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RESEARCH ARTICLE

An *n*-th section line search in conjugate gradient method for small-scale unconstrained optimization

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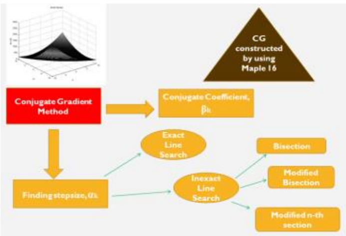
Graphical abstract



Abstract

Conjugate Gradient (CG) methods are well-known method for solving unconstrained optimization problem and popular for its low memory requirement. A lot of researches and efforts have been done in order to improve the efficiency of this CG method. In this paper, a new inexact line search is proposed based on Bisection line search. Initially, Bisection method is the easiest method to solve root of a function. Thus, it is an ideal method to employ in CG method. This new modification is named *n*-th section. In a nutshell, this proposed method is promising and more efficient compared to the original Bisection line search.

Keywords: Conjugate gradient; bisection method; line search; unconstrained optimization

INTRODUCTION

Optimization could be defined as the science of finding the best solution to mathematical problems which are the physical modelled from the real world. According to Snyman (2005), optimization includes the study of optimality criteria of problems, the determination of algorithmic methods, the study of structure of methods and its computer experimentation with methods both under trial conditions and also on real life problem.

Mathematically, in this study, we found the minimum solution to a given function which is

$$\min_{x\in R^n} f(x).$$

Using an initial guess or initial point, we try to get a new solution by using an appropriate method. In doing this, we basically return to the same calculation method but, using new initial guess. This returning procedure which is also known as an iterative method forms the basis of optimization that is to minimize $f(x)$ such that

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

The α_k is known as the stepsize and the d_k is known as the search direction. Different d_k give rise to different method of optimization.

The steepest descent is the earliest and recognized method, dated back in 1847 (Cauchy, 1847). Many other methods arise based on its modification. Conjugate Gradient (CG) method is one of it and dated back as early as 1952. Currently, this method seems to be the attention of many researches lately.

CONJUGATE GRADIENT METHOD

The initial calculation for conjugate gradient method starts with steepest descent direction and after that, the next search direction is calculated by adding the linear combination of the previous direction to the current gradient (Chong and Zak, 2013). The search directions defined is by

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

in which β_k is known as the CG coefficient while g_k is the gradient of f at point x_k (Hamoda *et. al*, 2015). Many researches have been conducted by researchers to find the best formula for β_k that will yield a better result. Some of the most well-known formulas are Fletcher-Reeves (FR), Polak-Ribière-Polyak (PRP) and Rivaie, Mustafa, Ismail and Leong (RMIL).

They are written as

$$\beta_k^{FR} = \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}} \qquad \text{(Fletcher –Reeves, 1964)}$$

$$\beta_k^{PRP} = \frac{g_k^T (g_k - g_{k-1})}{g_{k-1}^T g_{k-1}} \qquad \text{(Polak and Ribiere,1969;Polyak, 1969)}$$

$$\beta_k^{RMIL} = \frac{g_k^T (g_k - g_{k-1})}{\|d_{k-1}\|} \qquad \text{(Rivaie, Mustafa, Ismail and Leong, 2012)}$$

BISECTION AND *N*-th SECTION LINE SEARCH

In finding the step size in CG method, there are two line searches that can be applied which are exact and inexact line search. Exact line search is the exact value of step size, α_k , calculated analytically using $f'(\alpha_k) = 0$. While, inexact line search is the approximate value of α_k , calculated using numerical analysis such as Bisection, Newton and secant line search.

Bisection method is the easiest method using an interval which is divided into two or half. Doron (2010) assume that this method has opposite signs at both edges of the intervals where $f(a).f(b) < 0$. Then, it is known that $f(x)$ has at least one root in the interval, $[a, b]$. The existing method proceeds and continues iterating until it converges to a point within the tolerance range and finds the value of x such that $f(x) = 0$ or approximately 0.

The main advantage of Bisection method is the behaviour itself is always convergent since the method brackets the root much more quickly than the incremental search method does. Hence, Bisection method is easy to use, apply and has wide range of applications in other developments.

However, the division of the interval into two section leads to slow convergence of Bisection method. Hence, a new method is proposed called an *n*-th section method.This method is compared with the original Bisection method based on number iterations, CPU times and accuracy.

