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The Stability and Convergence Analysis of a New Conjugate Gradient Method for Solving Nonlinear Optimization Problems

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Abstract

The development of any conjugate gradient method could be viewed from the perspective of approximating an objective function $f(x)$ by a functional $F(x)$ noting that the properties of the functional can be used to characterize the method. Using the functional $F(x)$, the new conjugate gradient method was developed and used to solve many nonlinear optimization problems with high efficiency and accuracy. The numeric analysis of its stability and convergence becomes imperative in order to establish the reliability of the method and satisfy the yearnings of its increasing users. In this paper, we present the stability and convergence analysis of the new conjugate gradient method.

Keywords: Conjugate gradient method, convergence, stability, objective function.

1 Introduction

The new conjugate gradient method (NCGM) [1] is an effective iterative scheme for optimizing non-linear objective functions involved in many optimization problems. It is robust and generally able to achieve rapid convergence to an accurate solution. The traditional criterion for ensuring that a numerical method is stable is called absolute-stability [2]. A conjugate gradient method is

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said to be absolutely stable for given step lengths α if, for these α, the error bound $|E_j|$ satisfy the criterion $|E_j|<1,\ j=0,1,2,...,\ n$. An interval (a,b) of the real line is said to be an interval or region of absolute stability if the method is absolutely stable for all $\alpha \in (a,b)$ [3]. Numerical stability analysis of NCGM is carried out using the basic properties of Lanczos algorithm for tridiagonalizing a matrix while its absolute stability proof is derived from the error analysis.

Every conjugate gradient algorithm is known to be closely related to Lanczos algorithm for tridiagonalizing a matrix [4]. Greenbaum [5,6] have considered the close connection between the Lanczos and conjugate gradient algorithm in the analysis of stability of conjugate gradient computations under perturbations in finite arithmetic. Paige [7,8,2] stated that every conjugate gradient method (CGM) is a tridiagonalizing procedure. Greenbaum, amonst others, agreed with Paige and added that the symmetric tridiagonal matrix produced by symmetric Lanczos process gives the same pivot recurrence as the tridiagonal matrix produced by the CGM. They concluded that if the original matrix involved in the CGM is symmetric and positive definite, then, the CGM is absolutely stable.

In section 2, we describe the NCGM with its algorithm and how it satisfies the convergence theorem. In section 3, we explain the basic vector updates for the search directions. The natural association between the new conjugate gradient algorithm and the Lanczos process has been established in section 4. This exercise represents the stability proof of NCGM. Some numerical examples were considered in section 5. The examples confirmed that the error bound $|E_j|$, in each case, satisfy the criterion $|E_j|<1,\ j=0,1,2,...,\ n$. Section 6 summarizes the findings of this paper with a conclusion.

2 The New Conjugate Gradient Method

The new conjugate gradient method has been designed to optimize a non-linear objective functional, F:

$$\underset{x}{Optimize}\ F(x) \tag{1}$$

where $F(x)=\sum_{j=0}^{n}\frac{1}{j!}(x^{\frac{j}{2}})^T\nabla^j F(x_0)x^{\frac{j}{2}}$, $n>2$ is the degree of F. The gradient functional is

$$G(x)=F'(x)=\nabla F(x_0)+\sum_{j=2}^{n}\frac{1}{(j-1)!}\left(x^{\frac{j-1}{2}}\right)^T\nabla^j F(x_0)x^{\frac{j-1}{2}}. \tag{2}$$

$F(x)$ approximates $f(x)$ at point $x\in\Re^n$ and $g(x)=f'(x)$. The following algorithm characterizes the NCGM.

