{k+1})-\alpha_k \eta_k^T S_k/2}\right)\eta_{k+1}^T y_k+\eta_{k+1}^T y_k \\ \beta_k d_k^T y_k &= -\left(\frac{r_k^T r_k}{1/2 y_k^T r_k+3(f_k-f_{k+1})+3/2\eta_{k+1}^T r_k+\eta_k^T r_k}\right)\eta_{k+1}^T y_k+\eta_{k+1}^T y_k \end{aligned} \quad (17\text{ b})$$

then, the following equations are obtained:

$$\beta_k^{BTQ}=\left(1-\frac{r_k^T r_k}{f(x_k)-f(x_{k+1})-\lambda_k \eta_k^T S_k/2}\right)\frac{\eta_{k+1}^T y_k}{S_k^T y_k}, \beta_k^{BTC}=\left(1-\frac{r_k^T r_k}{\frac{1}{2}y_k^T r_k+3(f_k-f_{k+1})+\frac{3}{2}\eta_{k+1}^T r_k+\eta_k^T r_k}\right)\frac{g_{k+1}^T y_k}{S_k^T y_k} \quad (18)$$

putting (18) in (5), we obtained:

$$\begin{aligned} S_{k+1} &= -\eta_{k+1}+\left(1-\frac{r_k^T r_k}{f(x_k)-f(x_{k+1})-\lambda_k \eta_k^T S_k/2}\right)\frac{g_{k+1}^T y_k}{S_k^T y_k}S_k \\ S_{k+1} &= -g_{k+1}+\left(1-\frac{r_k^T r_k}{\frac{1}{2}y_k^T r_k+3(f_k-f_{k+1})+\frac{3}{2}\eta_{k+1}^T r_k+\eta_k^T r_k}\right)\frac{\eta_{k+1}^T y_k}{S_k^T y_k}S_k \end{aligned} \quad (19)$$

for simplicity, equation (19) is called by β_k method. Also, β_k can be written in this way and denoted by β_k^{BTQ} and β_k^{BTC}:

$$\beta_k^{BTQ}=\frac{1}{r_k^T y_k}\left(y_k-\tau_1\frac{\|y_k\|^2}{r_k^T y_k}r_k\right)^T\eta_{k+1}, \beta_k^{BTC}=\frac{1}{r_k^T y_k}\left(y_k-\tau_2\frac{\|y_k\|^2}{r_k^T y_k}r_k\right)^T\eta_{k+1}$$

where,

$$\tau_1=\frac{(r_k^T y_k)^2}{\|y_k\|^2}\left[\frac{r_k^T y_k}{r_k^T r_k}*\frac{r_k^T r_k}{f(x_k)-f(x_{k+1})-\frac{\lambda_k \eta_k^T S_k}{2}}\right], \tau_2=\frac{(r_k^T y_k)^2}{\|y_k\|^2}\left[\frac{r_k^T y_k}{r_k^T r_k}*\frac{r_k^T r_k}{\frac{1}{2}y_k^T r_k+3(f_k-f_{k+1})+\frac{3}{2}\eta_{k+1}^T r_k+\eta_k^T r_k}\right]$$

On the basis of above discussion, this section describes the algorithm frame of this study without fixed line search in this way. New algorithms (BTQ and BTC algorithms):
Step 1: Give$x_1 \in R^n$, $\varepsilon > 0$. Set$S_1 = -\eta_1, k = 1$. If $\|\eta_1\| \leq 10^{-6}$, then stop.
Step 2: Compute λ_k satisfying the conditions (3-4).
Step 3: Let $x_{k+1} = x_k + \lambda_k S_k$ and$\eta_{k+1} = \eta(x_{k+1})$. If $\|\eta_{k+1}\| \leq 10^{-6}$, then stop.
Step 4: Compute β_k by the formulae (12) then generate S_{k+1} b y equation (13)
Step 5: Set k = k + 1 and continue with stege 2

3. CONVERGENT ANALYSIS

The following section proves the property of global convergence of new method. Theorem 3.1 demonstrates that the direction of search in algorithms is continuously sufficient descent based on no line search. The property of sufficient descent is one of the important properties of the all conjugate gradient methods.

3.1. Theorem

Let $r_k, y_k, \eta_{k+1} \in R^n, \beta_k \in R$ and $\beta_k^{BTC} = \frac{1}{r_k^T y_k}\left(y_k - \tau \frac{\|y_k\|^2}{r_k^T y_k} r_k\right)^T \eta_{k+1}$, where $\tau \in (1/4, \infty)$. If $r_k^T y_k \neq 0$, then $S_{k+1}^T \eta_{k+1} \leq -[1 - 1/4\tau]\|\eta_{k+1}\|^2$.