An *n*-th section method is a modification from classical Bisection method which is fourth and sixth section method. This new scheme divided the interval into four and six section.The root is then identify either in the first, second, third, fourth, fifth or sixth interval. This will lead to faster convergence of the root and provide faster calculation of the roots. For an even number of *n*, the algorithm will be similar to Bisection method. However, the *n*-th section inherits the problems from the bisection itself and some modifications need to be implemented before fitting it as a line search. This modification has lead to an idea of an employment of a new line search in CG method. Fig. 1, Fig. 2 and Fig. 3 shows the schematic representation for Bisection method, 4th Section method and 6th Section method respectively.

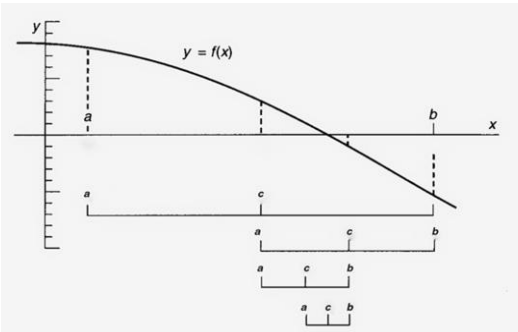


Fig. 1 The schematic representation of bisection method

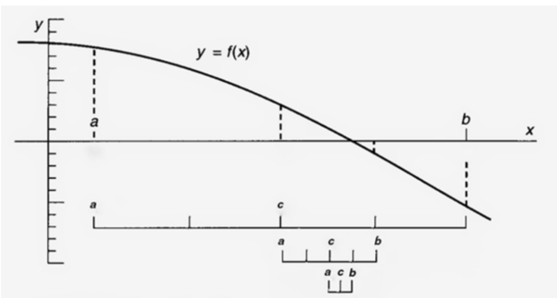


Fig. 2 The schematic representation of fourth section method

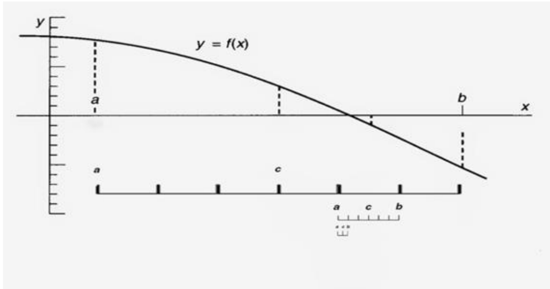


Fig. 3 The schematic representation of sixth section method

METHODOLOGY

The selected model to use in this research is CG method with the employment of classical Bisection, modified Bisection and modified *n*-th section line search. Since the classical Bisection and original *n*-th section might not always work and has some issues, some modifications need to be implemented before fitting it as a line search. Next, computer programming code will be constructed using Maple 16 software. Algorithm 1 shows CG method with an employment of original Bisection and *n*-th section line search Algorithm 1 and Algorithm 2 shows the proposed CG method under modified line search.

Algorithm 1: CG Method with an employment of original Bisection and *n*-th section line search algorithm

Step 1 Initialization.
Given x_0, set $k = 0$.

Step 2 Computing search direction.

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

Step 3 Computing step size α_k
Identify two numbers *a* and *b* as an interval at which $f'(\alpha_k)$ has different signs.

Divide into sections, m = $\frac{a+b}{n}$ where n=2,4, and 6

Determine if

i. $f'(a) . f'(a+m) < 0$ then $r \in (a, a+m)$
ii. $f'(a+m) . f'(a+2m) < 0$ then $r \in (a+m, a+2m)$
iii. $f'(a+2m) . f'(a+3m) < 0$ then $r \in (a+2m, a+3m)$
.
.

$f'(a+im) . f'(a+(i+1)m) < 0$ then $r \in (a+im, a+(i+1)m)$
where $i = 0,1,2,3, \ldots$

Define C_{mid} as midpoint, $C_{mid} = \frac{(a+im)+(a+(i+1)m)}{2}$

and $C_{mid} = \alpha_k$

Repeated until desired iteration/ accuracy

Step 4 Updating new point.
$x_{k+1} = x_k + \alpha_k d_k$

Step 5 Convergent test and stopping criteria.
If $f(x_{k+1}) < f(x_k)$ and $\|g_k\| \le \varepsilon$ then stop
Otherwise go to Step 1 with $k = k+1$.

