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for Singular Systems**

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Summary Consider applying the restarted Generalized Conjugate Residual (GCR(k)) method to systems of linear equations $A\mathbf{x} = \mathbf{b}$ or least squares problems $\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$, where $A \in \mathbf{R}^{n \times n}$ may be singular and/or nonsymmetric and $\mathbf{x}, \mathbf{b} \in \mathbf{R}^n$. Let $\mathcal{R}(A)$ and $\mathcal{N}(A)$ be the range and null space of A , respectively.

First, we prove that the necessary and sufficient condition for the method to converge to a least squares solution without breakdown for arbitrary \mathbf{b} and initial approximate solution \mathbf{x}_0 , is that A is definite in $\mathcal{R}(A)$, and $\mathcal{R}(A) \perp \mathcal{N}(A)$.

Next, we show that the necessary and sufficient condition for the method to converge to a solution without breakdown for arbitrary $\mathbf{b} \in \mathcal{R}(A)$ and arbitrary \mathbf{x}_0 , is that A is definite in $\mathcal{R}(A)$.

The main idea of the proofs is to decompose the algorithm into the $\mathcal{R}(A)$ and $\mathcal{R}(A)^\perp$ components.

Finally, we will give examples arising in the finite difference discretization of two-point boundary value problems of an ordinary differential equation, corresponding to the above two cases.

Key words: Krylov subspace method – GCR(k) method – singular systems – least squares problems – decomposition of algorithm

Mathematics Subject Classification (1991): 15A06, 15A09, 65F10, 65F20, 65F50

1 Introduction

Consider the system of linear equation

$$A\mathbf{x} = \mathbf{b}, \tag{1}$$

where $A \in \mathbf{R}^{n \times n}$, $\mathbf{x}, \mathbf{b} \in \mathbf{R}^n$, which arises, for instance, in the discrete approximation of partial differential equations.

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When A is nonsymmetric, there are Krylov subspace type iterative solvers for (1) based on biorthogonality, such as the Bi-CG method [9] and its modified versions such as the CGS [29], Bi-CGSTAB [33], QMR [13] and TFQMR [11] methods. There are also methods based on minimizing the residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$, such as the Generalized Conjugate Residual (GCR) method [8] and the Generalized Minimum Residual (GMRES) method [23]. When the coefficient matrix A is nonsingular, the behaviour of these methods is fairly well understood [8, 23].

On the other hand, in the discrete approximation of partial differential equations, the coefficient matrix of the resulting system of linear equations may be singular, depending on the boundary condition. For instance, when Neumann boundary conditions are imposed on the whole boundary, the system is rank one deficient. In the finite element electromagnetic analysis using edge elements, singular systems with null spaces of large dimensions may arise [2, 22, 17]. Such systems also arise when using redundant interpolation functions in the finite element method [30]. The computation of stationary probability vectors of stochastic matrices in the analysis of Markov chains also gives rise to singular systems [32, 12, 5]. The correction equations in the Jacobi-Davidson method [27] for eigenvalue problems are also singular systems.

For such singular systems, the system (1) does not always have solutions, so it is generally more appropriate to consider the least squares problem $\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$.

The analysis of linear stationary iterative methods on singular systems can be found, for instance, in [31, 6]. Work on semi-iterative methods for such systems was done in [7, 14, 26].

As for the analysis of Krylov subspace methods for singular systems, there are the works of [20, 32, 19, 10] for the conjugate gradient (CG) method, [12, 36] for methods based on biorthogonality such as the QMR and TFQMR methods. For residual minimization type methods, we refer to [1, 15, 16] for the conjugate residual (CR) method, [37] for the Orthomin(k) method, [24, 25] for the GCR method and [3, 28, 18, 4, 25] for the GMRES method.

When the system is singular, the CG method and methods based on biorthogonality may diverge [37], and one has to modify the system in order to guarantee convergence [19, 35]. On the other hand, for methods based on minimizing the residual, by principle, the residual is expected to decrease monotonically without such modifications [1, 37].

In [1], Abe et al. analysed the behaviour of the CR method for singular systems by decomposing the algorithm into the $\mathcal{R}(A)$ (range of A) component and its orthogonal complement, and derived necessary and sufficient conditions for the method to converge without breakdown for arbitrary right hand side and initial approximate solution.

In this paper, we will further clarify their arguments and apply their approach to the analysis of the restarted Generalized Conjugate Residual (GCR(k)) method. Further, we derive the necessary and sufficient condition for the method to converge without breakdown when \mathbf{b} is restricted in $\mathcal{R}(A)$ (the consistent case).

