Honam Mathematical J. 17(1995), No. 1,pp. 129–140

NUMERICAL RESULTS ON THE CONJUGATE GRADIENT METHOD OF SLIGHTLY NON–SYMMETRIC MATRICES

DO- HYUN KIM

Dept. of Mathematics Education, Cheju National Universty, Cheju 690-756, Korea.

1. Introduction and Preliminaries

It is known that the conjugate gradient(CG) method [1,2,8] converges when this method is applied to solve linear systems of the form Ax=b, where A is symmetric and positive definite. For some finite difference discretizations of elliptic problems, one gets positive definite matrices that are almost symmetric. Practically, the CG method work these matrices. However, the convergence of this method is not guaranteed theoretically. In this paper, we prove that the CG method converge when the l^2 matrix norm of the non-symmetric part of a positive definite matrix is less than some value related to the smallest and the largest eigenvalues of the symmetric part of the given matrix. We also illustrate numerical results for the CG method.

For non-symmetric matrices, many iterative methods [4,7] have been developed that come from the CG method by changing the number of terms, the number of iterations, or the inner product and so forth. The convergence of most of these CG-like methods were proven by the use of Krylov space techniques. The convergence proof that we do in this paper is done without the use of the Krylov space. Hence our setting and proof are much different from those that are done so far about the CG-like methods for non-symmetric matrices.

We begin with some notations. Let A be a positive definite matrix, then A can be represented as

$$A = A_s + A_n$$

where

$$A_s = \frac{A + A^t}{2} \quad \text{and} \quad A_n = \frac{A - A^t}{2}$$

Received March 2, 1995.

are the symmetric and nonsymmetric parts of A respectively. Since A is positive definite, the symmetric part A_s is also positive definite. Thus A_s is invertible and the eigenvalues of A_s are all positive real numbers. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A_s such that $0 < \lambda_1 \leq \ldots \leq \lambda_n$, then $\lambda_1^{-1}, \ldots, \lambda_n^{-1}$ are the eigenvalues of A_s^{-1}.

Define

$$(x, y) := x^t y$$

as the Euclidean inner product of two vectors $x, y \in R^n$ and let

$$\| x \| := \sqrt{(x, x)}$$

be the induced Euclidean norm. We need also the inner product

$$(x, y)_s := (x, A_s^{-1} y)$$

and the corresponding norm

$$\| x \|_s := \sqrt{(x, x)_s}$$

The associated matrix norms are given by

$$\| A \| = \sup_{\|x\|=1} \| Ax \| \quad \text{and} \quad \| A \|_s = \sup_{\|x\|_s=1} \| Ax \|_s$$

The condition number of A_s is defined as

$$\kappa = \| A_s \| \| A_s^{-1} \| = \lambda_n \lambda_1^{-1}$$

Note that $\kappa \geq 1$.

2. The CG Method for Slightly Nonsymmetric Matrices

We need the following lemmas to prove the theorem for the conjugate gradient method.

LEMMA 2.1. *For any vector x,*

$$(1) \quad (x, A_n x) = 0 \quad \textit{and}$$

$$(2) \quad (x, Ax) = (x, A_s x)$$

Proof. (1) Since $x^t A_n x$ is a real number,

$$x^t A_n x = (x^t A_n x)^t = x^t A_n^t x = -x^t A_n x$$

Hence $(x, A_n x) = 0$.

(2) By (1), $(x, Ax) = (x, A_s x) + (x, A_n x) = (x, A_s x)$.

LEMMA 2.2. *For any vector x,*

$$\lambda_1 \parallel x \parallel^2 \leq (x, Ax) \leq \lambda_n \parallel x \parallel^2 .$$

Proof. Since the Rayleigh quotients of a symmetric matrix are bounded by the smallest and the largest eigenvalues of the matrix,

$$\lambda_1 \leq \frac{(x, A_s x)}{\parallel x \parallel^2} \leq \lambda_n .$$

By Lemma 2.1, the claim follows.

