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A modified Block IDR(s) method for computing high accuracy solutions

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Abstract

In this paper, the difference between the residual and the true residual caused by the computation errors that arise in matrix multiplications for solutions generated by the Block IDR(s) method is analyzed. Moreover, in order to reduce the difference between the residual and the true residual, a modified Block IDR(s) method is proposed. Numerical experiments demonstrate that the difference under the proposed method is smaller than that of the conventional Block IDR(s) method.

Keywords Block Krylov subspace methods, Block IDR(s) method, linear systems with multiple right-hand sides, high accuracy solutions

Research Activity Group Algorithms for Matrix / Eigenvalue Problems and their Applications

1. Introduction

Linear systems with multiple right-hand sides of the form

$$AX = B,$$

where the coefficient matrix $A \in \mathbb{C}^{n\times n}$, $B \in \mathbb{C}^{n\times L}$, and $X \in \mathbb{C}^{n\times L}$ appear together in many problems, including lattice quantum chromodynamics calculation of physical quantities [1] and an eigensolver problem using contour integration [2]. To solve these linear systems, Block Krylov subspace methods such as Block BiCG [3] and Block BiCGSTAB [4] have been proposed. These methods can solve linear systems with multiple right-hand sides more efficiently than Krylov subspace methods for single right-hand side.

We consider the Block IDR(s) method [5] as a Block Krylov subspace method. A difference between the residual generated by the Block IDR(s) method and the true residual $B - AX$ obtained by the approximate solution occurs. When such a difference occurs, even if the residual generated by the Block IDR(s) method satisfies the convergence criterion, high accuracy approximate solutions cannot be obtained. In this paper, we analyze the difference between the residual and the true residual, and, based on the results of the analysis, a solution for reducing the difference is proposed.

The composition of this paper is as follows. In Section 2, the algorithm of the Block IDR(s) method is illustrated. In Section 3, the difference between the residual and the true residual caused by the computation errors that arise in matrix multiplications for solutions generated by the Block IDR(s) method is analyzed. In Section 4, to reduce this difference, a modified Block IDR(s) method is proposed. We show that the errors which arise in matrix multiplications for the proposed Block IDR(s) method do not influence between the residual and the true residual. In Section 5, some numerical experiments comparing the conventional Block IDR(s) method and the proposed Block IDR(s) method are described. In Section 6, this paper is concluded.

2. The Block IDR(s) method

In this section, we show the algorithm of the Block IDR(s) method [5]. Given $A \in \mathbb{C}^{n\times n}$ and $R_0 \in \mathbb{C}^{n\times L}$, and assuming that the residuals $R_{i-s}, \dots, R_i$ belong to subspace $\mathcal{G}_j$, the residual R_{i+1} which belongs to subspace $\mathcal{G}_j$ is constructed by setting

$$R_{i+1} = (I - \omega_{j+1}A)V_i,$$

where $V_i \in \mathbb{C}^{n\times L}$. Then let

$$\Delta R_k = R_{k+1} - R_k,$$
$$\Delta X_k = X_{k+1} - X_k,$$
$$G_k = (\Delta R_{k-s}, \Delta R_{k-s+1}, \dots, \Delta R_{k-1}),$$
$$U_k = (\Delta X_{k-s}, \Delta X_{k-s+1}, \dots, \Delta X_{k-1}).$$

Then V_i can be written as

$$V_i = R_i - G_iC_i. \quad (1)$$

Moreover, the condition on V_i can be written as

$$P^{\mathrm{H}}V_i = O, \quad (2)$$

where $P \in \mathbb{C}^{n\times sL}$. Then C_i can be obtained from (1) and (2).