The rest of this paper is organized as follows: In Section 2, we will review convergence results of the GCR(k) for nonsingular systems. In Section 3, we introduce the orthonormal basis for decomposing vector variables into the $\mathcal{R}(A)$ component and $\mathcal{R}(A)^\perp$ component. Then, in Section 3.1, we analyse the properties of the submatrices A_{11} and A_{12} thus obtained, in relation to $\mathcal{R}(A)$ and the nullspace $\mathcal{N}(A)$. In Section 3.2, we decompose the

GCR(k) algorithm into the $\mathcal{R}(A)$ and $\mathcal{R}(A)^\perp$ components using this basis. In Section 3.3, we derive convergence theorems for the general case when \mathbf{b} may not necessarily belong to $\mathcal{R}(A)$. In Section 3.4, we derive a convergence theorem for the consistent case when $\mathbf{b} \in \mathcal{R}(A)$. Finally, in Section 3.5, we give examples coming from the discretization of two-point boundary value problems of an ordinary differential equation.

In this paper, exact arithmetic (i.e. no rounding errors) will be assumed, and the following notations will be used.

$\langle \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_i \rangle$: the subspace spanned by the vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_i$.

V^\perp : orthogonal complement of subspace V of \mathbf{R}^n .

For $X \in \mathbf{R}^{n \times n}$,

$\mathcal{R}(X)$: the range space of X , i.e. the subspace spanned by the column vectors of X ,

$\mathcal{N}(X)$: the null space of X , i.e. the subspace of vectors $\mathbf{v} \in \mathbf{R}^n$ such that $X\mathbf{v} = \mathbf{0}$,

$M(X) := \frac{X + X^T}{2}$: the symmetric part of X ,

$\lambda_{\min}(X)$: the eigenvalue of X with minimum absolute value,

$\lambda_{\max}(X)$: the eigenvalue of X with maximum absolute value.

2 Convergence of the GCR(k) method on nonsingular systems

First, we will consider the convergence of the Generalized Conjugate Residual (GCR(k)) method for nonsingular systems according to [8, 21, 1].

For the system of linear equations

$$A\mathbf{x} = \mathbf{b}, \quad (2)$$

where $A \in \mathbf{R}^{n \times n}$ is nonsingular but not necessarily symmetric, $\mathbf{b} \in \mathbf{R}^n$ is the right hand side, and $\mathbf{x} \in \mathbf{R}^n$ is the solution, the GCR(k) method [8] is given as follows.

The GCR(k) algorithm

Choose \mathbf{x}_0

* $\mathbf{r}_0 := \mathbf{b} - A\mathbf{x}_0$

$\mathbf{p}_0 := \mathbf{r}_0$

For $i = 0, 1, \dots, k$ until the residual (\mathbf{r}) converges, do

begin

$$\alpha_i := \frac{(\mathbf{r}_i, A\mathbf{p}_i)}{(A\mathbf{p}_i, A\mathbf{p}_i)}$$

$$\mathbf{x}_{i+1} := \mathbf{x}_i + \alpha_i \mathbf{p}_i$$

$$\mathbf{r}_{i+1} := \mathbf{r}_i - \alpha_i A\mathbf{p}_i$$

$$\beta_j^i := -\frac{(A\mathbf{r}_{i+1}, A\mathbf{p}_j)}{(A\mathbf{p}_j, A\mathbf{p}_j)} \quad (0 \leq j \leq i)$$

$$\mathbf{p}_{i+1} := \mathbf{r}_{i+1} + \sum_{j=0}^i \beta_j^i \mathbf{p}_j$$

end

$\mathbf{x}_0 := \mathbf{x}_{k+1}$
Go to *.

(3)

The method is a Krylov subspace method which minimizes the residual norm $\|\mathbf{r}_i\|_2$ over $\mathbf{x}_i = \mathbf{x}_0 + \langle \mathbf{r}_0, A\mathbf{r}_0, \dots, A^{i-1}\mathbf{r}_0 \rangle$, satisfying the orthogonality $(A\mathbf{p}_l, A\mathbf{p}_m) = 0$ ($l < m$), within the same cycle. The method restarts every $k+1$ iterations, instead of doing the full orthogonalization, in order to save storage and computation time. The full GCR method without restarts may be considered as GCR(∞).

When $(A\mathbf{p}_i, A\mathbf{p}_i) = 0$, the GCR(k) method is said to break down, and no further computation can be performed.

If the (full) GCR method does not break down, it gives the exact solution to (2) in at most n iterations [8].

First, note the following lemmas.