Algorithm 2: Proposed CG method with improvement of Bisection and *n*-th section line search

Step 1 Initialization.
Given x_0, set $k = 0$.

Step 2 Computing search direction.

$$d_k = \begin{cases} -g_k, & if\ k = 0; \\ -g_k + \beta_k d_{k-1}, & if\ k \ge 1 \end{cases}$$

Step 3 Computing step size α_k

Identify two numbers *a* and *b* as an interval at which $f'(\alpha_k)$ has different signs.

Divide into sections, m = $\frac{a+b}{n}$ where n = 2,4 and 6

Determine if
i. $f'(a) . f'(a+m) > 0$ then continue
ii. $f'(a+m) . f'(a+2m) > 0$ then continue
iii. $f'(a+2m) . f'(a+3m) > 0$ then continue
.
.
$f'(a+im) . f'(a+(i+1)m) < 0$ $then\ r \in (a+im,\ a+(i+1)m)$ then stop
where $i = 0,1,2,3, \ldots$

Define C_{mid} as midpoint, $C_{mid} = \frac{(a+im)+(a+(i+1)m)}{2}$

and $C_{mid} = \alpha_k$

Repeated until desired iteration/ accuracy

Step 4 Updating new point.
$x_{k+1} = x_k + \alpha_k d_k$

Step 5 Convergent test and stopping criteria.
If $f(x_{k+1}) < f(x_k)$ and $\|g_k\| \le \varepsilon$ then stop
Otherwise go to Step 1 with $k = k+1$.

The stopping criteria for the standard test problem is $\|g_k\| \le 10^{-6}$ as suggested by Andrei (2011) is applied. The initial points in a single quadrant are then tested from a point that is closer to the solution point to the one that is furthest. There is a tendency that an algorithm will found the solution point when we used an initial point which is closer. In this case, four other initial points which is spread further apart is chosen to see the behaviour of the method. Comparison of both method are based on its efficiency in terms of number of iterations. A comparison between existing methods and proposed method based on its efficiency and convergence properties are studied. Performance profile introduced by Dolan & Moré will be also be featured and conducted in this paper. The numerical results is tested on a same computer with Core i5 processor 3337U with 4GB RAM.

STANDARD OPTIMIZATION TEST PROBLEM

The quality of an optimization methods are frequently evaluated using standard optimization test problems. In this research, all methods have been tested using four different functions. In this section, we shall discuss about the main criteria of the selected test problems. We have also plot the test problems with two variables using *Maple 16* to show the different shape of the functions which has been selected.

Problem 1: Tridiagonal Function with *n*=2 (Andrei, 2008)

Function: $f(x) = \sum_{i=1}^{n/2} (x_{2i-1} - x_{2i} - 3)^2 + (x_{2i-1} - x_{2i} + 1)^4$

Global minimum is $x^* = (0,0)$ and minimum function values is $f(x^*) = 0$, which lies inside the bottom curve, see Fig. 4.

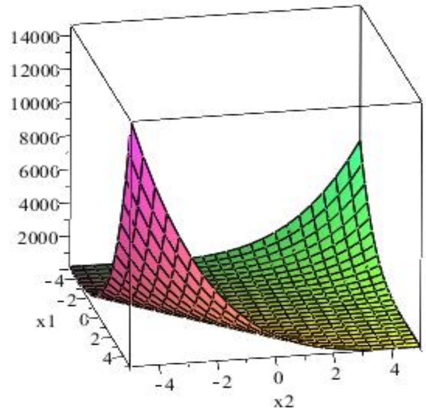


Fig. 4 Tridiogonal function in 3D

Problem 2: Booth Function with *n*=2 (Witte and Holst, 1964)

Function: $f(x) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2$

Global minimum is $x^* = (1,3)$ and minimum function values is $f(x^*) = 0$, which lies inside the bottom curve, see Fig. 5.