LEMMA 2.3. *For any vector x, the followings hold.*

$$(1) \quad \lambda_n^{-1} \parallel x \parallel^2 \leq \parallel x \parallel_s^2 \leq \lambda_1^{-1} \parallel x \parallel^2 \quad \text{and}$$
$$(2) \quad \lambda_1 \parallel x \parallel_s^2 \leq \parallel x \parallel^2 \leq \lambda_n \parallel x \parallel_s^2 .$$

Proof. (1) Since the Rayleigh quotients of a symmetric matrix A_s^{-1} are bounded by the smallest and the largest eigenvalues of the matrix,

$$\lambda_n^{-1} \leq \frac{(x, A_s^{-1} x)}{\parallel x \parallel^2} \leq \lambda_1^{-1} .$$

Thus

$$\lambda_n^{-1} \parallel x \parallel^2 \leq \parallel x \parallel_s^2 \leq \lambda_1^{-1} \parallel x \parallel^2 .$$

(2) From (1),

$$\lambda_1 \leq [\frac{(x, A_s^{-1} x)}{\parallel x \parallel^2}]^{-1} \leq \lambda_n .$$

The Schwarz inequality for a symmetric positive definite matrix is stated in the next lemma.

LEMMA 2.4. *If P is a symmetric positive definite matrix, then*

$$| (x, Py) | \leq \sqrt{(x, Px)(y, Py)} \quad \text{for any } x \text{ and } y.$$

LEMMA 2.5. *For any x and y,*

$$|(x,y)| \leq \sqrt{(x, A_s x)(y, A_s^{-1} y)}.$$

Proof. By Lemma 2.4,

$$\begin{aligned} |(x,y)| &= |(x, A_s(A_s^{-1}y))| \\ &\leq \sqrt{(x, A_s x)(A_s^{-1}y, A_s(A_s^{-1}y))} = \sqrt{(x, A_s x)(A_s^{-1}y, y)}. \end{aligned}$$

We will use the notations.

$$\epsilon := \| A_n \| \quad \text{and} \quad a_k := (r^k, A_s^{-1} r^k)$$

LEMMA 2.6. *For any positive integer k,*

$$|\alpha_k| \leq \sqrt{\frac{a^k}{\lambda_1 \| p^k \|^2}}.$$

Proof. By Lemma 2.1, Lemma 2.2 and Lemma 2.5,

$$\begin{aligned} |\alpha_k| &= \frac{|(p^k, r^k)|}{(p^k, Ap^k)} \leq \frac{\sqrt{(p^k, A_s p^k)(r^k, A_s^{-1} r^k)}}{(p^k, Ap^k)} \\ &= \frac{\sqrt{(p^k, A_s p^k) a^k}}{(p^k, A_s p^k)} = \sqrt{\frac{a^k}{(p^k, A_s p^k)}} \leq \sqrt{\frac{a^k}{\lambda_1 \| p^k \|^2}}. \end{aligned}$$

