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# SOME METHODS OF KRYLOV SUBSPACE AND IT'S COMPARISON IN APPLICATION

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*ABSTRACT*

*In this paper, we mainly introduce several kinds of the Krylov subspace algorithms, the most representative are: CGNR algorithm, GMRES algorithm, BiCG algorithm, CGS algorithm, BiCGSTAB algorithm and QMR algorithm, and discuss the relationships between these algorithms and their respective advantages and disadvantages, and finally verify the correctness of the conclusions for a class of numerical examples.*

***Key words:*** *Krylov subspace methods; WQMR algorithm; CGNR algorithm.*

## 1. CONJUGATE GRADIENT METHOD OF NORMAL EQUATION (CGNR)

We know that the conjugate gradient method (CG) combining the proper preprocessing techniques is an effective way to solve large symmetric positive definite (s.p.d) linear equation set, such as incomplete LU decomposition. But, According to the foregoing description, for asymmetrical linear equation set:

$$Ax = b \qquad (1.1)$$

It's efficient solution is still an important subject to numerical calculation workers. A direct idea is that the original equations (1.1) can be pre multiplied by transpostion $A^T$ in to as .p.d equation with the same solution, and then solve the equivalent equation set by C Galgorithm:

$$A^T Ax = A^T b \qquad (1.2)$$

or through variable substitution, we can solve the equivalent equation set:

$$AA^T y = b, x = A^T y \qquad (1.3)$$

We call equation (1.2) as Normal Equations. Two typical algorithms of iteration methods which based on the normal equations are CGNR algorithm solving (1.2) and CGNE algorithm solving (1.3). CGNR method is discussed emphatically in this paper.

### 1.1 Algorithm Introduction CGNR Algorithm

1. Compute $r_0 = b - Ax_0, z_0 = A^T r_0, p_0 = z_0$
2. Let $i = 0,1,\ldots,$ until problem converges
3. $w_i = Ap_i$
4. $\alpha_i = \|z_i\|^2 / \|w_i\|_2^2$
5. $x_{i+1} = x_i + \alpha_i p_i$

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6. $r_{i+1} = r_i - \alpha_i w_i$
7. $z_{i+1} = A^T r_{i+1}$
8. $\beta_i = \|z_{i+1}\|_2^2 / \|z_i\|_2^2$
9. $p_{i+1} = z_{i+1} + \beta_i p_i$

### 1.2. Algorithm analyze

The convergence of conjugate gradient algorithm largely depends on the condition number of coefficient matrix. The smaller the condition number, the convergence of conjugate gradient algorithm is better. CGNR algorithm is to use CG algorithm to solve the equivalent equation set $A^T Ax = A^T b$, but the condition number of matrix is the square of the condition number of matrix, it can slow down the convergence speed of the CGNR iterative greatly, this is the so-called "square condition number" effect. However, although it makes the condition number into the the square of the condition number of original equation, but the method of solving linear equations method sometimes performed very well in the competition, such as Trefe then pointed out that the convergence rate of the CGNR method only is determined by the singular value of matrix $A$ [1], this is why, in some cases, especially when the matrix singular value's distribution is concentrated, the convergence of this method will perform better than other methods, the numerical example of this chapter also validates it.

## 2. THE GENERALIZED MINIMAL RESIDUAL ALGORITHM (GMRES)

In Krylov subspace methods, if let $L_m = \kappa_m$ and use the Arnoldi process make the matrix $A$ into upper Hessenbergmatrix, then we can get the Arnoldi method, the corresponding algorithm is FOM algorithm; If let $L_m = A\kappa_m$ combining Arnoldi process and the least square method, we can get the GMRES method. Let $V_m = [v_1, v_2, ..., v_m]$ be the matrix of standard orthogonal vector generated in the process of Arnoldi, $\overline{H}_m$ is the upper Hessenberg matrix with $(m+1)\times m$ order which is gotten in this process, let $AV_m = V_{m+1}\overline{H}_m$ Then, the approximate solution of the GMRES method are as follows:

$$x_m = x_0 + V_m y_m \text{ of which, } \quad y_m = \arg\min \left\| \beta e_1 - \overline{H}_m \right\|_2, \quad \beta = \|r_0\|_2$$

and solve the least square problem with Givens rotation method. As you can see, this method in Krylov subspace $\kappa_m$ has the minimum residual, but it is recurrence based on the Longformula, the vector stored and the computation increase rapidly with the iterative steps, when m is large, for example, need to save all the calculation $\{v_i\}_{i=1}^m$, for a large matrix, this will cause too much storage space requirements. In order to overcome this difficulty, Saad proposed GMRES method, namely the GMRES (m) algorithm [2].

## 3. BIORTHOGONAL LANCZOS ALGORITHM

When taking $L_m = A^T \kappa_m$, we can get a series of method based on biorthogonal Lanczos process, such as BiCG, CGS, BiCGSTAB and QMR algorithm, etc. Here we will introduce these algorithms and give the relationships between the several methods.

### 3.1. BiCGalgorithm

BiCG algorithm is the process of projection in

$\kappa_m = span\{v_1, Av_1, A^2v_1, \ldots, A^{m-1}v_1\}$ and it's residual orthogonaled in

$\kappa_m = span\{w_1, A^T w_1, (A^T)^2 w_1, \ldots, (A^T)^{m-1} w_1\}$

We usually let $v_1 = r_0 / \|r_0\|_2$, $w_1$ is arbitrary, and make $(v_1, w_1) \neq 0$, $v_1 = w_1$. The derivation is similar with the conjugate gradient method, the $LU$ decomposition of $T_m = L_m U_m$, of which $T_m$ is a tridiagonal matrix which is biorthogonaled by the asymmetric matrix $A$, we define $P_m = V_m U_m^{-1}$, the expressions of the solutions of solving the equation (1.1) as follows:

$$x_m = x_0 + V_m T_m^{-1}(\beta e_1) = x_0 + V_m U_m^{-1} L_m^{-1}(\beta e_1) = x_0 + P_m L_m^{-1}(\beta e_1)$$

With the same method ,we define the matrix $P_m^* = W_m L_m^{-1}$, the column vector and the row vector of $P_m^*$ is $A$ - conjugate, this is because:

$$(P_m^*)^T AP_m = L_m^{-1} W_m^T A V_m U_m^{-1} = L_m^{-1} T_m U_m^{-1} = I$$

Thus, similar to the CG algorithm, BiCG algorithm can be get from the Lanczos process.

**BiCGalgorithm**[3]

1. Compute $r_0 = b - Ax_0$, get $r_0^*$, let $(r_0, r_0^*) \neq 0$
2. Let $p_0 = r_0, p_0^* = r_0^*$
3. For $j = 0, 1, \cdots$ until problem converges
4. $\alpha_j = (r_j, r_j^*) / (Ap_j, p_j^*)$
5. $x_{j+1} = x_j + \alpha_j p_j$
6. $r_{j+1} = r_j - \alpha_j Ap_j$
7. $r_{j+1}^* = r_j^* - \alpha_j A^T p_j^*$
8. $\beta_j = (r_{j+1}, r_{j+1}^*) / (r_j, r_j^*)$
9. $p_{j+1} = r_{j+1} + \beta_j p_j$
10. $p_{j+1}^* = r_{j+1}^* + \beta_j p_{j+1}^*$