Lemma 1 *If the symmetric part $M(A)$ of a matrix A is definite, then the matrix A is nonsingular.*

Proof. Denote $M := M(A)$. Note that $(\mathbf{x}, M\mathbf{x}) = \frac{1}{2}(\mathbf{x}, A\mathbf{x}) + \frac{1}{2}(\mathbf{x}, A^T\mathbf{x}) = (\mathbf{x}, A\mathbf{x})$. If A is singular, there exists $\mathbf{x} \neq \mathbf{0}$ such that $A\mathbf{x} = \mathbf{0}$. Hence, for such $\mathbf{x} \neq \mathbf{0}$, $(\mathbf{x}, M\mathbf{x}) = (\mathbf{x}, A\mathbf{x}) = 0$, which contradicts with the definiteness of M . Thus, A is nonsingular. \square

Lemma 2 [8] *The following relations hold within the same cycle of the GCR(k) method if $M(A)$ is definite.*

$$(A\mathbf{p}_l, A\mathbf{p}_m) = 0 \quad (l \neq m, 0 \leq l, m \leq k+1) \quad (4)$$

$$(\mathbf{r}_l, A\mathbf{p}_m) = 0 \quad (0 \leq m < l \leq k+1) \quad (5)$$

$$(\mathbf{r}_l, A\mathbf{r}_l) = (\mathbf{r}_l, A\mathbf{p}_l) \quad (0 \leq l \leq k+1) \quad (6)$$

When A is nonsingular, the sufficient condition for the residual vector of the GCR(k) method to converge to $\mathbf{0}$ is given by the following theorem [8, 21].

Theorem 1 *If the symmetric part $M(A)$ of A is definite, either of the following holds for the GCR(k) method ($k \geq 0$).*

1. *There exists $l \geq 0$, such that $\mathbf{p}_i \neq \mathbf{0}$ ($0 \leq i < l$) and $\mathbf{r}_l = \mathbf{0}$. Further,*

$$\frac{\|\mathbf{r}_{i+1}\|_2^2}{\|\mathbf{r}_i\|_2^2} \leq 1 - \frac{\{\lambda_{\min}(M(A))\}^2}{\lambda_{\max}(A^T A)} \quad (7)$$

holds for $0 \leq i < l$.

2. *For all $i \geq 0$, $\mathbf{p}_i \neq \mathbf{0}$, $\mathbf{r}_i \neq \mathbf{0}$ and (7) hold.*

Proof. To show that the method does not break down, it is sufficient to show that, when $\mathbf{p}_i \neq \mathbf{0}$ ($0 \leq i \leq l-1$) and $\mathbf{p}_l = \mathbf{0}$, then $\mathbf{r}_l = \mathbf{0}$. From (6) of Lemma 2, $(\mathbf{r}_l, M\mathbf{r}_l) = (\mathbf{r}_l, A\mathbf{r}_l) = (\mathbf{r}_l, A\mathbf{p}_l)$. Hence, if $\mathbf{p}_l = \mathbf{0}$, we have $\mathbf{r}_l = \mathbf{0}$, since $M := M(A)$ is definite. The proof of the inequality (7) is given in [8]. \square

Next, note the following lemma.

Lemma 3 *If $M(A) := \frac{A + A^T}{2}$ is not definite, there exists $\mathbf{v} \neq \mathbf{0}$ such that $(\mathbf{v}, A\mathbf{v}) = 0$.*

Proof. Since $M := M(A)$ is symmetric, its eigenvalues are all real. If M has a zero eigenvalue, let the corresponding eigenvector be $\mathbf{x} \neq \mathbf{0}$. Then, there exists $\mathbf{x} \neq \mathbf{0}$ such that $(\mathbf{x}, A\mathbf{x}) = (\mathbf{x}, M(A)\mathbf{x}) = 0$.

If M has positive and negative eigenvalues, i.e.

$$\exists \lambda_1 > 0, \exists \mathbf{v}_1; \|\mathbf{v}_1\| = 1; M\mathbf{v}_1 = \lambda_1\mathbf{v}_1,$$

$$\exists \lambda_2 < 0, \exists \mathbf{v}_2; \|\mathbf{v}_2\| = 1; M\mathbf{v}_2 = \lambda_2\mathbf{v}_2,$$

$\lambda_1 \neq \lambda_2$ so that $(\mathbf{v}_1, \mathbf{v}_2) = 0$. Hence, letting $c \neq 0$ an arbitrary constant, and $\mathbf{x} := c(\sqrt{-\lambda_2}\mathbf{v}_1 + \sqrt{\lambda_1}\mathbf{v}_2)$ we have, $\mathbf{x} \neq \mathbf{0}$, and $(\mathbf{x}, A\mathbf{x}) = (\mathbf{x}, M\mathbf{x}) = 0$. \square

Theorem 1 and Lemma 3 give the following theorem which gives the necessary and sufficient condition for the GCR(k) method to converge without breakdown [1].