Proof: Since $S_0 = -\eta_0$, we have $\eta_0^T S_0 = -\|\eta_0\|^2$, satisfying (6). Through multiplying (19) by η_{k+1} (20) is obtained:

$$S_{k+1}^T \eta_{k+1} = -\|\eta_{k+1}\|^2 + \left(\frac{\eta_{k+1}^T y_k}{r_k^T y_k} - \tau \frac{\|y_k\|^2}{(r_k^T y_k)^2} \eta_{k+1}^T r_k\right) r_k^T \eta_{k+1} \tag{20}$$

yielding

$$S_{k+1}^T \eta_{k+1} = \frac{(\eta_{k+1}^T y_k)(r_k^T \eta_{k+1})(r_k^T y_k) - \|\eta_{k+1}\|^2 (r_k^T y_k)^2 - \tau \|y_k\|^2 (\eta_{k+1}^T r_k)^2}{(r_k^T y_k)^2} \tag{21}$$

The inequality $\omega^T \upsilon \leq \frac{1}{2}(\|\omega\|^2 + \|\upsilon\|^2)$ is applied with $\omega = \frac{1}{\delta}(r_k^T y_k)\eta_{k+1}$ and $\upsilon = \delta(\eta_{k+1}^T r_k) y_k$, where $\delta \in (\frac{1}{\sqrt{2}}, \sqrt{2t}]$, to the first term of the above equality, the (23) is obtained:

$$(\eta_{k+1}^T y_k)(r_k^T \eta_{k+1})(r_k^T y_k) \leq \frac{1}{2}\left[\frac{1}{\delta^2}(r_k^T y_k)^2 \|\eta_{k+1}\|^2 + \delta^2 (r_k^T \eta_{k+1})^2 \|y_k\|^2\right] \tag{22}$$

this yields,

$$S_{k+1}^T \eta_{k+1} \leq \frac{\left[\frac{1}{2\delta^2} - 1\right](r_k^T y_k)^2 \|\eta_{k+1}\|^2 + \left[\frac{\delta^2}{2} - \tau\right](r_k^T \eta_{k+1})^2 \|y_k\|^2}{(r_k^T y_k)^2} \tag{23}$$

From (18), the (24) is derived as follows:

$$S_{k+1}^T \eta_{k+1} \leq \left[\frac{1}{2\delta^2} - 1\right] \|\eta_{k+1}\|^2 \leq -\left[1 - \frac{1}{2\delta^2}\right] \|\eta_{k+1}\|^2 \tag{24}$$

Therefore, the (25) is obtained:

$$S_{k+1}^T \eta_{k+1} \leq -\left[1 - \frac{1}{4\tau}\right] \|\eta_{k+1}\|^2 \tag{25}$$

Consequently, it is necessary to have Assumption 3.2 for analyzing the global convergence of algorithms.

3.2. Assumption

i. The level set$L = \{x \in R^n | f(x) \leq f(x_0)\}$ is constrained.
ii. In a number of areas, U and $L, f(x)$ are continuously differentiable and their gradient id Lipschitz is continuous, i.e., a constant $L > 0$ exists, like that:

$$\|\eta(z)-\eta(o)\| \le L\|z-o\|, \forall z, o \in U \quad (26)$$

Under the above assumptions on f, a constant $\Gamma > 0$ exists, like that:

$$\|\eta_{k+1}\| > \Gamma \quad (27)$$

for all $x \in L$. More details can be found in [13] verified that the next general result is applied to any CG method with strong Wolfe line search:

3.3. Lemma

Supposing that assumptions (i) and (ii) are held, then consider any method of conjugate gradient (2) and (5) where S_{k+1} is a descent direction and λ_k is achieved by the strong Wolfe line search (3) and (4). If:

$$\sum_{k\ge 0} \frac{1}{\|S_{k+1}\|^2} = \infty, \quad (28)$$

then,

$$\lim_{k\to\infty} inf\|\eta_{k+1}\| = 0 \quad (29)$$

3.4. Theorem

Supposing that assumptions are held, then consider methods (2) and (5), where is a descent direction with and given by (18), and λ_k is found by the Wolfe line search. If the objective function is uniformly, then $\lim_{n\to\infty} inf\|\eta_{k+1}\| = 0$.

$$\begin{aligned}
&\|S_{k+1}\| = \|-\eta_{k+1} + \beta_k S_k\| \le \|\eta_{k+1}\| + |\beta_k|\|S_k\| \\
&\le \|\eta_{k+1}\| + \left\|\left(y_k - \tau\frac{\|y_k\|^2}{r_k^T y_k} r_k\right)\right\| \frac{\|\eta_{k+1}\|}{\|r_k\|\|y_k\|}\|r_k\| \\
&\le \|\eta_{k+1}\| + \frac{\|y_k\|\|\eta_{k+1}\| + \tau\frac{\|\eta_{k+1}\|\|y_k\|^2\|r_k\|}{\|r_k\|\|y_k\|}}{\|r_k\|\|y_k\|}\|r_k\| \\
&\le \|\eta_{k+1}\| + \frac{\|y_k\|\|\eta_{k+1}\| + \tau\|\eta_{k+1}\|\|y_k\|}{\|r_k\|\|y_k\|}\|r_k\| \\
&\le [1+1+\tau]\|\eta_{k+1}\| \le [2+\tau]\|\eta_{k+1}\|
\end{aligned} \quad (30)$$