2.1 Algorithm (NCGM)

i. Input initial values x_0 *and* $D_0 = -G_0 = -g_0$.

ii. Repeat:

a. Find step length α_k such that

$$F(x_k + \alpha_k D_k) = \min_{\alpha > 0} F(x_k + \alpha D_k)$$

b. Compute new point:

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

c. Update search direction:

$$D_{k+1} = -G_{k+1} + \beta_k D_k,$$

$$G_{k+1} = \frac{1}{2!}\left[g(x_k + 2\Delta x_k) + g(x_k)\right]$$

$$\beta_k = \frac{\|G_{k+1}\|^2}{D_k{}^T y_k};\ \|G_k\| = \left(G_k{}^T G_k\right)^{\frac{1}{2}}.$$

$$y_k = G_{k+1} - G_k$$

d. Check for optimality of g:

Terminate iteration at step m when $\|g_m\|$ is so small that x_m is an acceptable estimate of the optimal point x^* of F. If not optimal set $k = k+1$.

2.2 Convergence of the New Conjugate Gradient Method

In order to establish the convergence of the above algorithm, we assume that the objective function satisfies the following conditions:

1. F is bounded below in $\Re^N$ and is continuously differentiable in a neighborhood Z of the level set $L = \{x_1, x \in \Re^N : F(x) \le F(x_1)\}$
2. The gradient $\nabla F(x)$ is Lipschitz continuous in Z, namely, there exists a constant $L > 0$ such that

$$\| \nabla F(x) - \nabla F(y) \| \le L \| x - y \|, \textit{ for any } x, y \in Z \tag{3}$$

2.3 Lemma (Existence of a Global Optimum of f)

Suppose that x_1 is a starting point for which the above assumptions are satisfied. Consider the conventional conjugate gradient method where d_k is the descent direction and α_k (the step length of line search) satisfies the standard Wolfe conditions. Then, we have that

$$\sum_{k\geq 1} \frac{(g_k{}^T d_k)^2}{\| d_k \|^2} < \infty \tag{4}$$

Proof. (See the proof by Dai and Yuan [9])

Dai and Yuan proved this lemma for the algorithm of any conventional conjugate gradient method (CGM). The proof for our algorithm is same when we put $G(x_k)$ in place of $g(x_k)$ and D_k in place of d_k . Dai and Yuan made it simple to see that with $G_{k+1} = \frac{1}{2!}\left[g(x_k + 2\Delta x_k) + g(x_k)\right]$ we have

$$\sum_{k\geq 1} \frac{\left(G_{k+1}{}^T D_k\right)^2}{\left\|D_k\right\|^2} = \sum_{k\geq 1} \frac{\left[\left(g\left(x_k + 2\Delta x_k\right)^T + g(x_k)^T\right) D_k / 2\right]^2}{\left\|D_k\right\|^2}$$

$$= \sum_{k\geq 1} \frac{\left[g(x_k + 2\Delta x_k)^T D_k / 2\right]^2}{\left\|D_k\right\|^2} + \sum_{k\geq 1} \frac{\left[g(x_k)^T D_k / 2\right]^2}{\left\|D_k\right\|^2} < \infty$$

Hence,

$$\sum_{k\geq 1} \frac{\left(G_{k+1}{}^T D_k\right)^2}{\left\|D_k\right\|^2} < \infty. \tag{5}$$

2.4 Theorem (Convergence of A Conventional CGM)

Suppose that x_1 is a starting point for which the above assumptions and the lemma are satisfied. Let $\{x_k, k = 1, 2, ...\}$ be generated by an algorithm for a conventional CGM. Then, the algorithm either terminates at a stationary point or converges in the sense that

$$\lim_{k\to\infty} \inf \| g(x_k) \| = 0 \tag{6}$$

Proof: (See the proof by Dai and Yuan [9])

Dai and Yuan used proof by contradiction to prove this theorem for a conventional CGM. The proof of this theorem for the above algorithm is same when we put $G(x_k)$ in place of $g(x_k)$ and D_k in place of d_k. It is not difficult to see that

$\lim_{k\to\infty} \inf \| g(x_k) \| = 0$ when $g(x_k)$ =0(zero vector) and Δx_k =0 (zero vector, no further improvement on x_k). Hence, with $G_{k+1} = \frac{1}{2!}\left[g(x_k + 2\Delta x_k) + g(x_k)\right]$ we have

$$\liminf_{k\to\infty} \| G(x_{k+1}) \| = \liminf_{k\to\infty} \| g(x_k + 2\Delta x_k) + g(x_k) \| / 2 = 0$$

This implies that $\liminf_{k\to\infty} \| G(x_k) \| = 0$. We conclude that the new conjugate gradient method will converge to the global optimum of F and hence f.