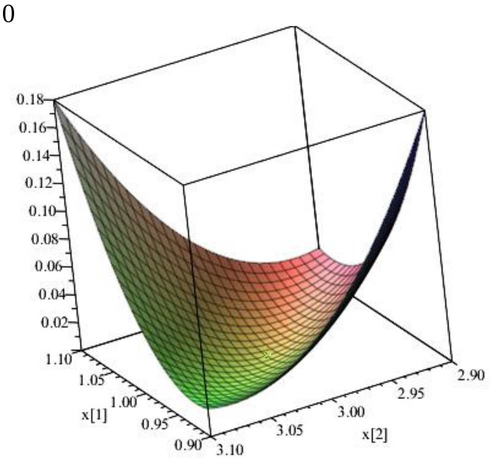


Fig. 5 Booth function in 3D

Problem 3: Bukin Function with *n*=2 (as cited in Mishra, 2006)

Function: $f(x) = 100(x_2 - 0.01x_1^2 + 1) + 0.01(x_1 + 10)^2$

Global minimum is $x^* = (-10,0)$ and minimum function values is $f(x^*) = 0$, see Fig. 6.

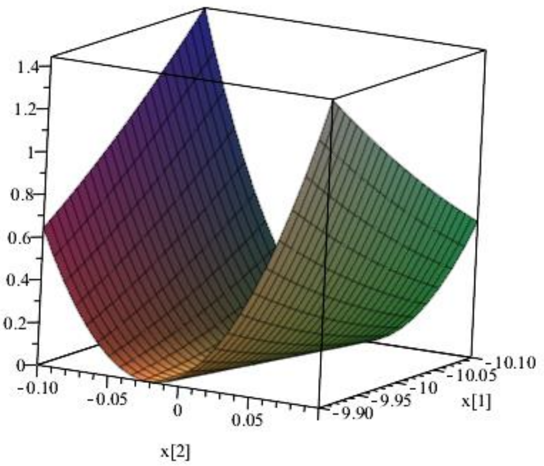


Fig. 6 Bukin function in 3D

Problem 4: Three-hump Function with n=2 (Jasson & Knuppel, 1992)

Function: $f(x) = 2x_1^{\ 2} - 1.05x_1^{\ 4} + \frac{x_1^{\ 6}}{6} - x_1x_2 + x_2^{\ 2}$

Global minimum is $x^* = (0,0)$ and minimum function values is $f(x^*) = 0$, see Fig. 7.

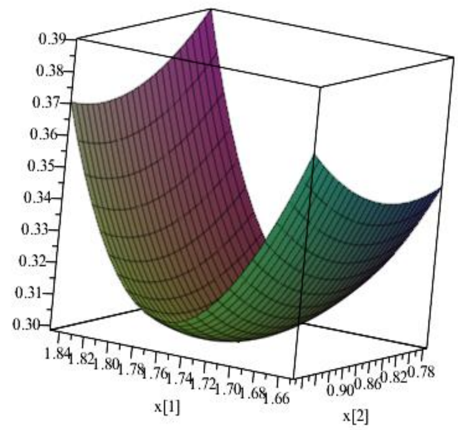


Fig. 7 Three-hump function in 3D

RESULTS AND DISCUSSION

The results are presented for CG-FR, CG-PRP and CG-RMIL based on the functions that have been discussed in previous section.Table 1, Table 2 and Table 3 shows the number iterations for CG-FR method, CG-PRP method and CG-RMIL method respectively. Fig. 8 shows the performance profile involving the classical Bisection, modified Bisection, modified 4-th section and modified 6-th section. The abbreviation of CB, MB, M4 and M6 are denoted as classical Bisection, modified Bisection, modified 4^{th} Section and modified 6^{th} Section line search respectively. In each table, F is denoted as failure to converge in which the method could not reach the solution point.

For CG-FR method using the Tridiagonal function, the number of iterations is equivalent for all line searches using any initial points. Both Tridiagonal and Bukin function possess global convergence properties since all the tested initial points converges to the solution point. However, some of the initial ponts failed to converge for Bukin and Threehump function. In this results, the application of modified 6^{th} Section line search in CG-FR method is quite promising since the convergence is unlikely to fail when compared to the classical Bisection.

For CG-PRP method, only booth function possess global convergence properties. For Tridiagonal function, only the nearest point tend to fail. Some of the initial points are also fail to converge for Bukin and Threehump function. In bukin function, it is obvious that the application of n^{th} Section line search can be a problem solver when using modified 6^{th} Section line search.