The approximate solution X_{i+1} can be written as

$$X_{i+1} = X_i + \omega_{j+1}V_i - U_iC_i,$$

$X_0 \in \mathbb{C}^{n\times L}$ is an initial guess
$R_0 = B - AX_0, P \in \mathbb{C}^{n\times sL}$
for $i = 0$ to $s-1$ **do**
  $V_i = AR_i, \omega = \mathrm{Tr}(V_i^{\mathrm{H}} R_i)/\mathrm{Tr}(V_i^{\mathrm{H}} V_i)$
  $\Delta X_i = \omega R_i, \Delta R_i = \omega V_i$
  $X_{i+1} = X_i + \Delta X_i, R_{i+1} = R_i + \Delta R_i$
end for
$G_{i+1} = (\Delta R_{i-s+1}, \Delta R_{i-s+2}, \ldots, \Delta R_i)$
$U_{i+1} = (\Delta X_{i-s+1}, \Delta X_{i-s+2}, \ldots, \Delta X_i)$
$M = P^{\mathrm{H}} G_{i+1}, F = P^{\mathrm{H}} R_{i+1}$
$i = s$
while $\|R_i\|_{\mathrm{F}} < \epsilon \|B\|_{\mathrm{F}}$ **do**
  for $k = 0$ to s **do**
    solve C_i from $MC_i = F$
    $V_i = R_i - G_i C_i$
    if $k = 0$ **then**
      $T_i = AV_i$
      $\omega = \mathrm{Tr}(T_i^{\mathrm{H}} V_i)/\mathrm{Tr}(T_i^{\mathrm{H}} T_i)$
      $\Delta R_i = -G_i C_i - \omega A V_i$
      $\Delta X_i = -U_i C_i + \omega V_i$
    else
      $\Delta X_i = -U_i C_i + \omega V_i$
      $\Delta R_i = -A \Delta X_i$
    end if
    $X_{i+1} = X_i + \Delta X_i, R_{i+1} = R_i + \Delta R_i$
    $M = P^{\mathrm{H}} G_i, F = P^{\mathrm{H}} R_{i+1}$
    $G_{i+1} = (\Delta R_{i-s+1}, \Delta R_{i-s+2}, \ldots, \Delta R_i)$
    $U_{i+1} = (\Delta X_{i-s+1}, \Delta X_{i-s+2}, \ldots, \Delta X_i)$
    $i = i + 1$
  end for
end while

Fig. 1. Algorithm of the Block IDR(s) method.

where the scalar parameter ω_{j+1} is

$$\omega_{j+1} = \mathrm{Tr}\big[(AV_i)^{\mathrm{H}} V_i\big]/\mathrm{Tr}\big[(AV_i)^{\mathrm{H}} AV_i\big].$$

The algorithm of the Block IDR(s) method is shown in Fig. 1. Here, $\|\cdot\|_{\mathrm{F}}$ denotes the Frobenius norm of a matrix and $\mathrm{Tr}[\,\cdot\,]$ denotes the trace of a matrix.

3. Analysis of the difference between the residual and the true residual

The relation between the residual R_k and the approximate solution X_k can be written as

$$R_k = B - AX_k. \tag{3}$$

However, a difference between the residual generated by the Block IDR(s) method and the true residual obtained by the approximate solution occurs. In this section, we analyze this difference based on an analysis method of the Block BiCGGR method [6].

We define $\tilde{X}_0$ and $\tilde{R}_0$ as

$$\tilde{X}_0 = X_0 + \Delta X_0 + \Delta X_1 + \cdots + \Delta X_{s-1},$$

$$\tilde{R}_0 = R_0 + \Delta R_0 + \Delta R_1 + \cdots + \Delta R_{s-1}.$$

The residual R_{i+1} and the approximate solution X_{i+1} generated by the Block IDR(s) method are written as

$$\begin{aligned} X_{i+1} &= X_i + \omega_{j+1} V_i - U_i C_i \\ &= \tilde{X}_0 + \sum_{k=s}^{i} \omega_m V_k - \sum_{k=s}^{i} U_k C_k, \end{aligned} \tag{4}$$

and

$$\begin{aligned} R_{i+1} &= R_i - \omega_{j+1} A V_i - G_i C_i \\ &= \tilde{R}_0 - \sum_{k=s}^{i} \omega_m A V_k - \sum_{k=s}^{i} G_k C_k, \end{aligned} \tag{5}$$