3 Basic Vector Updates

The two basic vector updates needed to update the search direction and the computed solutions by NCGM are

$$D_{k+1} = r_{k+1} + \beta_k D_k \tag{7}$$

and

$$r_{k+1} = r_k - \alpha_k W P_k \tag{8}$$

where $r_k = -G_k$

Equation (4) is an implicit vector update since

$$F(x) = \sum_{j=0}^{n} \frac{1}{j!} (x^{\frac{j}{2}})^T \nabla^j F(x_0) x^{\frac{j}{2}}$$

$$F'(x) = \nabla F(x_0) + \sum_{j=2}^{n} \frac{1}{(j-1)!} \left(x^{\frac{j-1}{2}} \right)^T \nabla^j F(x_0) x^{\frac{j-1}{2}}$$

$$F'(x_0) = \nabla F(x_0) + \sum_{j=2}^{n} \frac{1}{(j-1)!} \left(x_0^{\frac{j-1}{2}} \right)^T \nabla^j F(x_0) x_0^{\frac{j-1}{2}} = 0$$

$$\nabla F(x_0) = -\sum_{j=2}^{n} \frac{1}{(j-1)!} \left(x_0^{\frac{j-1}{2}} \right)^T \nabla^j F(x_0) x_0^{\frac{j-1}{2}};$$

$$b = -\sum_{j=2}^{n} \frac{1}{(j-1)!} \left(x_0^{\frac{j-1}{2}} \right)^T \nabla^j F(x_0) x_0^{\frac{j-1}{2}};$$

$$\begin{aligned} r(x) &= -F'(x) \\ &= -(b + \sum_{j=2}^{n} \frac{1}{(j-1)!} \left(x^{\frac{j-1}{2}} \right)^T \nabla^j F(x_0) x^{\frac{j-1}{2}}) \\ &= -(\sum_{j=2}^{n} \frac{1}{(j-1)!} \left((x-x_0)^{\frac{j-1}{2}} \right)^T \nabla^j F(x_0) (x-x_0)^{\frac{j-1}{2}}) \end{aligned}$$

$$r(x_k) = -(\sum_{j=2}^{n} \frac{1}{(j-1)!}\left((x_k - x_0)^{\frac{j-1}{2}}\right)^T \nabla^j F(x_0)(x_k - x_0)^{\frac{j-1}{2}})$$

$$r(x_{k+1}) = -F'(x_{k+1}) = -F'(x_k + \alpha_k P_k)$$

$$= -(\sum_{j=2}^{n} \frac{1}{(j-1)!}\left((x_k + \alpha_k P_k - x_0)^{\frac{j-1}{2}}\right)^T \nabla^j F(x_0)(x_k + \alpha_k P_k - x_0)^{\frac{j-1}{2}})$$

$$= -((\sum_{j=2}^{n} \frac{1}{(j-1)!}\left((x_k - x_0)^{\frac{j-1}{2}}\right)^T \nabla^j F(x_0)(x_k - x_0)^{\frac{j-1}{2}}) +$$

$$(\sum_{j=2}^{n} \frac{1}{(j-1)!}\left((\alpha_k P_k)^{\frac{j-1}{2}}\right)^T \nabla^j F(x_0)(\alpha_k P_k)^{\frac{j-1}{2}}))$$

$$r(x_{k+1}) = r(x_k) - (\sum_{j=2}^{n} \frac{1}{(j-1)!}\left((\alpha_k P_k)^{\frac{j-1}{2}}\right)^T \nabla^j F(x_0)(\alpha_k P_k)^{\frac{j-1}{2}}))$$