Theorem 2 *Let $A \in \mathbf{R}^{n \times n}$ be nonsingular. Then, the GCR(k) method converges to the solution of $A\mathbf{x} = \mathbf{b}$ without breakdown for arbitrary right hand side $\mathbf{b} \in \mathbf{R}^n$ and initial approximate solution $\mathbf{x}_0 \in \mathbf{R}^n$, if and only if the symmetric part $M(A)$ of A is definite.*

Proof. First, we will prove the necessity of the condition.

Assume that $M(A)$ is not definite. Then, by Lemma 3, there exists $\mathbf{v} \neq \mathbf{0}$ such that $(\mathbf{v}, A\mathbf{v}) = 0$. In the GCR(k) method, let $\mathbf{x}_0 = A^{-1}(\mathbf{b} - \mathbf{v})$. Then, $A\mathbf{x}_0 = \mathbf{b} - \mathbf{v}$, so that $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0 = \mathbf{v} \neq \mathbf{0}$. Hence, $\mathbf{p}_0 = \mathbf{r}_0 = \mathbf{v} \neq \mathbf{0}$, and $(\mathbf{r}_0, A\mathbf{p}_0) = (\mathbf{v}, A\mathbf{v}) = 0$. Note also that, since A is nonsingular and $\mathbf{p}_0 \neq \mathbf{0}$, $A\mathbf{p}_0 \neq \mathbf{0}$, and $(A\mathbf{p}_0, A\mathbf{p}_0) \neq 0$.

Then, for step $i = 0$, $\alpha_0 = 0$, so that $\mathbf{x}_1 = \mathbf{x}_0 \neq A^{-1}\mathbf{b}$, and $\mathbf{r}_1 = \mathbf{r}_0 = \mathbf{p}_0 \neq \mathbf{0}$. Thus, we have $\beta_0^0 = -\frac{A\mathbf{r}_1, A\mathbf{p}_0}{(A\mathbf{p}_0, A\mathbf{p}_0)} = -1$, so that $\mathbf{p}_1 = \mathbf{r}_1 + \beta_0^0\mathbf{p}_0 = \mathbf{r}_1 - \mathbf{p}_0 = \mathbf{p}_0 - \mathbf{p}_0 = \mathbf{0}$.

Hence, for $k \geq 1$, in step $i = 1$, the denominator of α_1 becomes 0 and the method breaks down, even though $\mathbf{r}_1 \neq \mathbf{0}$.

For $k = 0$, breakdown does not occur, but the solution remains $\mathbf{x}_i = \mathbf{x}_0$, and the residual $\mathbf{r}_i = \mathbf{r}_0 = \mathbf{v} \neq \mathbf{0}$, so that the solution never converges to the true solution, which proves the necessity of the condition.

The sufficiency of the condition is a consequence of Theorem 1. \square

The GCR method is a simple and useful implementation of the Krylov subspace method for nonsymmetric matrices. Although the GCR method is “mathematically equivalent” to the GMRES method [23], the GCR has breakdowns unique to the method, which may occur when the system is indefinite, as shown in the theorem above, whereas the GMRES never breaks down for nonsingular systems. This character is reflected in the singular case, as will be shown in the following section.

3 Convergence of the GCR(k) method on singular systems

In this section, we will consider the convergence of the GCR(k) method when it is applied to the least squares problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2 \quad (8)$$

where $A \in \mathbf{R}^{n \times n}$ may be singular and $\mathbf{b} \in \mathbf{R}^n$, as a generalization of the system of linear equations (2).

Following [1], we will analyse the convergence of the method on singular systems by decomposing the method into its $\mathcal{R}(A)$ component and its $\mathcal{R}(A)^\perp$ component.

Let $\text{rank}A = \dim \mathcal{R}(A) = r > 0$, and

$$\mathbf{q}_1, \dots, \mathbf{q}_r : \text{orthonormal basis of } \mathcal{R}(A), \quad (9)$$

$$\mathbf{q}_{r+1}, \dots, \mathbf{q}_n : \text{orthonormal basis of } \mathcal{R}(A)^\perp, \quad (10)$$

$$Q_1 := [\mathbf{q}_1, \dots, \mathbf{q}_r] \in \mathbf{R}^{n \times r}, \quad (11)$$

$$Q_2 := [\mathbf{q}_{r+1}, \dots, \mathbf{q}_n] \in \mathbf{R}^{n \times (n-r)}, \quad (12)$$

so that,

$$Q := [Q_1, Q_2] \in \mathbf{R}^{n \times n} \quad (13)$$

is an orthogonal matrix satisfying

$$Q^T Q = Q Q^T = I_n, \quad (14)$$

where I_n is the identity matrix of order n .