where $m = \lfloor (k+1)/(s+1) \rfloor$. From (4) and (5), the true residual $B - AX_k$ for the Block IDR(s) method is given by

$$\begin{aligned} B - AX_{i+1} &= \tilde{R}_0 - \sum_{k=s}^{i} A(\omega_m V_k) - \sum_{k=s}^{i} A(U_k C_k) \\ &= R_{i+1} + \sum_{k=s}^{i} [\omega_m (AV_k) - A(\omega_m V_k)] \\ &\quad + \sum_{k=s}^{i} [G_k C_k - A(U_k C_k)]. \end{aligned} \tag{6}$$

From (3) and (6), the difference between the residual and the true residual is given by $\sum_{k=s}^{i} [\omega_m (AV_k) - A(\omega_m V_k)] + \sum_{k=s}^{i} [G_k C_k - A(U_k C_k)]$, in (6).

4. Derivation of a modified Block IDR(s) method

In this section, from the analysis of the difference between the residual generated by the Block IDR(s) method and the true residual obtained from the approximate solution, a modified Block IDR(s) method is proposed to reduce this difference.

To reduce the difference, the proposed method negates the influence of the computation error generated by the multiplication with C_i in the Block IDR(s) method.

Then the proposed method satisfies

$$G_k C_k - A(U_k C_k) = O.$$

We define the following equation

$$Q_k = -U_k - \omega_{j+1} G_k. \tag{7}$$

From (7), the residual R_{i+1} and the approximate solution X_{i+1} generated by the Block IDR(s) is written as

$$\begin{aligned} X_{i+1} &= X_i + \omega_{j+1} R_i + Q_i C_i \\ &= \tilde{X}_0 + \sum_{k=s}^{i} \omega_m R_k + \sum_{k=s}^{i} Q_k C_k. \end{aligned} \tag{8}$$

$$\begin{aligned} R_{i+1} &= R_i - \omega_{j+1} A R_i - A(Q_i C_i) \\ &= \tilde{R}_0 - \sum_{k=s}^{i} \omega_m (AR_k) - \sum_{k=s}^{i} A(Q_k C_k). \end{aligned} \tag{9}$$

From (8) and (9), the true residual $B - AX_k$ is written

$X_0 \in \mathbb{C}^{n\times L}$ is an initial guess
$R_0 = B - AX_0, P \in \mathbb{C}^{n\times sL}$
for $i = 0$ to $s-1$ **do**
  $V_i = AR_i, \omega = \mathrm{Tr}(V_i^{\mathrm{H}}R_i)/\mathrm{Tr}(V_i^{\mathrm{H}}V_i)$
  $\Delta X_i = \omega R_i, \Delta R_i = \omega V_i$
  $X_{i+1} = X_i + \Delta X_i, R_{i+1} = R_i + \Delta R_i$
end for
$G_{i+1} = (\Delta R_{i-s+1}, \Delta R_{i-s+2}, \dots, \Delta R_i)$
$U_{i+1} = (\Delta X_{i-s+1}, \Delta X_{i-s+2}, \dots, \Delta X_i)$
$M = P^{\mathrm{H}}G_{i+1}, F = P^{\mathrm{H}}R_{i+1}$
$i = s$
while $\|R_i\|_{\mathrm{F}} < \epsilon\|B\|_{\mathrm{F}}$ **do**
  for $k = 0$ to s **do**
    solve C_i from $MC_i = F$
    if $k = 0$ **then**
      $Q_i = -U_i - \omega G_i$
      $W = AR_i$
      $\omega = \mathrm{Tr}(W^{\mathrm{H}}R_i)/\mathrm{Tr}(W^{\mathrm{H}}W)$
      $\Delta R_i = -\omega W - A(Q_iC_i)$
      $\Delta X_i = \omega R_i + Q_iC_i$
    else
      $V_i = R_i - G_iC_i$
      $\Delta X_i = -U_iC_i + \omega V_i$
      $\Delta R_i = -A\Delta X_i$
    end if
    $X_{i+1} = X_i + \Delta X_i, R_{i+1} = R_i + \Delta R_i$
    $M = P^{\mathrm{H}}G_i, F = P^{\mathrm{H}}R_{i+1}$
    $G_{i+1} = (\Delta R_{i-s+1}, \Delta R_{i-s+2}, \dots, \Delta R_i)$
    $U_{i+1} = (\Delta X_{i-s+1}, \Delta X_{i-s+2}, \dots, \Delta X_i)$
    $i = i + 1$
  end for
end while