But

$$(\sum_{j=2}^{n} \frac{1}{(j-1)!}\left((\alpha_k P_k)^{\frac{j-1}{2}}\right)^T \nabla^j F(x_0)(\alpha_k P_k)^{\frac{j-1}{2}})) =$$

$$\alpha_k\left(\nabla^2 F(x_0) + \frac{1}{2!}\alpha_k P_k{}^T \nabla^3 F(x_0) + \ldots + \frac{1}{(j-1)!}(\alpha_k P_k)^{j-2})^T \nabla^j F(x_0)\right) P_k$$

$$= \alpha_k W P_k$$

where

$$W = \left(\nabla^2 F(x_0) + \frac{1}{2!}\alpha_k P_k{}^T \nabla^3 F(x_0) + \ldots + \frac{1}{(j-1)!}(\alpha_k P_k)^{j-2})^T \nabla^j F(x_0)\right)$$

$$r(x_{k+1}) = r(x_k) - \alpha_k W P_k \tag{9}$$

4 An Absolute-Stability Proof: (A New Conjugate Gradient Method)

Here, we need to show that the symmetric tridiagonal matrix produced by the symmetric Lanczos process gives the same pivot recurrence as the tridiagonal matrix produced by the NCGM. Also, we need to show that the error bound $| E_j |$ satisfy the criterion $| E_j | < 1,\ j = 0, 1, 2, \ldots,\ n$.

In line with Hageman [10] and Paige [2], the two basic vector updates of the NCGM given in equations (3) and (4) can be summarized as

$$R(I - J) = WPV, \quad PU = R \tag{10}$$

where R and P are matrices containing the vector sequences $\{r_k\}$ and $\{p_k\}$ as columns. $J = (\delta_{i,j+1})$, $V = diag(\alpha_k), c = (\frac{1}{\beta_k})$ *and* $U = \frac{1}{c} diag(\| (J^{-1} - cI) \|)$. It follows from equation (10) that

$$
\begin{aligned}
I - J &= R^{-1}WPV \\
(I - J)V^{-1} &= R^{-1}WP \\
(I - J)V^{-1}U &= R^{-1}WPU \\
&= R^{-1}WR \text{, a tridiagonal matrix}
\end{aligned}
$$

With $H = (I - J)V^{-1}U$, a tridiagonal matrix, we have that

$$WR = RH$$

since

$$
\begin{aligned}
RH &= R(I - J)V^{-1}U \\
&= WPVV^{-1}U \\
&= WPU \\
&= WR
\end{aligned}
$$

The Lanczos method for constructing an orthonormal matrix Q that reduces W to symmetric tridiagonal form T by $T = Q^T WQ$ could be constructed from the NCGM by letting $q_i = D_i$ be the diagonal elements of Q. The orthonormal tridiagonalization becomes $WQ = QT$ with $Q = RC^{-1}, T = C^{-1}HC$. Using the fact that H is tridiagonal and that $H = C^{-1}TC$ with C diagonal, we see that the factorization of T generates the same pivot sequence as W. This is true since

$$
\begin{aligned}
H &= C^{-1}TC; CH = TC \\
WQ &= WRC^{-1} \\
&= RHC^{-1}; \; WR = RH \\
&= QCHC^{-1}; \; R = QC \\
&= QTCC^{-1}; \; CH = TC
\end{aligned}
$$

For the region of absolute stability, we recall the step length $\alpha_c = \frac{2(1-\varepsilon)}{M}$, $0 < \varepsilon \, 1$ and error function defined by $E_k = E(x_k) = x_k - x^*$ where $\frac{\| E_{k+1} \|}{\| E_k \|} \leq Z = \| I - \frac{\alpha_c F''_{kc}}{\| F'_{opt} \|} \|$ and $Z = \max(| 1 - \frac{\alpha_c m}{\| F'_{opt} \|} |, | 1 - \frac{M\alpha_c}{\| F'_{opt} \|} |)$ from [1]. M and m are the biggest and smallest eigenvalues of F''_{kc} respectively. x^* is the exact solution of the optimization problem stated in equation (1). It follows that