Orthogonal transformation of the coefficient matrix A using Q gives

$$\tilde{A} := Q^T A Q = \begin{bmatrix} Q_1^T A Q_1 & Q_1^T A Q_2 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ 0 & 0 \end{bmatrix}, \quad (15)$$

since $Q_2^T A Q = 0$. Here, $A_{11} := Q_1^T A Q_1$ and $A_{12} := Q_1^T A Q_2$.

3.1 Properties concerning A_{11} and A_{12}

First, we will clarify some properties concerning the sub-matrices A_{11} and A_{12} , which appeared in (15).

Theorem 3 $A_{11} := Q_1^T A Q_1 : \text{nonsingular} \iff \mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$.

Proof.

$Q_1^T A Q_1 : \text{nonsingular}$

$\iff Q_1^T [A\mathbf{q}_1, \dots, A\mathbf{q}_r] = [Q_1^T A\mathbf{q}_1, \dots, Q_1^T A\mathbf{q}_r] : \text{nonsingular}$

$\iff \left[\sum_{i=1}^r c_i (Q_1^T A\mathbf{q}_i) = \mathbf{0} \implies c_1 = \dots = c_r = 0 \right]$

$$\begin{aligned}
&\iff \left[Q_1^T A \left(\sum_{i=1}^r c_i \mathbf{q}_i \right) = \mathbf{0} \implies c_1 = \dots = c_r = 0 \right] \\
&\iff \left[A \left(\sum_{i=1}^r c_i \mathbf{q}_i \right) \in R(A) \cap R(A)^\perp \implies c_1 = \dots = c_r = 0 \right] \\
&\iff \left[A \left(\sum_{i=1}^r c_i \mathbf{q}_i \right) = \mathbf{0} \implies c_1 = \dots = c_r = 0 \right] \\
&\iff \left[\sum_{i=1}^r c_i \mathbf{q}_i \in \mathcal{N}(A) \implies c_1 = \dots = c_r = 0 \right] \\
&\iff [\mathbf{x} \in \mathcal{R}(A) \cap \mathcal{N}(A) \implies \mathbf{x} = \mathbf{0}] \\
&\iff \mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}. \quad \square
\end{aligned}$$

We give an example where A_{11} is singular.

Example 1 Let

$$A := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix},$$

and $\mathbf{e}_1 := (1, 0, 0)^T$, $\mathbf{e}_2 := (0, 1, 0)^T$, $\mathbf{e}_3 := (0, 0, 1)^T$. Then, we have $A\mathbf{e}_1 = \mathbf{e}_1$, $A\mathbf{e}_2 = \mathbf{0}$, $A\mathbf{e}_3 = \mathbf{e}_2$.

Hence, $\mathcal{R}(A) = \langle \mathbf{e}_1, \mathbf{e}_2 \rangle$, so that $r = 2$, and $\mathcal{N}(A) = \langle \mathbf{e}_2 \rangle$. Hence, neither $\mathcal{R}(A) \perp \mathcal{N}(A)$ nor $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$ holds.

If we let $\mathbf{q}_1 := \mathbf{e}_1$, $\mathbf{q}_2 := \mathbf{e}_2$, $\mathbf{q}_3 := \mathbf{e}_3$, so that $Q_1 := [\mathbf{q}_1, \mathbf{q}_2] = [\mathbf{e}_1, \mathbf{e}_2]$, $Q_2 := [\mathbf{q}_3] = [\mathbf{e}_3]$. Since $Q := [Q_1, Q_2] = I_3$ and $Q^T A Q = A$, we have

$$A_{11} := Q_1^T A Q_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix},$$

and A_{11} is singular.

Note also that in this example,

$$A_{12} := Q_1^T A Q_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \neq \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

In fact, the following holds.

Theorem 4 $A_{12} := Q_1^T A Q_2 = 0 \iff \mathcal{R}(A) \perp \mathcal{N}(A)$.