Fig. 2. Algorithm of the proposed method.

as

$$\begin{aligned} B - AX_{i+1} &= \tilde{R}_0 - \sum_{k=s}^{i} A(\omega_m R_k) - \sum_{k=s}^{i} A(Q_kC_k) \\ &= R_{i+1} + \sum_{k=s}^{i}[\omega_m(AR_k) - A(\omega_m R_k)] \\ &\quad + \sum_{k=s}^{i}[A(Q_kC_k) - A(Q_kC_k)] \\ &= R_{i+1} + \sum_{k=s}^{i}[\omega_m(AR_k) - A(\omega_m R_k)]. \end{aligned}$$

By comparing (6) with the above equation, we see that the influence of the computation error generated by the multiplication with C_i in the Block IDR(s) method is negated.

The algorithm of the proposed Block IDR(s) method is shown in Fig. 2.

5. Numerical experiments

In this section, we verify that the proposed Block IDR(s) method can reduce the difference between the residual and the true residual relative to the conventional Block IDR(s) method through comparative experiments.

Table 1. Size and number of nonzero elements of test matrices.

Matrix name	Size	Number of nonzero elements
poisson2D	367	2,417
CONF5.0-00L8X8-1000	49,152	1,916,928

Table 2. Results of the Block IDR(s) method for poisson2D.

s	L	Iter.	Res.	True Res.
1	1	140	8.73×10^{-15}	9.84×10^{-15}
	2	105	1.39×10^{-14}	1.44×10^{-14}
	4	79	1.86×10^{-15}	4.87×10^{-15}
8	1	100	2.92×10^{-15}	4.52×10^{-14}
	2	79	7.30×10^{-15}	3.15×10^{-13}
	4	57	9.89×10^{-15}	6.34×10^{-14}
16	1	99	6.30×10^{-15}	2.34×10^{-13}
	2	77	4.89×10^{-15}	2.58×10^{-13}
	4	57	2.88×10^{-15}	4.59×10^{-13}
32	1	98	3.77×10^{-15}	1.47×10^{-10}
	2	75	9.10×10^{-15}	6.72×10^{-11}
	4	57	3.30×10^{-15}	1.86×10^{-11}

Table 3. Results of the Block IDR(s) method for CONF5.0-00L8X8-1000.

s	L	Iter.	Res.	True Res.
1	1	1140	7.43×10^{-15}	1.12×10^{-14}
	2	895	1.85×10^{-14}	3.95×10^{-14}
	4	847	8.57×10^{-15}	2.47×10^{-11}
8	1	904	7.67×10^{-15}	1.09×10^{-14}
	2	710	1.89×10^{-14}	5.04×10^{-14}
	4	550	9.70×10^{-15}	1.42×10^{-12}
16	1	867	5.75×10^{-15}	2.69×10^{-14}
	2	697	2.71×10^{-15}	4.08×10^{-13}
	4	539	3.31×10^{-15}	2.58×10^{-13}
32	1	851	9.16×10^{-15}	1.05×10^{-5}
	2	692	2.59×10^{-15}	1.14×10^{-3}
	4	527	6.08×10^{-15}	1.40×10^{-4}

The test matrices used in the numerical experiments are poisson2D and CONF5.4-00L8X8-1000 from the MATRIX MARKET collection [7]. The size and the number of nonzero elements of these matrices are shown in Table 1. The matrix CONF5.0-00L8X8-1000 is constructed as $I_n - \kappa D$, where $D \in \mathbb{C}^{n\times n}$ is a non-Hermitian matrix and κ is a real-valued parameter. The parameter κ was set to 0.1782.