$$Z_k = \max(|1 - \frac{2m(1-\varepsilon)}{\| F'_k \| M}|, |1 - \frac{2(1-\varepsilon)}{\| F'_k \|}|), \; k = 0, 1, 2, ..., n$$

and

$$|E_{k+1}| \le Z_k |E_k|, \; k = 0, 1, ..., n; \; |E_0| = |x_0 - x^*| \text{ or}$$
$$|E_k| \le Z_{k-1} |E_{k-1}|, \; k = 0, 1, ..., n; \; |E_0| = |x_0 - x^*|$$

defines the region of absolute stability of the method. This is true since, with $0 < \varepsilon 1$ and $M \ge m > 0$,

$$Z_{k-1} = \frac{1}{|F'_{k-1}|} \max(\| F'_{k-1}| - \frac{2m(1-\varepsilon)}{M}|, || F'_{k-1}| - 2(1-\varepsilon)|), \; k = 1, 2, ..., n$$

$$|F'_{k-1}| > \| F'_{k-1}| - \frac{2m(1-\varepsilon)}{M}| \; and \; |F'_{k-1}| > \; || F'_{k-1}| - 2(1-\varepsilon)|), \; k = 1, 2 ..., n$$

implies that $Z_{k-1} < 1$. Convergence of the new conjugate gradient method ensures that $|E_{k-1}| \to 0 \; as \; k \to \infty$. We have shown that the error bound

$$|E_k| \le Z_{k-1} |E_{k-1}| < 1, \; k = 1, 2, ..., n$$

defines the region of absolute stability of the new conjugate gradient method. We note that $\nabla^j F(x), \; j = 3, 4, ..., n$ are the matrix vector differentials of $\nabla^2 F(x)$. Therefore, if $\nabla^2 F(x)$ is symmetric, then, W must be symmetric too. Also, W must be positive definite since A = $\nabla^2 F(x_0)$ must be positive definite for an optimal point of F to exist. Since W is symmetric and positive definite, we conclude that the new conjugate gradient method is absolutely stable.

5 Numerical Examples

Numerical results obtained from the optimization of the following problems [11] are hereby presented.

Problem 1(Rastrigin function; n=2):

Minimize $F(x, y) = 20 + x_1^{\,2} + x_2^{\,2} - 10\left(Cos(2\pi x_1) + Cos(2\pi x_2)\right)$,

$x_0 = [0.1, \; 0.1], \; x^* = [0, \; 0]$

Problem 2:

Minimize $F(x_1, x_2) = Exp(x_1)\left(4x_1^{\,2} + 2x_2^{\,2} + 4x_1 x_2 + 2x_2 + 1\right)$,

$x_0 = [-1,\ 1],\ \ x^* = [-1.5,\ 1]$

Problem 3:

Minimize $F(x_1, x_2) = (x_1{}^2 - x_2)^2 + (x_2 - 1)^2$,

$x_0 = [1,\ 0],\ \ x^* = [1,\ 1]$

Problem 4:

Minimize $f(x_1, x_2) = (x_1 + 1)^3 + x_2$

Subject to

$x_1 - 1 \geq 0, x_2 \geq 0.$

$x^* = [1,\ 0]$

Problem 5:

Minimize $J(x,u) = 0.1\sum_{i=1}^{10}\left(x(i)^2 + u(i)^2\right)$

Subject to

$x_i = x_{i-1} + 0.1u_{i-1}$

$x_0 = 1, u_0 = 0.5; i = 1, 2, ..., 10.$

Problem 6:

Minimize $I(x,u) = \frac{1}{4}\int_0^1 u^4(t)dt$

Subject to

$\dot{x} = x(t) + u(t);\ \ 0 \leq t \leq 1;\ x(0) = 1,\ x(1) = 0;\ u(0) = -2,\ \Delta t = 0.1$