As you can see, be similar to the GMRES algorithm, BiCG algorithm also meet Petrov-Galerkinconditions, only the residual polynomial satisfy the following biorthogonal conditions:

$$r_m \perp span\{w_1, A^T w_1, (A^T)^2 w_1, \ldots, (A^T)^{m-1} w_1\}.$$

The difference is BiCG is based on the short form of recursive method, to some problem, it's convergence speed faster but it doesn't satisfy the optimal conditions. The problem of the curve characteristic of the residual norm is instability, turbulence in the iterative process, serious even not sure when the terminating. In order to improve the residual conditions, Freund proposed the QMR (Quasi Minimal Residual) method in 1991, its form is very similar to the GMRES method. Another disadvantage of BiCG method is using transposed matrix $A^T$ in the iterative process, which is inconvenient in some cases, Sonneveld observed by residual polynomial's square of the BiCG algorithm to construct a new iterative format, which can avoid to use $A^T$, thus we can get the square of the conjugate gradient method (CGS).

**3.2. CGSalgorithm[4]**

1. Compute $r_0 = b - Ax_0$, choose $r_0^*$, let $(r_0, r_0^*) \neq 0$
2. Let $p_0 = u_0 = r_0$
3. For $j = 0,1,\cdots$ until problem converges
4. $\alpha_j = (r_j, r_0^*) \big/ (Ap_j, r_0^*)$
5. $q_j = u_j - \alpha_j Ap_j$
6. $x_{j+1} = x_j + \alpha_j (u_j + q_j)$
7. $r_{j+1} = r_j - \alpha_j A(u_j + q_j)$
8. $\beta_j = (r_{j+1}, r_0^*) \big/ (r_j, r_0^*)$
9. $u_{j+1} = r_{j+1} + \beta_j q_j$
10. $p_{j+1} = u_{j+1} + \beta_j (q_{j+1} + \beta_j p_j)$

Compared with BiCG algorithm, the above CGS algorithm on the one hand, doesn't have to Compute another group of vector $r_j^*$ which is correspond with $r_j$, simplify the programming code; On the other hand, it can avoid the product of the vector and the transposed matrix $A^T$ and improve operation efficiency. So that, if BiCG algorithm has a better convergence and stability, the absolute convergence speed of CGS is almost twice the BiCG. At the same time, we noticed that the convergence of the CGNR algorithm is strictly monotone decreasing, however, BiCG and CGS algorithm are both likely to disruptions, and its residual curve performance of ups and downs, turbulence, there is a potential instability.

**3.3. BiCGSTAB algorithm**

In order to overcome the potential instability of BiCG and the CGS method, Vander Vorst proposed the stable biorthogonal conjugate gradient algorithm, namely BiCGSTAB algorithm. The residual $r_m$ of CGS satisfy the relation $r_m = (p_m(A))^2 r_0$, of which, $(p_m(A))^2 r_0$ is the residual amount in the BiCG. But the residual of CGS is almost approximate square of BiCG, which leads to the oscillation of the convergence, in order to avoid the big oscillation, the residual amount written in the form:

$$r_m = q_m(A) p_m(A) r_0$$

$(p_m(A))^2 r_0$ is the residual of BiCG, but we let $q_m(A)$ be

$$q_m(A) = (1-\omega_1 A)(1-\omega_2 A)\cdots(1-\omega_m A)$$

and makes the residual $r_m$ still has the fast convergence of the CGS, that is the coefficient $\omega_i$ $i = 1,\ldots,m$ meet the condition:

$$\min_{\omega_m} \|r_m\|_2 = \min_{\omega_m} \|(1-\omega_m) q_{m-1}(A) p_m(A) r_0\|_2$$

this leads to the following BiCGSTAB algorithm.

**BiCGSTAB algorithm [5]**

1. Compute $r_0 = b - Ax_0$, select $r_0^*$
2. Let $p_0 = r_0$
3. For $j = 0,1,\cdots$ unit problem converges
4. $\alpha_j = (r_j, r_0^*) \big/ (Ap_j, r_0^*)$

5. $s_j = r_j - \alpha_j A p_j$
6. $\omega_j = (As_j, s_j)/(As_j, As_j)$
7. $x_{j+1} = x_j + \alpha_j p_j + \omega_j s_j$
8. $r_{j+1} = s_j - \omega_j A s_j$
9. $\beta_j = \dfrac{(r_{j+1}, r_0^*)}{(r_j, r_0^*)} \times \dfrac{\alpha_j}{\omega_j}$
10 $p_{j+1} = r_{j+1} + \beta_j (p_j - \omega_j A p_j)$

BiCGSTAB algorithm effectively overcomes the residual's oscillation of CGS algorithm, at the same time, due to the character of the minimization, the convergence of the BiCG algorithm is more smooth than BiCG .