The initial solution X_0 was set to the zero matrix. The right-hand side B is given by $B = [\boldsymbol{e}_1, \boldsymbol{e}_2, \dots, \boldsymbol{e}_L]$, where $\boldsymbol{e}_j$ is the jth unit vector. The convergence criterion of the residual was set with 1.0×10^{-14}.

All experiments were performed on an Intel Core i7 2.8 GHz CPU with 8 GB of memory using MATLAB 7.12.0.635 (R2011a).

The results of the conventional Block IDR(s) method are shown in Tables 2 and 3. In this Table, Iter., Res., and True Res. denote the number of iterations, the relative residual norm $\|R_k\|_{\mathrm{F}}/\|B_k\|_{\mathrm{F}}$, and the true relative residual norm $\|B - AX_k\|_{\mathrm{F}}/\|B_k\|_{\mathrm{F}}$, respectively. As shown in Tables 2 and 3, the relative residual norms of the conventional Block IDR(s) method satisfy the convergence criterion. However, because of the difference between the true residual and the residual generated by the Block IDR(s) method, the true residual norms do

Table 4. Results of the proposed Block IDR(s) method for poisson2D.

s	L	Iter.	Res.	True Res.
1	1	139	8.47×10^{-15}	8.95×10^{-15}
	2	103	3.99×10^{-15}	4.61×10^{-15}
	4	77	6.93×10^{-15}	7.31×10^{-15}
8	1	100	2.65×10^{-15}	1.53×10^{-15}
	2	79	6.34×10^{-16}	1.85×10^{-15}
	4	60	2.43×10^{-16}	1.89×10^{-15}
16	1	100	6.72×10^{-16}	1.27×10^{-15}
	2	77	5.02×10^{-15}	5.22×10^{-15}
	4	59	4.48×10^{-15}	4.67×10^{-15}
32	1	97	9.35×10^{-15}	9.50×10^{-15}
	2	77	8.14×10^{-16}	1.48×10^{-15}
	4	61	5.10×10^{-15}	5.25×10^{-15}

Table 5. Results of the proposed Block IDR(s) method for CONF5.0-00L8X8-1000.

s	L	Iter.	Res.	True Res.
1	1	1127	9.24×10^{-15}	1.74×10^{-14}
	2	991	6.86×10^{-15}	7.15×10^{-15}
	4	813	3.10×10^{-14}	3.19×10^{-14}
8	1	901	5.86×10^{-15}	6.04×10^{-15}
	2	710	1.08×10^{-14}	1.09×10^{-14}
	4	557	1.58×10^{-14}	1.62×10^{-14}
16	1	868	7.61×10^{-15}	7.69×10^{-15}
	2	703	8.11×10^{-15}	8.18×10^{-15}
	4	530	9.14×10^{-15}	9.21×10^{-15}
32	1	689	8.20×10^{-15}	8.36×10^{-15}
	2	524	8.57×10^{-15}	8.67×10^{-15}
	4	404	7.71×10^{-15}	8.57×10^{-15}

not satisfy the convergence criterion.

The results of the proposed Block IDR(s) method are shown in Tables 4 and 5. As shown, the relative residual norms of the proposed Block IDR(s) method satisfy the convergence criterion. Moreover, the proposed Block IDR(s) method reduced the differences between the residual and the true residual relative to the conventional Block IDR(s) method.

6. Conclusion

A difference between the residual generated by the Block IDR(s) method and the true residual $B-AX$ may occur. If so, even if the residual generated by the Block IDR(s) method satisfies the convergence criterion, high accuracy approximate solutions cannot be obtained.

Therefore, in this paper, we analyzed the difference between the residual generated by the Block IDR(s) method and the true residual. From the analysis results, we were able to propose a modified Block IDR(s) method. The proposed method can negate the influence of the computation error generated by the multiplication with C_i in the Block IDR(s) method. Through numerical experiments, we verified that the proposed method can reduce the difference relative to the conventional method.

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