LEMMA 2.7. *For any positive integer k,*

$$(p^k, r^k) = (r^k, r^k).$$

Proof. Note that for any k,

$$(p^k, r^{k+1}) = (p^k, r^k) - \alpha_k (p^k, Ap^k) = 0$$

by the definition of α_k.
Thus,

$$(p^k, r^k) = (r^k, r^k) + \beta_{k-1}(p^{k-1}, r^k) = (r^k, r^k).$$

LEMMA 2.8. *For any positive integer k,*

$$(p^k, Ap^k) = (p^k, Ar^k).$$

Proof. By the definition of β_k,

$$(p^{k+1}, Ap^k) = (r^{k+1}, Ap^k) + \beta_k(p^k, Ap^k) = 0$$

for any k.
Hence,

$$(p^k, Ap^k) = (p^k, Ar^k) + \beta_{k-1}(p^k, Ap^{k-1}) = (p^k, Ar^k)$$

LEMMA 2.9. *For any positive integer k,*

$$\alpha_k(p^k, r^k) \geq \kappa^{-1} a^k$$

Proof. By Lemma 2.4 and Lemma 2.8,

$$(p^k, A_s p^k) = (p^k, A_s r^k) \leq \sqrt{(p^k, A_s p^k)(r^k, A_s r^k)}.$$

Using Lemma 2.1, we get

$$(p^k, Ap^k) \leq (r^k, Ar^k) \qquad (2.1).$$

Hence, by (2.1), Lemma 2.2, Lemma 2.3 and Lemma 2.7,

$$\alpha_k(p^k, r^k) = \frac{(r^k, r^k)^2}{(p^k, Ap^k)} \geq \frac{(r^k, r^k)^2}{(r^k, Ar^k)} \geq \frac{(r^k, r^k)}{\lambda_n} \geq \frac{\lambda_1}{\lambda_n} a^k.$$

With the above lemmas, the convergence for the CG method applied to the linear system Ax=b is shown in the next theorem.

THEOREM 2.10. *If*

$$\| A_n \| < \lambda_1 \left(-1 + \sqrt{1+\kappa^{-1}}\right)$$

then the CG method, defined by

$$p^0 = r^0 = b - Ax^0$$

$$x^{k+1} = x^k + \alpha_k p^k$$

$$r^{k+1} = r^k - \alpha_k A p^k$$

$$p^{k+1} = r^{k+1} + \beta_k p^k$$

$$\alpha_k = \frac{(p^k, r^k)}{(p^k, Ap^k)}$$

$$\beta_k = -\frac{(r^{k+1}, Ap^k)}{(p^k, Ap^k)}$$

converges.

Proof. We have

$$\begin{aligned}
(r^{k+1}, A_s^{-1} r^{k+1}) =& (r^k - \alpha_k A p^k, A_s^{-1} r^k - \alpha_k A_s^{-1} A p^k) \\
=& (r^k, A_s^{-1} r^k) - 2\alpha_k (Ap^k, A_s^{-1} r^k) + \alpha_k^2 (Ap^k, A_s^{-1} A p^k) \\
=& (r^k, A_s^{-1} r^k) - 2\alpha_k (p^k, r^k) - 2\alpha_k (A_n p^k, A_s^{-1} r^k) \\
&+ \alpha_k^2 (Ap^k, p^k) + \alpha_k^2 (Ap^k, A_s^{-1} A_n p^k) \\
=& (r^k, A_s^{-1} r^k) - \alpha_k (p^k, r^k) - 2\alpha_k (A_n p^k, A_s^{-1} r^k) \qquad (2.2) \\
&+ \alpha_k^2 (Ap^k, A_s^{-1} A_n p^k) \\
=& (r^k, A_s^{-1} r^k) - \alpha_k (p^k, r^k) - 2\alpha_k (A_n p^k, A_s^{-1} r^k) \\
&+ \alpha_k^2 (p^k, A_n p^k) + \alpha_k^2 (A_n p^k, A_s^{-1} A_n p^k) \\
=& (r^k, A_s^{-1} r^k) - \alpha_k (p^k, r^k) - 2\alpha_k (A_n p^k, A_s^{-1} r^k) \\
&+ \alpha_k^2 (A_n p^k, A_s^{-1} A_n p^k).
\end{aligned}$$

By lemma 2.3,

$$|(A_n p^k, A_s^{-1} A_n p^k)| \le \lambda_1^{-1} \| A_n p^k \|^2 \le \lambda_1^{-1} \epsilon^2 \| p^k \|^2 \qquad (2.3).$$

Using (2.3) and Lemma 2.4,

$$|(A_n p^k, A_s^{-1} r^k)| \leq \sqrt{(A_n p^k, A_s^{-1} A_n p^k) a^k} \leq \sqrt{\lambda_1^{-1} \epsilon^2 \parallel p^k \parallel^2 a^k} \quad (2.4).$$

By Lemma 2.6, Lemma 2.9, and equations from (2.2) to (2.4), one gets

$$\begin{aligned} a^{k+1} &\leq a^k - \kappa^{-1} a^k + 2\sqrt{\frac{a^k}{\lambda_1 \parallel p^k \parallel^2}} \sqrt{\lambda_1^{-1} \epsilon^2 \parallel p^k \parallel^2 a^k} \\ &\quad + \frac{a^k}{\lambda_1 \parallel p^k \parallel^2} \lambda_1^{-1} \epsilon^2 \parallel p^k \parallel^2 \\ &= a^k (1 - \kappa^{-1} + 2\lambda_1^{-1} \epsilon + \lambda_1^{-2} \epsilon^2) \end{aligned}$$