Proof.

$$\begin{aligned}
&Q_1^T A Q_2 = 0 \\
&\iff Q_1^T [A\mathbf{q}_{r+1}, \dots, A\mathbf{q}_n] = 0 \\
&\iff A\mathbf{q}_j \in \mathcal{R}(A)^\perp \quad (r+1 \leq j \leq n) \\
&\iff A\mathbf{q}_j \in \mathcal{R}(A) \cap \mathcal{R}(A)^\perp = \{\mathbf{0}\} \quad (r+1 \leq j \leq n) \\
&\iff \langle \mathbf{q}_{r+1}, \dots, \mathbf{q}_n \rangle = \mathcal{N}(A) \\
&\iff \mathcal{R}(A) \perp \mathcal{N}(A). \quad \square
\end{aligned}$$

Corollary 1 $\mathcal{R}(A) \perp \mathcal{N}(A) \implies A_{11} : \text{nonsingular}$

Proof. $\mathcal{R}(A) \perp \mathcal{N}(A) \implies \mathcal{R}(A) \cap \mathcal{N}(A) = \mathbf{0} \iff A_{11} : \text{nonsingular}$. \square

Hence,

$$\tilde{A} := Q^T A Q = \begin{bmatrix} A_{11} & 0 \\ 0 & 0 \end{bmatrix} \quad (16)$$

holds if and only if $\mathcal{R}(A) \perp \mathcal{N}(A)$, and then, A_{11} is nonsingular.

We give an example where the opposite of Corollary 1 is not true.

Example 2 Let

$$A := \begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix}.$$

Note $\text{rank} A = 1$. Let $\mathbf{q}_1 := (1, 0)^T$. Then, $\mathcal{R}(A) = \langle \mathbf{q}_1 \rangle$. Let $\mathbf{q}_2 := (0, 1)^T$. Then, $\mathcal{R}(A)^\perp = \langle \mathbf{q}_2 \rangle$. On the other hand, $\mathcal{N}(A) = \langle (1, 1)^T \rangle$. Hence, $\mathcal{R}(A) \perp \mathcal{N}(A)$ does not hold. However, since $Q_1 := [\mathbf{q}_1]$, $A_{11} := Q_1^T A Q_1 = [1]$, so that A_{11} is nonsingular and $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$ holds.

The following identity holds.

Lemma 4 $\mathcal{R}(A)^\perp = \mathcal{N}(A^T)$.

Proof.

$$\begin{aligned} \mathbf{x} \in \mathcal{R}(A)^\perp & \\ \iff (A^T \mathbf{x}, \mathbf{y}) = (\mathbf{x}, A\mathbf{y}) = 0 \quad \forall \mathbf{y} \in \mathbf{R}^n & \\ \iff A^T \mathbf{x} = \mathbf{0} & \\ \iff \mathbf{x} \in \mathcal{N}(A^T). \quad \square & \end{aligned}$$

Hence, we have the following lemma.

Lemma 5 *The following (1), (2), (3), (4) are equivalent.*

- (1) $\mathcal{R}(A) \perp \mathcal{N}(A)$,
- (2) $A_{12} = 0$,
- (3) $\mathcal{N}(A^T) = \mathcal{N}(A)$,
- (4) $\mathcal{R}(A^T) = \mathcal{R}(A)$.

Proof. (1) \iff (2) is Theorem 4. (1) \iff (3) follows from Lemma 4.

Applying Lemma 4 to A^T gives $\mathcal{R}(A^T)^\perp = \mathcal{N}(A)$.

Hence, (1) $\iff \mathcal{R}(A)^\perp = \mathcal{N}(A) \iff \mathcal{R}(A)^\perp = \mathcal{R}(A^T)^\perp \iff$ (4). \square

Below are examples (cf. [3]) of classes of matrices which satisfy the condition: $\mathcal{R}(A) \perp \mathcal{N}(A)$.

Lemma 6 $A : \text{normal} \implies \mathcal{R}(A) \perp \mathcal{N}(A)$.

Proof. If A is normal,

$$\begin{aligned} \mathbf{x} \in \mathcal{N}(A) &\iff A\mathbf{x} = \mathbf{0} \iff (A\mathbf{x}, A\mathbf{x}) = 0 \iff (A^T A\mathbf{x}, \mathbf{x}) = 0 \\ &\iff (AA^T \mathbf{x}, \mathbf{x}) = 0 \iff (A^T \mathbf{x}, A^T \mathbf{x}) = 0 \iff A^T \mathbf{x} = \mathbf{0} \iff \mathbf{x} \in \mathcal{N}(A^T). \end{aligned}$$

Hence, $\mathcal{N}(A) = \mathcal{N}(A^T)$, so that $\mathcal{R}(A) \perp \mathcal{N}(A)$. \square

Corollary 2 A : symmetric $\implies \mathcal{R}(A) \perp \mathcal{N}(A)$.

Proof. If A is symmetric, then A is normal. Hence, Lemma 6 implies $\mathcal{R}(A) \perp \mathcal{N}(A)$.