$x^* = 0,\ \ u^* = -1.29735$

The following Tables (1-6) and Figs. (1-6) confirm the fact that the error bounds generated by NCGM satisfy the condition $|E_k| \leq Z_{k-1}|E_{k-1}| < 1,\ \ k = 1, 2, ..., n$

Table 1. Solution of problem 1 by NCGM

No. of iterations	x_1	x_2	$F(x_1, x_2)$	**Error bound** $\|E_k\| = \|x_k - x^*\|$
1	0.1	0.1	3.824634	0.141421
2	0.001849	0.001849	0.001351	2.615534E-03
3	0.000037	0.000037	0.000001	5.166958E-05
4	0.000001	0.000001	0	1.020735E-06

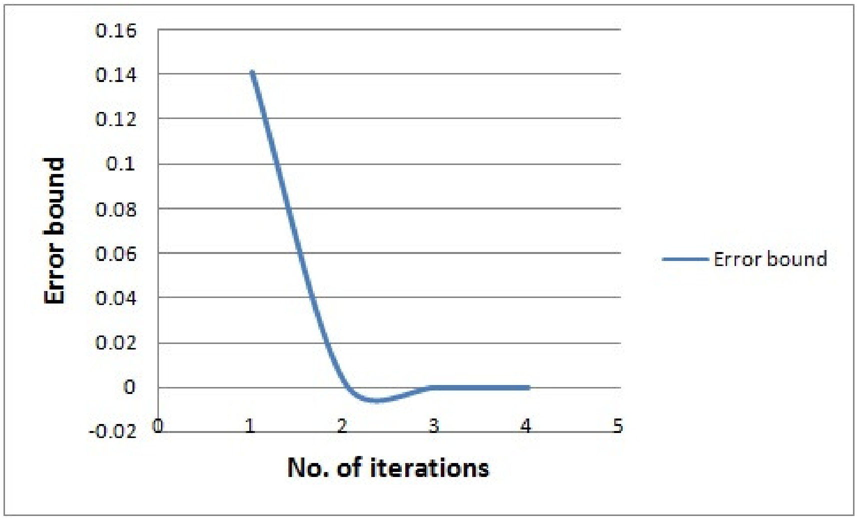

Fig. 1. Error bound of problem 1 by NCGM

Table 2. Solution of problem 2 by NCGM

No. of iterations	x_1	x_2	$F(x_1,x_2)$	Error bound
				$\lvert E_k \rvert = \lvert x_k - x^* \rvert$
1	-1	1	1.839397	0.5
2	-1.133956	0.732088	1.724263	0.453613
3	-1.547138	0.938846	1.789058	7.721252E-02
4	-1.512419	1.008243	1.78498	1.490518E-02
5	-1.498656	1.001342	1.785044	1.899201E-03
6	-1.499497	0.999665	1.785041	6.045778E-04
7	-1.500055	0.999945	1.785041	7.752504E-05
8	-1.50002	1.000013	1.785041	2.429327E-05