## 4. NUMERICAL EXAMPLES

To illustrate the merits and demerits of the above algorithm, we present numerical examples to verify it. we select the right vector $b$ which makes the exact solutions of the equation set is $x = (1,1,\ldots,1)^T$ .

**Example 1:** Solve the equation set, $Ax = b$ , of which, the coefficient matrix is the following block tridiagonal matrix:

$$A = \begin{pmatrix} B & -I & & & & \\ I & \ddots & \ddots & & O & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & O & & \ddots & \ddots & -I \\ & & & & I & B \end{pmatrix} \quad B = \begin{pmatrix} 4 & -2 & & & & \\ -1.01 & 4 & -2 & & 0 & \\ & -1.01 & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & \ddots & 2 \\ & & & & -1.01 & 4 \end{pmatrix}$$

$I$ is a unit matrix with ten order, $O$ is a zero matrix with ten order, $B$ is a tridiagonal matrix with ten order. Firstly, we will compare these three short recursion algorithm. The results of the iterations and residual curve as shown against (4.1).

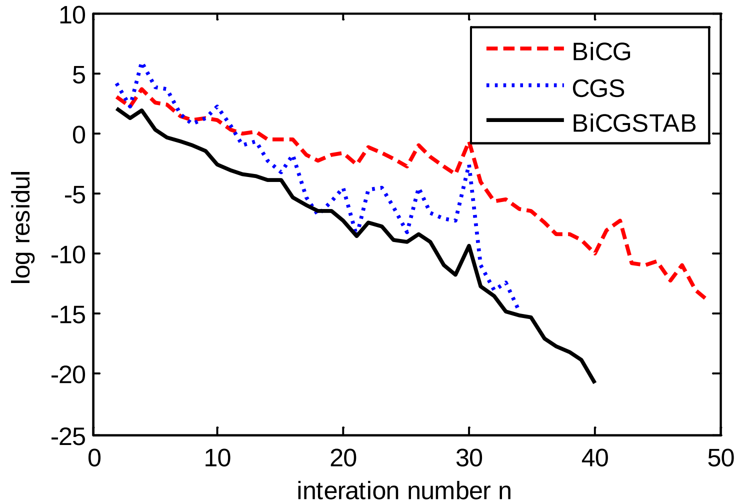


**Figure-4.1:** Iterations and residual curve of the three kind of Lanczos class

Since QMR algorithm also belongs to the Lanczos algorithm, but it has the optimum properties which is similar to the GMRES algorithm, so the algorithm obtained is different with the above three short recursive, hence, we compare QMR algorithm and BiCGSTAB algorithm, get the residual curve is as follow:

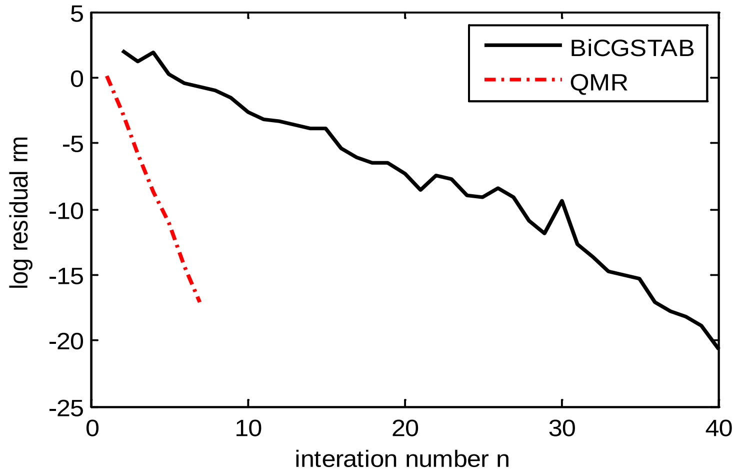


**Figure-4.2:** The iterations and residual curve of BiCGSTAB and QMR

Secondly, to illustrate the computational efficiency of Lanczos algorithm andnon-Lanczos class, and BiCGSTAB has better convergence in Lanczos algorithm, BiCGSTAB, GMRES and CGNR are compared, in order to find the pros and cons of these two kinds of algorithms. For the coefficient matrix in case 1, BiCGSTAB, the residual graph of GMRES and CGNR algorithm is show below (4.3):

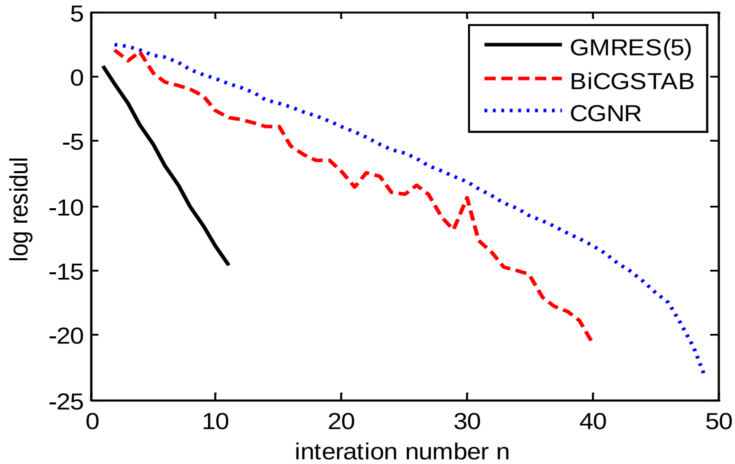


**Figure-4.3:** The iterations and residual curve of GMRES, BiCGSTAB and CGNR

Comparison of the following two examples are similar with the example 1.

**Example 2:** In this case, the matrix from matrix market (http://math.nist. gov/Matrix Market/), the condition number is 1.7637 e+004, the number of non-zero element is 13151, order number is 2395, its structure as shown in the following figure (4.4):

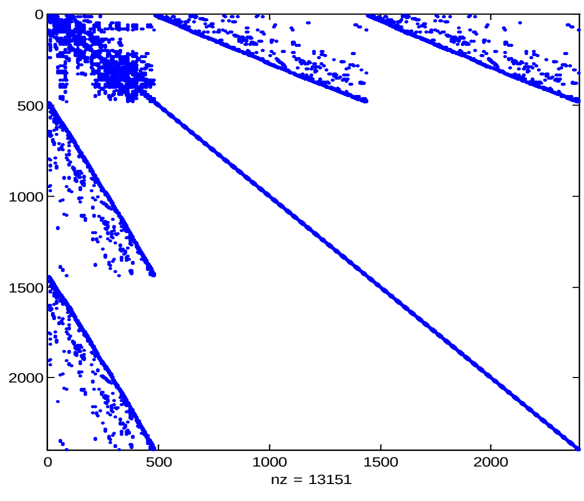


**Figure-4.4:** the structure of the matrix in example 2

The residual graph of Lanczos class algorithms is compared in the following figure (4.5):