For convergence, we require

$$1 - \kappa^{-1} + 2\lambda_1^{-1}\epsilon + \lambda_1^{-2}\epsilon^2 < 1$$

$$\lambda_1^{-2}\epsilon^2 + 2\lambda_1^{-1}\epsilon - \kappa^{-1} < 0$$

$$\epsilon^2 + 2\lambda_1\epsilon - \kappa^{-1}\lambda_1^2 < 0$$

Hence, the sufficient condition for convergence is

$$\epsilon < -\lambda_1 + \sqrt{\lambda_1^2 + \kappa^{-1}\lambda_1^2} = \lambda_1(-1 + \sqrt{1 + \kappa^{-1}}).$$

3. Numerical Results

Consider the one-dimensional boundary value problem given by

$$-\nu u_{xx} + u_x = f(x) \quad \text{for} \quad 0 \leq x \leq 1 \qquad (3.1)$$

$$u(0) = A, \quad u(1) = B$$

where A, B are constants and f is a given function. The equation (3.1) describes the motion of a fluid with viscosity.

We wish to find numerical solution of the equation (3.1) by finite difference method.

Let

$$u_l = u(x_l), f_l = f(x_l).$$

Replacing u_x and u_{xx} by backward difference approximation and central difference approximation respectively, the equation (3.1) is

$$-\nu\frac{u_{l+1}-2u_l+u_{l-1}}{h^2}+\frac{u_l-u_{l-1}}{h}=f_l \quad (l=1,...,n-1)$$
$$u_0=A, u_n=B.$$

Simplifying the above expression,

$$-(\nu+h)u_{l-1}+(2\nu+h)u_l-\nu u_{l+1}=h^2f_l \quad (l=1,...,n-1) \qquad (3.2).$$

If

$$A=\begin{pmatrix} 2\nu+h & -\nu & & & \\ -\nu-h & 2\nu+h & -\nu & & \\ & \ddots & \ddots & \ddots & \\ & & -\nu-h & 2\nu+h & -\nu \\ & & & -\nu-h & 2\nu+h \end{pmatrix}$$

$$U=\begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \end{pmatrix} \quad \text{and} \quad F=\begin{pmatrix} h^2f_1+(\nu+h)A \\ h^2f_2 \\ \vdots \\ h^2f_{n-2} \\ h^2f_{n-1}+\nu B \end{pmatrix}$$

this equations (3.2) can be written in the matrix notation

$$AU=F$$

By the definition of A_s and A_n, we can write

$$A_s=(\nu+\frac{h}{2})\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

$$\text{and} \quad A_n=\frac{h}{2}\begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ & & & -1 & 0 \end{pmatrix}$$

Since

$$\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

is an (n-1)×(n-1) matrix, there should be n-1 eigenvalues and eigenvectors. It is easy to check that the eigenvectors are given by

$$v_a = (\sin \frac{al\pi}{n})_{l=1}^{n-1}, \quad (a = 1, ..., n-1)$$

and the corresponding eigenvalues are

$$\lambda_a = 2(1 - \cos \frac{a\pi}{n}).$$

Hence, we can see that

$$\lambda_{min}(A_s) = (\nu + \frac{h}{2})\lambda_1 = (2\nu + h)(1 - \cos \frac{\pi}{n}) = (2\nu + h)(1 - \cos \pi h)$$

$$\lambda_{max}(A_s) = (\nu + \frac{h}{2})\lambda_{n-1} = (2\nu + h)(1 + \cos \frac{\pi}{n}) = (2\nu + h)(1 + \cos \pi h).$$

Thus

$$\kappa(A_s)^{-1} = \lambda_{min}\lambda_{max}^{-1} = \frac{1 - \cos \pi h}{1 + \cos \pi h}.$$