An alternative proof using Theorem 4 is as follows.

$$A^T = A$$

\implies

$$\begin{bmatrix} A_{11}^T & 0 \\ A_{12}^T & 0 \end{bmatrix} = (Q^T A Q)^T = Q^T A^T Q = Q^T A Q = \begin{bmatrix} A_{11} & A_{12} \\ 0 & 0 \end{bmatrix}$$

$$\implies A_{12} = 0$$

$$\iff \mathcal{R}(A) \perp \mathcal{N}(A). \quad \square$$

Lemma 7 A : nonsingular $\implies \mathcal{R}(A) \perp \mathcal{N}(A)$.

Proof. If A is nonsingular, $\mathcal{R}(A) = \mathbf{R}^n$, and $\mathcal{N}(A) = \{\mathbf{0}\}$. Hence, $\mathcal{R}(A) \perp \mathcal{N}(A)$. \square

3.2 Decomposition of the GCR(k) algorithm into the $\mathcal{R}(A)$ and $\mathcal{R}(A)^\perp$ components

Now we will consider decomposing the GCR(k) algorithm into the $\mathcal{R}(A)$ and $\mathcal{R}(A)^\perp$ components. In order to do so, we will use the transformation

$$\tilde{\mathbf{v}} := Q^T \mathbf{v} = [Q_1, Q_2]^T \mathbf{v} = \begin{bmatrix} Q_1^T \mathbf{v} \\ Q_2^T \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{v}^1 \\ \mathbf{v}^2 \end{bmatrix},$$

$$\mathbf{v} = Q \tilde{\mathbf{v}} = [Q_1, Q_2] \begin{bmatrix} \mathbf{v}^1 \\ \mathbf{v}^2 \end{bmatrix} = Q_1 \mathbf{v}^1 + Q_2 \mathbf{v}^2,$$

cf. (9)-(14). Here, \mathbf{v}^1 corresponds to the $\mathcal{R}(A)$ component $Q_1 \mathbf{v}^1$ of \mathbf{v} , and \mathbf{v}^2 corresponds to the $\mathcal{R}(A)^\perp$ component $Q_2 \mathbf{v}^2$ of \mathbf{v} .

Using this transformation, we will decompose the vector variables $\mathbf{x}, \mathbf{p}, \mathbf{b}, \mathbf{r}$ into the $\mathcal{R}(A)$ component and the $\mathcal{R}(A)^\perp$ component.

Note, for instance, that the residual vector $\mathbf{r} := \mathbf{b} - A\mathbf{x}$ is transformed into

$$\tilde{\mathbf{r}} := Q^T \mathbf{r} = Q^T \mathbf{b} - Q^T A Q (Q^T \mathbf{x}),$$

or

$$\begin{bmatrix} \mathbf{r}^1 \\ \mathbf{r}^2 \end{bmatrix} = \begin{bmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \end{bmatrix} - \begin{bmatrix} A_{11} & A_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{x}^1 \\ \mathbf{x}^2 \end{bmatrix},$$

i.e.,

$$\begin{aligned} \mathbf{r}^1 &= \mathbf{b}^1 - A_{11} \mathbf{x}^1 - A_{12} \mathbf{x}^2 \\ \mathbf{r}^2 &= \mathbf{b}^2. \end{aligned} \tag{17}$$

Hence, in the least squares problem (8),

$$\begin{aligned}
\|\mathbf{b} - A\mathbf{x}\|_2^2 &= \|\mathbf{r}\|_2^2 = \mathbf{r}^T \mathbf{r} = \mathbf{r}^T Q Q^T \mathbf{r} = (Q^T \mathbf{r})^T Q^T \mathbf{r} \\
&= \tilde{\mathbf{r}}^T \tilde{\mathbf{r}} = \|\mathbf{r}^1\|_2^2 + \|\mathbf{r}^2\|_2^2 = \|\mathbf{r}^1\|_2^2 + \|\mathbf{b}^2\|_2^2 \\
&\geq \|\mathbf{b}^2\|_2^2.
\end{aligned} \tag{18}$$

Note also that the quantities in the GCR(k) algorithm (3) can now be expressed as follows.