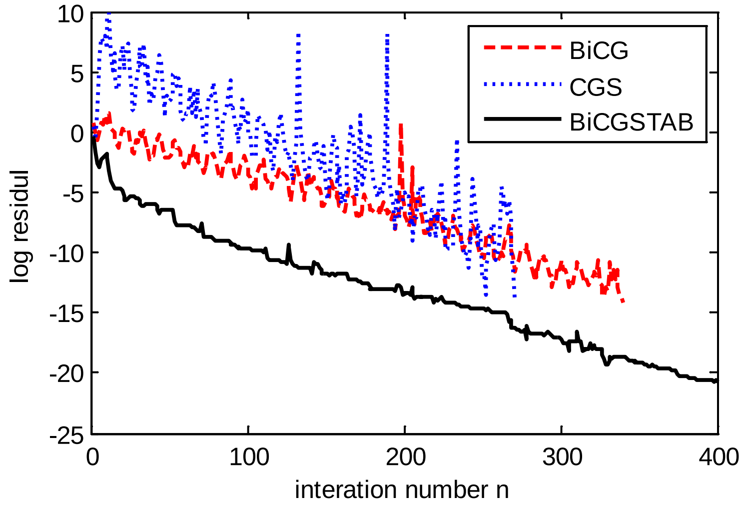


**Figure-4.5:** The iterations and residual curve of Lanczos class algorithms

The residual graph of QMR algorithm and BiCGSTAB are compared in the following figure (4.6):

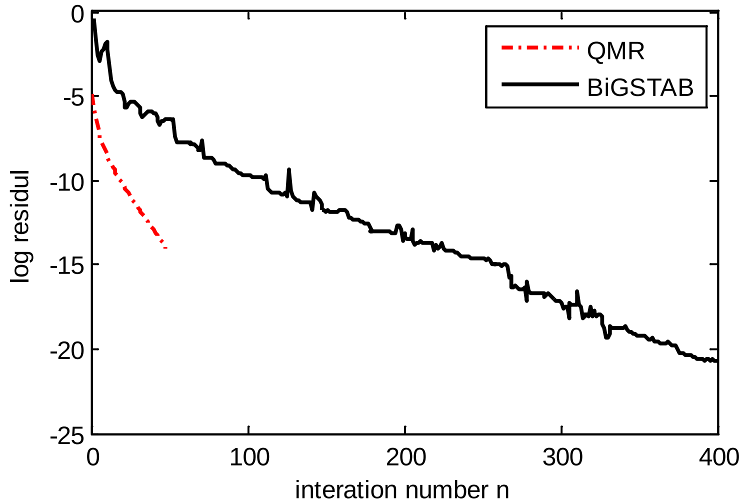


**Figure-4.6:** The iterations and residual curve of BiCGSTAB and QMR

The residual curve of BiCGSTAB, GMRES and CGNR algorithms are compared in the following figure (4.7):

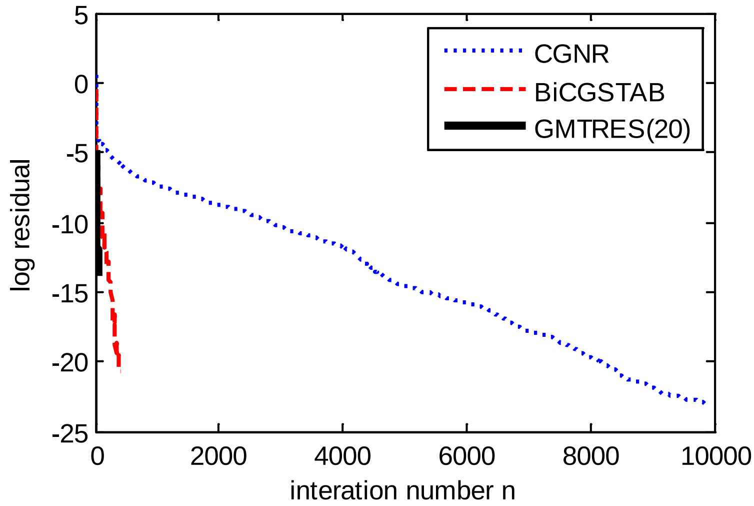


**Figure-4.7:** The iterations and residual curve of GMRES, BiCGSTAB and CGNR

**Example 3:** in this case, the matrix also from matrix market, the condition number is213.6310, the number of non-zero element is 19848, order number is 4960, its structure as shown in the figure (4.8) below:

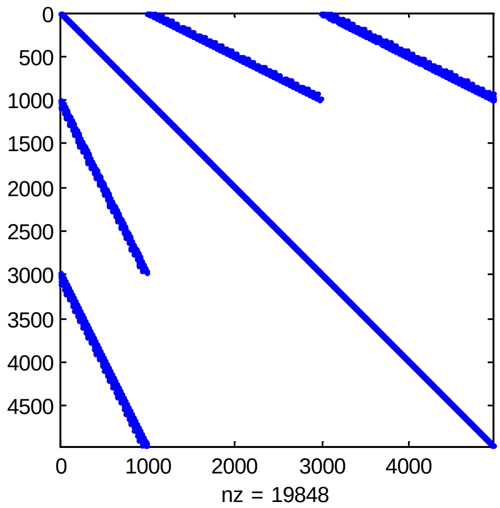


**Figure-4.8:** the structure of the matrix in example 3

The residual curve of Lanczos class algorithms are compared in the following figure (4.9):

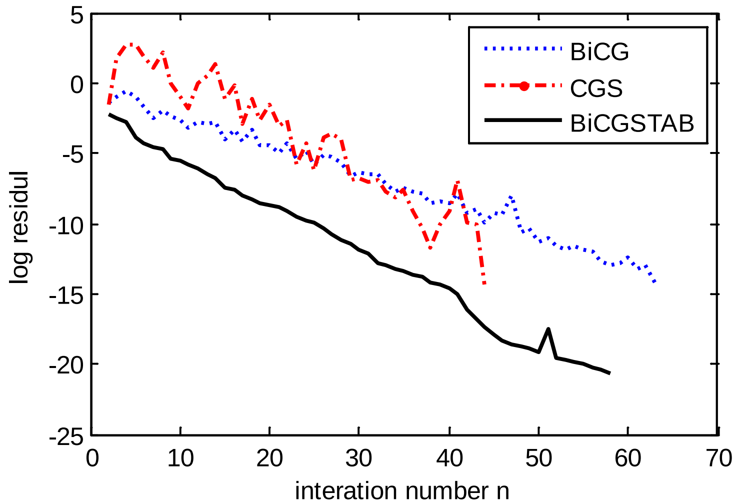


**Figure-4.9:** The iterations and residual curve of Lanczos class algorithms

The residual curve of QMR and BiCGSTAB algorithms are compared in the following figure (4.10):

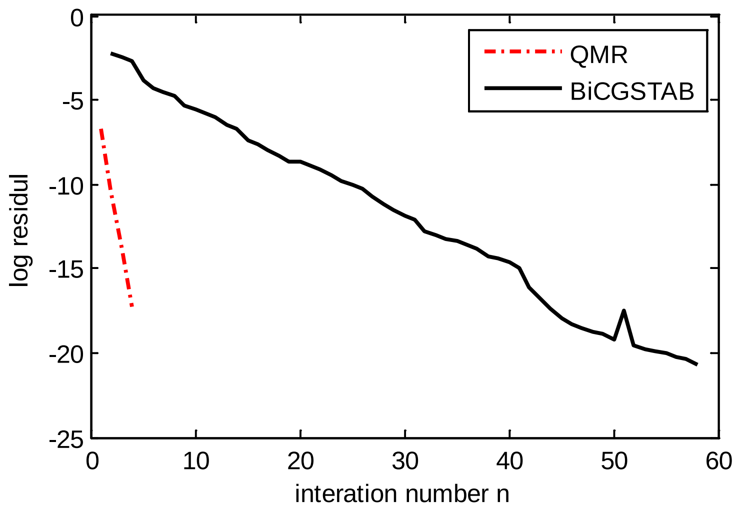


**Figure-4.10:** The iterations and residual curve of QMR and BiCGSTAB

The residual curve of BiCGSTAB, GMRES and CGNR algorithms are compared in the following figure (4.11):

