

Conjugate gradient method for ill – conditioned linear system

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Abstract

In this article, an iterative method - Conjugate Gradient Method is used to deal 4 by 4 Wilkinson matrix and 10 by 10 Hilbert matrix during solving ill- conditioned linear systems. The work has been carried out in FORTRAN on new computational facilities. All calculations have been done in double precision. It is found that, this method is very efficient, fast converging and less time consuming.

Keywords: Conjugate Gradient Method, Wilkinson Matrix, Hilbert Matrix

INTRODUCTION

Consider the following system of linear equations

$$AX = B \quad \text{----(1.1)}$$

where A is n by n matrix, X and B are n-dimensional column vectors.

Our concern is here to yield the solution of (1.1) if A is either 4 by 4 Wilkinson matrix or 10 by 10 Hilbert matrix. That is the coefficient matrix of the system (1.1) is restricted to be only 4 by 4 Wilkinson matrix or 10 by 10 Hilbert matrix. The various direct/iterative methods for solving linear equations get failed or give solutions which are not good. It is investigated that various factorization methods are failed to solve this problem. Among the iterative methods, Conjugate Gradient Method has been found to be most efficient, fast converging and less time consuming.

METHOD AND ALGORITHM

Before conjugate gradient method, it is necessary to discuss 'Steepest Descent Method'.

Steepest Descent Method

Using the fact that gradient vector represents the direction of 'steepest descent', where direction for minimization will be taken as negative of gradient vector. In this method, starting with an initial trial point 'X' and iteratively move towards the optimum point according to the rule-

$$X_{k+1} = X_k + \lambda_k S_k = X_k - \lambda_k \nabla f_k \quad \text{----(2.1)}$$

where λ_k is the optimal step length along the search direction

$$S_k = -\nabla f_k \quad \text{----(2.2)}$$

The phenomenon of function for solution of linear

simultaneous equation is as follows-

To minimize the function $f(x)$ defined by

$$f(X) = \frac{1}{2} X^T A X - X^T B \quad \text{----(2.3)}$$

where $B \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n \times n}$ is assumed to be positive definite and symmetric. The minimum value of 'f' is $-(B^T A^{-1} B)/2$ achieved by setting $X = A^{-1} B$. Thus minimizing 'f' and solving $AX = B$ are equivalent problems.

In the direction of negative gradient

$$-\nabla f(X_c) = B - AX_c \quad \text{----(2.4)}$$

The residual at $X = X_c$ is defined as

$$r_c = B - AX_c \quad \text{----(2.5)}$$

If the residual is non-zero, then there exists a positive 'α' such that

$$f(X_c + \alpha r_c) < f(X_c) \quad \text{----(2.6)}$$

The optimal step length λ_k is the scalar α.

At each point X_i , find

$$S_k = -\nabla f_k \quad \text{----(2.7)}$$

To find X_{k+1} , find the optimal step length λ_k . For this minimize $f(X_k + \lambda_k S_k)$ with respect to λ_k . Then using (2.1) calculate X_{k+1} .

This process has to be continued until the optimum point 'X' is reached. Any one of convergence criteria can be used to terminate the process-

$$(a) |(f(X_{k+1}) - f(X_k))/f(X_k)| \leq \epsilon_1$$

$$(b) |X_{k+1} - X_k| \leq \epsilon_2$$

$$(c) |X_{k+1} - X_k|^2 / |X_{k+1}|^2 \leq \epsilon_3$$

The Conjugate Gradient method

The convergence characteristics of 'steepest descent method' that can be greatly improved by modifying it into conjugate gradient method. Any minimization method that makes use of conjugate directions is quadratically convergent; this property ensures that the method will minimize a function in 'n' steps or less. The following result is important in developing the conjugate gradient method.

If the search directions used in minimization process, S_1, S_2, \dots, S_k , are mutually conjugate with respect to A then

$$S_k^T \nabla f_{i+1} = 0, \text{ for } k = 1, 2, \dots, i \quad \text{----(2.8)}$$

Procedure

Starting with an initial point X_1 , calculate the first search

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direction

$$S_1 = -\nabla f(X_1) = -\nabla f_1 \quad (\text{say})$$

The point X_2 is calculated according as-

$$X_2 = X_1 + \lambda_1 S_1$$

where λ_1 is the optimal step length in the direction S_1 .