If

$$B_n = \begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ & & & -1 & 0 \end{pmatrix}$$

then $\| B_n \|$ is the largest singular value of B_n. Using the mathematica, we can find an approximation of $\| B_n \|$. In case of the equation (3.1), the condition of theorem 2.10 is

$$\frac{h}{2} \| B_n \| < (2\nu + h)(1 - \cos \pi h) \left(-1 + \sqrt{\frac{2}{1 + \cos \pi h}} \right) \qquad (3.3).$$

Let

$$M_c = (1 - \cos \pi h)\left(-1 + \sqrt{\frac{2}{1 + \cos \pi h}}\right),$$

then the expression (3.3) is $\nu > \overline{M}_c$,

where

$$\overline{M}_c = \frac{h}{4M_c} \| B_n \| - \frac{h}{2}.$$

Mathematica has been used to find $\overline{M}_c$ for some values of h, which we show in the next table.

Table 3.1

ν for the CG method

h	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{30}$
$\overline{M}_c$	78.5858	649.324	2205.55

To show that the CG method converges when

$$\nu > \overline{M}_c,$$

we choose the numerical problem as follows :

$$u(x) = \frac{1}{2\pi} \sin 2\pi x \quad , \quad f(x) = 2\pi\nu \sin 2\pi x + \cos 2\pi x \qquad (3.4)$$

Since the functions u(x) and f(x) defined on [0,1] are given with change of sign and is not a brief polynomial form, (3.4) is used to discuss the numerical methods in this thesis.

Table 3.2 shows the numerical results when applied to the CG method

Table 3.2-1
The CG method with tolerance = 10^{-6}
(h = 1/10)

ν	No. of Iterations	l_2-error
79	19	0.00482118
100	18	0.00484001
500	15	0.000489684
1000	14	0.00490376
5000	14	0.00490961
10000	13	0.00491033
50000	11	0.00491091

Table 3.2-2
The CG method with tolerance = 10^{-6}
(h = 1/20)

ν	No. of Iterations	l_2-error
650	29	0.00101046
700	29	0.00101079
1000	29	0.00101209
5000	27	0.00101452
10000	26	0.00101483
50000	21	0.00101506
100000	19	0.00101507

References

1. Owe Axelsson, *Solution of Linear Systems of Equations:iterative methods Sparse Matrix Techniques,*, Springer-Verlag, New York, 1976.
2. Rati Chandra, *Conjugate Gradient Methods for Partial Differential Equations Ph.D.Thesis Department of Computer Science, Yale University.*
3. A.J.Chorin and J.E.Marsden, *A Mathematical Introduction to Fluid Mechanics*, Springer-Verlag, 1990.
4. H.C. Elman, *Iterative Methods for Large,Sparse,Nonsymmetric Systems of Linear Equations, Ph.D. Dissertation, Yale University*, 1982.

5. G.H. Golub and C.F.Van loan, *Matrix Computations*, Johns Hopkins University Press, Baltimore, 1983.
6. W.Joubert, *Generalized Conjugate Gradient Methods for the Solution of Nonsymmetric Systems of Linear Equations*, CNA-238, 1990.
7. W.Joubert, *Iterative Methods for the Solution of Nonsymmetric Systems of Linear Equations*, CNA-242, The Center for Numerical Analysis, The University of Texas at Austin, Texas, 1990.
8. J.k. Reid, *On the Method of Conjugate Gradients for the Solution of Large Sparse Systems of Linear Equations, Large Sparse Sets of Linear Equations*, Academic Press, New York, 1971, pp. 231-254.
9. J.C. Strikwerda, *Finite Difference Schemes and Partial Differential Equations*, Wadoworth & Brooks, 1989.
10. R.S. Varga, *Matrix Iterative Analysis*, Prentice-Hall,Inc., 1962.
11. Chia-Shun Yih, *Fluid Mechanics*, West River Press, 1988.
12. D.M.Young, *Iterative Solution of Large Linear Systems*, Academic Press Inc., 1971.