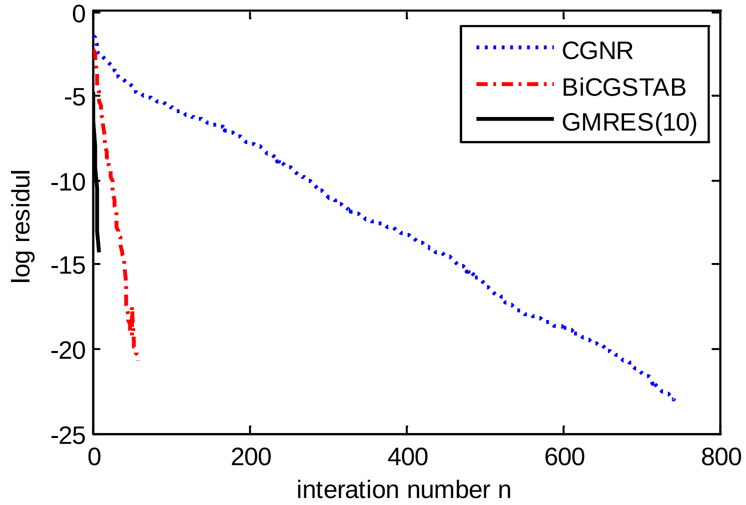


**Figure-4.11:** The iterations and residual curve **of** BiCGSTAB GMRES and CGNR

In the above three examples, the CPU time executing each algorithm and the number of iterations is given in the following table (4.1):

**Table-4.1: CPU time and the number of iterations**

| example | algorithm | CPU time(s) | iteration number |
|---|---|---|---|
| example1 | CGNR | 0.003109 | 49 |
| | GMRES(5) | 0.020313 | 11 |
| | BiCG | 0.017026 | 49 |
| | CGS | 0.010129 | 34 |
| | BiCGSTAB | 0.017262 | 40 |
| | QMR | 0.062379 | 7 |
| example2 | CGNR | 6.773385 | 9869 |
| | GMRES(20) | 1.335291 | 47 |
| | BiCG | 0.549048 | 340 |
| | CGS | 0.319929 | 271 |
| | BiCGSTAB | 0.697247 | 400 |
| | QMR | 2.116118 | 48 |
| example3 | CGNR | 0.532815 | 63 |
| | GMRES(10) | 0.147617 | 8 |
| | BiCG | 0.145476 | 63 |
| | CGS | 0.071777 | 44 |
| | BiCGSTAB | 0.147617 | 58 |
| | QMR | 0.403715 | 4 |

## 5. RESULTS ANALYSIS

1. Figure 4.1, figure 4.5 and figure 4.9 are iterations and residual curves which are Lanczos classalgorithms namely BiCG, CGS and BiCGSTAB, from the comparison we can see that the CGS needs the smallest number of iterations, but its residual turbulence is the most serious; BiCGSTAB needs more iterationnumber than CGS, but its residual has the beststability.
2. Figure4.2, figure 4.6 and figure 4.10 are the residual diagram of QMR and BiCGSTAB algorithm in Lanczos algorithm, in this example we given, iterations of QMR algorithm is much less than the iterations of BiCGSTAB algorithm, but it need more CPU time.
3. Figure 4.3, figure 4.7 and figure 4.11 give the iterations and residual curves of BiCGSTAB and GMRES (m) and CGNR, seen from the figure, in solving theequations which have banded or claw structure matrix, GMRES (m) needs the least number of iterations required for convergence, hence, it has the best convergence; CGNR algorithm needs the most number of iteration required for convergence, but in case 1, although it needs the most number of iteration, its calculation speed is the fastest. Can also be concluded from the figure, compared with GMRES (m) and CGNR algorithm, BiCGSTAB has the oscillation residual error.

 

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