Now, calculate S_2 by formula

$$S_k = \nabla f_k + \{ |\nabla f_k|^2 / |\nabla f_{k-1}|^2 \} S_{k-1} \quad \text{----(2.9)}$$

Now, to find λ_2 , minimize $f(X_2 + \lambda_2 S_2)$ after getting λ_2 , calculate

$$X_3 = X_2 + \lambda_2 S_2$$

and repeat the above process till the optimum is reached as given by desired accuracy.

The convergence of the conjugate gradient iterates $\{X_k\}$ depends upon the fact that- "If $A = I + B$ is an $n \times n$ symmetric positive matrix and $\text{rank}(B) = r$, then method converges in at most ' r ' steps".

The method performs well when A is near the identity either in the sense of a low rank perturbation matrix or in the sense of norm.

Algorithm

If $A \in \mathbb{R}^{n \times n}$ is symmetric positive definite and $B \in \mathbb{R}^n$, then the following algorithm computes $X \in \mathbb{R}^n$ so $AX = B$.

- (i) start $k = 0$; $X(0) = 0$; $r(0) = B$
- (ii) if $(r(k) \neq 0)$
- (iii) $k = k+1$
- (iv) if $k = 1$
 - $p(1) = r(0)$
 - else
 - $\beta(k) = r(k-1)^T r(k-1) / r(k-2)^T r(k-2)$
 - $p(k) = r(k-1) + \beta(k) p(k-1)$
 - (end of if statement)
- (v) $\alpha(k) = r(k-1)^T r(k-1) / p(k)^T A p(k)$
- (vi) $x(k) = x(k-1) + \alpha(k) p(k)$
- (vi) $r(k) = r(k-1) - \alpha(k) A p(k)$
- (vii) for $i = 1, n$
 - calculate $\text{eps} = \{ \sum (x(i)^{(k+1)} - x(i)^{(k)})^2 \} / \sum (x(i)^{(k+1)})^2$
- (ix) if eps is less than given accuracy
 - goto(x)
 - else
 - goto(ii)
- (x) $X = X(k)$

RESULTS AND DISCUSSION

The equation systems containing 4 by 4 Wilkinson matrix and 10 by 10 Hilbert matrix as coefficient matrix have been experimented in order to estimate the potential of Conjugate Gradient method.

The 4 by 4 Wilkinson matrix

The following matrix is deceptively simple, as it is already in lower triangular form. However, it possesses severe computational problems.

$$A = \begin{bmatrix} 0.9143\text{E-4} & 0 & 0 & 0 \\ 0.8762 & 0.7156\text{E-4} & 0 & 0 \\ 0.7943 & 0.8143 & 0.9504\text{E-4} & 0 \\ 0.8017 & 0.6123 & 0.7165 & 0.7123\text{E-4} \end{bmatrix}$$

$$B = [0.00009143 \quad 0.87627156 \quad 1.60869504 \quad 2.13057123]^T$$

This makes true solution of $AX = B$, the vector $[1, 1, 1, 1]^T$.

When this problem is solved by Direct methods, it is observed that factorization methods do not give a good result. This is due to, in the step of triangulization the diagonal element of last row tends to zero. Therefore one of the factors goes to singular. Thus, perhaps all factorization methods are failed to solve this problem.

For this matrix, we have-

$$\|A\| = 2.13$$

$$\|A^{-1}\| = 1.15 \times 10^{16}$$

$$\|r\| = 1.46 \times 10^{-14}$$

$$\|X - \underline{X}\| = 0.00177$$

$$(\|X - \underline{X}\|) / \|X\| = 0.0017$$

The 10 by 10 Hilbert matrix

It is defined by as follows-

$$h(i, j) = 1 / ((i + j) - 1); \quad i, j = 1, 2, \dots, 10.$$

$$\text{Taking } B = [1, 0, 0, \dots, 0]^T,$$

When we try to solve this problem by Direct methods, we observe that elimination process with S.P.P. gives close result while factorization method failed.

For this matrix, we have-

$$\|A\| = 2.93$$

$$\|A^{-1}\| = 1.21 \times 10^{13}$$

$$\|r\| = 5.12 \times 10^{-19}$$

$$\|X - \underline{X}\| = 9.61 \times 10^6$$

$$(\|X - \underline{X}\|) / \|X\| = 2.77 \times 10^{-4}$$

It is observed that Conjugate Gradient method is very efficient, fast converging, less time consuming and gives very good results.

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