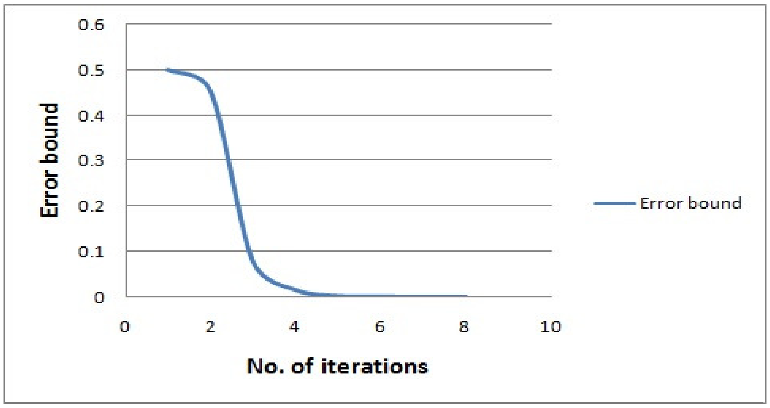

Fig. 2. Error bound of problem 2 by NCGM

Table 3. Solution of problem 3 by NCGM

No. of iterations	x_1	x_2	$F(x_1, x_2)$	Error bound $\lvert E \rvert = \lvert x - x^* \rvert$
1	1	0	2	1
2	0.5002	0.4998	0.3125	0.707107
3	0.99997	1.001372	0.000004	1.371892E-03
4	1.00054	1.000814	0.000001	9.764222E-04
5	0.999993	1.000252	0	2.523227E-04
6	1.000099	1.000149	0	1.789777E-04
7	0.999999	1.000046	0	4.554963E-05
8	1.000018	1.000027	0	3.219506E-05
9	1	1.000008	0	8.070761E-06
10	1.000003	1.000005	0	5.683448E-06
11	1	1.000001	0	1.402926E-06
12	1.000001	1.000001	0	9.841288E-07

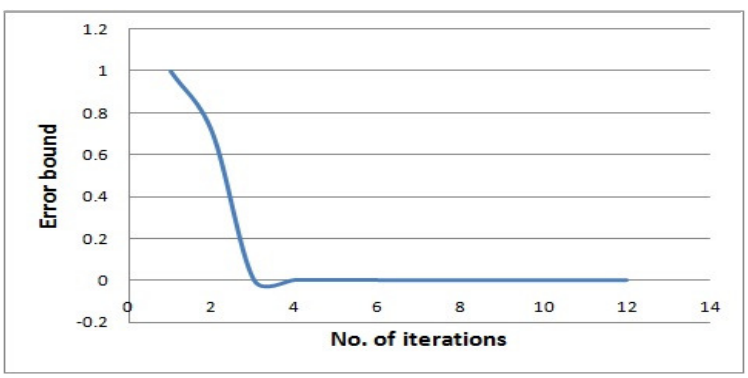

Fig. 3. Error bound of problem 3 by NCGM

Table 4. Solution of problem 4 by NCGM

No. of iterations	x_1	x_2	$F(x_1,x_2)$	Error bound $\lvert E_k \rvert = \lvert x_k - x^* \rvert$
1	1.2	0.2	3.749334	0.2
2	1.139556	0.2604439	3.525193	0.139556
30	1.000002	0.03880354	2.705478	1.788139E-06
31	1.000002	0.0388035	2.705478	1.788139E-06
32	1.000002	0.0388035	2.705478	1.788139E-06
33	1.000002	0.0388035	2.705478	2.026558E-06
34	1.000002	5.871513E-06	2.66668	2.026558E-06
35	1.000002	3.903678E-06	2.66668	2.026558E-06
36	1.000002	3.928141E-06	2.66668	2.026558E-06
37	1.000002	3.928141E-06	2.66668	2.026558E-06