This relation shows that:

$$\sum_{k\ge 1} \frac{1}{\|S_{k+1}\|^2} \ge \left(\frac{1}{2+\tau}\right)\frac{1}{\Gamma}\sum_{k\ge 1} 1 = \infty \quad (31)$$

based on Lemma 1, $\lim_{k\to\infty} inf\|\eta_{k+1}\| = 0$ is derived, which equals $\lim_{k\to\infty}\|\eta_{k+1}\| = 0$ for uniformly convex function.

4. NUMERICAL RESULTS

This section explains some numerical experiments conducted for testing BTQ and BTC algorithms. Some test problems studied by Andrei [11] were used in this study (see Table 1) to analyze the efficiency of the new formula formed in this study in comparison to the method of FR. Comparison is based on iterations number (NI) and function evaluations number (NF) the CG algorithms by teepest descent directions. In all CG, the step length λ_k is yielded by Wolfe line search with $\alpha = 0.001$ and $\sigma = 0.9$, and the termination condition is $\|\eta_{k+1}\| \le 10^{-6}$. Some noted papers can be see [14]-[25].

Tables 1 present list of some numerical results of this study. Based on the current numerical results, the proposed methods, BTQ and BTC, have minimum numbers of iterations, restarts and function evaluations in all implemented test problems in this study, except for problems 7 and 10, where the FR algorithm has less numbers of iterations, restarts and function evaluations against the new proposed BTQ and BTC algorithms. Generally, the percentage performance of the new proposed algorithms BTQ and BTC can be computed as compared to the standard FR algorithm for the general Tools NI, NR and NF shown in Table 2.

Table 1. Comparison of FR and new algorithms (BTQ and BTC) with n=100 and n=1000, test function

P. No	n	FR algorithm		BTQ algorithm		BTC algorithm	
		NI	NR	NF	NI	NR	NF
1	100	47	93	38	84	39	82
	1000	78	131	37	87	33	75
2	100	43	88	43	95	45	100
	1000	46	92	40	87	37	79
3	100	32	52	15	30	13	25
	1000	22	42	24	47	16	32
4	100	25	43	23	45	22	44
	1000	46	741	30	204	29	52
5	100	37	67	39	60	43	63
	1000	73	115	66	110	63	98
6	100	15	31	11	23	9	19
	1000	8	17	8	17	7	15
7	100	89	174	75	165	73	160
	1000	107	211	72	155	61	139
8	100	71	110	40	79	31	60
	1000	47	84	68	131	30	57
9	100	32	65	21	50	30	70
	1000	53	116	37	87	37	85
10	100	74	123	92	141	75	115
	1000	370	616	345	583	277	456
11	100	69	1202	30	56	26	47
	1000	98	1967	33	57	55	837
12	100	49	80	10	19	17	32
	1000	129	166	12	24	14	27
13	100	12	25	11	23	10	21
	1000	11	23	11	23	10	21
14	100	122	156	14	28	11	20
	1000	130	166	15	29	15	27
15	100	112	147	43	66	34	54
	1000	110	145	40	60	38	60
Total		**2157**	**7090**	**1343**	**2666**	**1199**	**2972**

Table 2. Relative efficiency of the new algorithms

	FR algorithm	BTQ algorithm	BTC algorithm
NI	100%	62.26%	55.58%
NF	100%	37.60%	41.91%

Problems numbers indicator (Table 1): 1) is the extended Rosenbrock, 2) is the extended White & Holst, 3) is the extended Beale, 4) is the generalized tridiagonal 1, 5) is the generalized tridiagonal 2, 6) is the extended PSC1, 7) is the extended Maratos, 8) is the extended Wood, 9) is the extended quadratic penalty QP2, 10) is the partial perturbed quadratic, 11) is the EDENSCH (CUTE), 12) is the DENSCHNC (CUTE), 13) is the DENSCHNB (CUTE), 14) is the extended block-diagonal BD2, and 15) is the generalized quartic GQ2. Full details of these test problems can be found in Andrie [11].

5. CONCLUSIONS

Practically, when the complexity and size of the test problem increase, greater improvements could be realized by the new algorithms because the new proposed algorithm is more stable and always preserves the descent search directions. Our reported results showed that the proposed methods are efficient for solving large-scalc unconstrained optimization. Generally, the percentage performance of the new proposed algorithms BTQ and BTC can be computed as compared to the standard FR algorithm for the general tools NI, NR and NF.

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