Table 1 Number of iterations of CG-FR method

Initial Points	CB	MB	M4	M6
Tridiagonal				
(12,12)	5	5	5	5
(50,50)	2	2	2	2
(100,100)	2	2	2	2
(500,500)	2	2	2	2
Booth				
(12,12)	2	3	3	3
(50,50)	3	3	3	3
(100,100)	3	3	3	3
(500,500)	2	3	3	3
Bukin				
(7,7)	F	38	28	F
(15,15)	F	F	39	220
(30,30)	F	F	80	24
(50,50)	F	F	172	290
Threehump				
(-1,1)	F	F	12	12
(-10,10)	8	8	F	6
(-30,30)	F	F	F	10
(-100,100)	8	8	F	33

Table 2 Number of iterations of CG-PRP method

Initial Points	CB	MB	M4	M6
Tridiagonal				
(12,12)	F	F	F	F
(50,50)	2	2	2	2
(100,100)	2	2	2	2
(500,500)	3	3	2	2
Booth				
(12,12)	2	3	3	3
(50,50)	2	3	3	3
(100,100)	2	3	3	3
(500,500)	2	3	3	3
Bukin				
(7,7)	F	F	38	22
(15,15)	F	F	25	22
(30,30)	F	F	F	36
(50,50)	F	F	F	111
Threehump				
(-1,1)	F	F	4	4
(-10,10)	4	4	F	4
(-30,30)	5	5	4	F
(-100,100)	7	7	F	F

Table 3 Number of iterations of CG-RMIL method

Initial Points	CB	MB	M4	M6
Tridiagonal				
(12,12)	F	F	5	5
(50,50)	2	2	2	2
(100,100)	2	2	2	2
(500,500)	3	3	2	2
Booth				
(12,12)	2	3	3	3
(50,50)	2	3	3	3
(100,100)	2	3	3	3
(500,500)	2	3	3	3
Bukin				
(7,7)	F	F	F	F
(15,15)	F	F	F	F
(30,30)	F	F	F	F
(50,50)	F	F	F	F
Threehump				
(-1,1)	F	F	6	6
(-10,10)	6	6	F	6
(-30,30)	5	5	5	F
(-100,100)	F	F	F	F

For CG-RMIL method, only booth function possess global convergence properties. For Tridiagonal function, only the application of modified 4th Section and 6th Section are capable to reach its minimum solution. Some of the intial points in Threehump function failed to converge. CG-RMIL with this line searches is unlikely to be the ideal as a problem solver for Bukin function since none of the intial points succeed to converge.

Other than that, the performance results are shown in Fig. 8 using the performance profile introduced by Dolan and More (2002). The performance profile seeks to find how well the solvers perform relative to the other solvers on the problems. In this performance profile, they introduced the notion of a means to evaluate and compare
the performance of the set solver S on a test set P. Assume that s_n solvers and p_n problems exists, for each problem p and solver s, define that

$t_{p,s}$ = computing time (the number of iterations or CPU time or others) required to solve problems p by solver s .

The performance of solver s on any given problem might be of interest, but because want to obtain an overall assessment of the performance of the solver, then it was defined

$$p_s(t) = \frac{1}{n_p} size\{p \in P : r_{p,s} \leq t\}$$

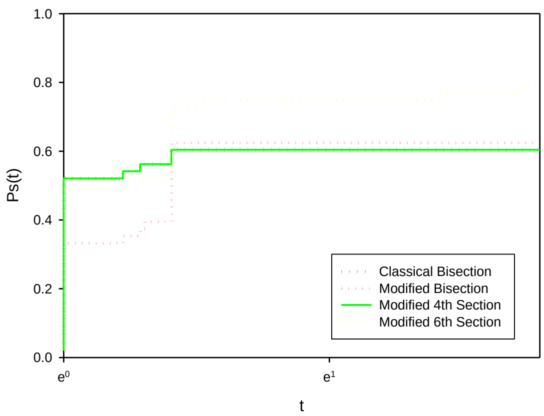


Fig. 8 Performance profile

Based on this performance profile, the best method is determined based on the right side of figure which has the highest curve value. In this case, it shows that the best line search is modified 6th section with 0.8. This means that this method is able to solve 80% of the given problems. Based on the left side, it shows that the classical Bisection, 4th section and 6th section possess the top curve which means that this method is competetively fast. However, the classical Bisection and 4th section are the lowest curve on the right side which implies the least problem solver.

CONCLUSION

In this paper, a new line search has been proposed which is the modified *n*-th section method that is applied in CG method. It shows that this method could be used as a line search for CG method with superior performance. It is believe that some improvement could also be done in future research to enhance the performance of these line searches.

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