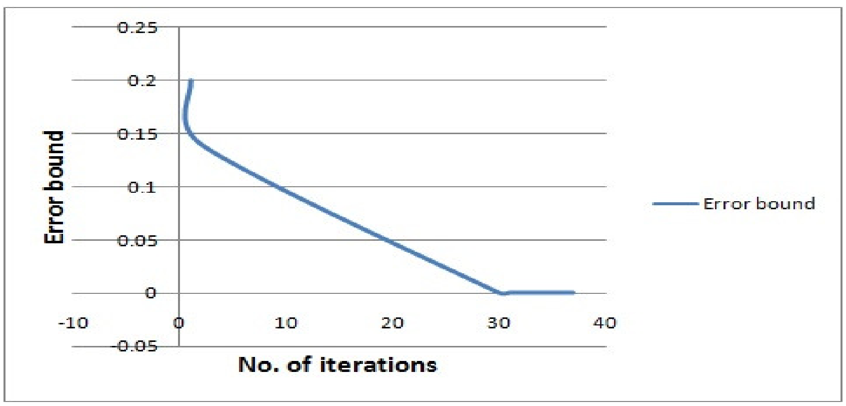

Fig. 4. Error bound of problem 4 by NCGM

Table 5. Solution of problem 5 by NCGM

No. of iterations	x	u	$F(x,u)$	Error bound $\lvert E_k \rvert$
1	1.011796	4.084E-04	0.102373	1.346319E-02
2	0.974485	4.27E-7	0.197335	1.3985E-2
3	0.969326	9.77E-12	0.291295	1.13E-4
4	0.947307	3.927E-15	0.381034	5.838E-3
5	0.890482	1.068E-17	0.460329	0.015985
6	0.878034	1.652E-21	0.537424	1.239899E-2
7	0.825365	4.942E-24	0.605546	0.004888
8	0.775855	1.221E-26	0.665741	3.398E-03
9	0.729315	3.32E-29	0.718931	6.397E-03
10	0.658226	2.346E-31	0.762258	1.4801E-03

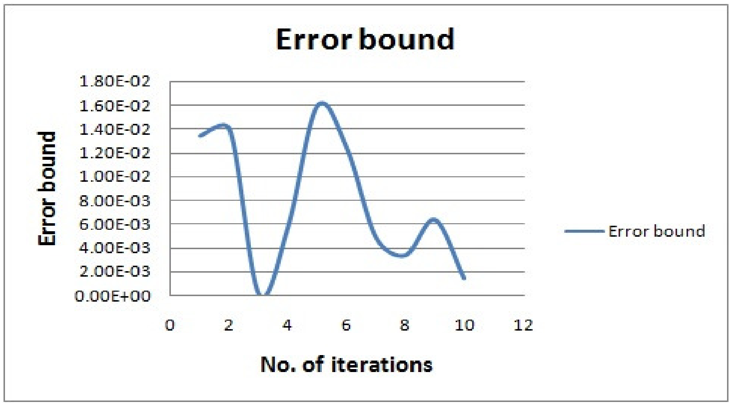

Fig. 5. Error bound of problem 5 by NCGM

Table 6. Solution of problem 6 by NCGM

No. of iterations	x	u	$F(x,u)$	Error bound $\vert E_k \vert$
1	1	-2	4	0.702651
2	0.000000001	-1.330793	0.784119	3.344284E-02
3	0.000000001	-1.306902	0.729310	9.552149E-03
4	0.000000001	-1.300079	0.714199	2.728966E-03
5	0.000000001	-1.298130	0.709926	7.802653E-04
6	0.000000001	-1.297573	0.708709	2.237162E-04
7	0.000000001	-1.297415	0.708362	6.476587E-05
8	0.000000001	-1.297369	0.708263	1.936964E-05
9	0.000000001	-1.297356	0.708235	6.404475E-06
10	0.000000001	-1.297353	0.708227	2.701624E-06
11	0.000000001	-1.297353	0.708227	2.689312E-06
12	0.000000001	-1.297352	0.708227	2.676999E-06

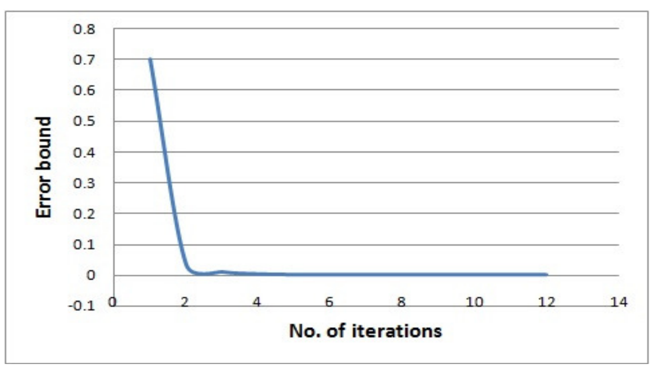

Fig. 6. Error bound of problem 6 by NCGM

6 Conclusion

The new conjugate gradient method has a natural connection with the Lanczos process for solving systems of equations. Also, it satisfies the traditional criterion for ensuring that a numerical method is stable. Therefore, the NCGM is efficient, accurate, reliable and absolutely stable.

Competing Interests

Authors have declared that no competing interests exist.

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