First,

$$\begin{aligned}
(\mathbf{r}, A\mathbf{p}) &= (Q\tilde{\mathbf{r}}, AQ\tilde{\mathbf{p}}) = \tilde{\mathbf{r}}^T Q^T AQ\tilde{\mathbf{p}} \\
&= \begin{bmatrix} \mathbf{r}^{1T} & \mathbf{r}^{2T} \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{p}^1 \\ \mathbf{p}^2 \end{bmatrix} = (\mathbf{r}^1, A_{11}\mathbf{p}^1 + A_{12}\mathbf{p}^2).
\end{aligned}$$

Next,

$$(A\mathbf{p}, A\mathbf{p}) = (AQ\tilde{\mathbf{p}}, AQ\tilde{\mathbf{p}}) = \tilde{\mathbf{p}}^T Q^T A^T AQ\tilde{\mathbf{p}} = \tilde{\mathbf{p}}^T Q^T A^T Q Q^T AQ\tilde{\mathbf{p}} = (\tilde{A}\tilde{\mathbf{p}}, \tilde{A}\tilde{\mathbf{p}}),$$

where,

$$\tilde{A}\tilde{\mathbf{p}} = \begin{bmatrix} A_{11} & A_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{p}^1 \\ \mathbf{p}^2 \end{bmatrix} = \begin{bmatrix} A_{11}\mathbf{p}^1 + A_{12}\mathbf{p}^2 \\ \mathbf{0} \end{bmatrix},$$

so that

$$(A\mathbf{p}, A\mathbf{p}) = (A_{11}\mathbf{p}^1 + A_{12}\mathbf{p}^2, A_{11}\mathbf{p}^1 + A_{12}\mathbf{p}^2).$$

Further,

$$\begin{aligned}
(A\mathbf{r}, A\mathbf{p}) &= (AQ\tilde{\mathbf{r}}, AQ\tilde{\mathbf{p}}) = \tilde{\mathbf{r}}^T Q^T A^T Q Q^T AQ\tilde{\mathbf{p}} \\
&= (\tilde{A}\tilde{\mathbf{r}}, \tilde{A}\tilde{\mathbf{p}}) = (A_{11}\mathbf{r}^1 + A_{12}\mathbf{r}^2, A_{11}\mathbf{p}^1 + A_{12}\mathbf{p}^2).
\end{aligned}$$

Hence, the GCR(k) algorithm can always be decomposed into the $\mathcal{R}(A)$ and $\mathcal{R}(A)^\perp$ components as follows.

Decomposed GCR(k) algorithm (the general case)

Choose initial approximate solution \mathbf{x}_0 .

<u>$\mathcal{R}(A)$ component</u>	<u>$\mathcal{R}(A)^\perp$ component</u>
$\mathbf{b}^1 := Q_1^T \mathbf{b}$	$\mathbf{b}^2 := Q_2^T \mathbf{b}$
$\mathbf{x}_0^1 := Q_1^T \mathbf{x}_0$	$\mathbf{x}_0^2 := Q_2^T \mathbf{x}_0$
$* \mathbf{r}_0^1 := \mathbf{b}^1 - A_{11}\mathbf{x}_0^1 - A_{12}\mathbf{x}_0^2$	$\mathbf{r}_0^2 := \mathbf{b}^2$
$\mathbf{p}_0^1 := \mathbf{r}_0^1$	$\mathbf{p}_0^2 := \mathbf{r}_0^2 = \mathbf{b}^2$

For $i = 0, 1, \dots, k$ until convergence do

begin

$$\alpha_i := \frac{(\mathbf{r}_i^1, A_{11}\mathbf{p}_i^1 + A_{12}\mathbf{p}_i^2)}{(A_{11}\mathbf{p}_i^1 + A_{12}\mathbf{p}_i^2, A_{11}\mathbf{p}_i^1 + A_{12}\mathbf{p}_i^2)}$$

$$\mathbf{x}_{i+1}^1 := \mathbf{x}_i^1 + \alpha_i \mathbf{p}_i^1$$

$$\mathbf{x}_{i+1}^2 := \mathbf{x}_i^2 + \alpha_i \mathbf{p}_i^2$$

$$\mathbf{r}_{i+1}^1 := \mathbf{r}_i^1 - \alpha_i (A_{11}\mathbf{p}_i^1 + A_{12}\mathbf{p}_i^2)$$

$$\mathbf{r}_{i+1}^2 := \mathbf{r}_i^2 = \mathbf{b}^2$$

$$\beta_j^i := -\frac{(A_{11}\mathbf{r}_{i+1}^1 + A_{12}\mathbf{r}_{i+1}^2, A_{11}\mathbf{p}_j^1 + A_{12}\mathbf{p}_j^2)}{(A_{11}\mathbf{p}_j^1 + A_{12}\mathbf{p}_j^2, A_{11}\mathbf{p}_j^1 + A_{12}\mathbf{p}_j^2)} \quad (0 \leq j \leq i)$$

$$\mathbf{p}_{i+1}^1 := \mathbf{r}_{i+1}^1 + \sum_{j=0}^i \beta_j^i \mathbf{p}_j^1$$

$$\mathbf{p}_{i+1}^2 := \mathbf{r}_{i+1}^2 + \sum_{j=0}^i \beta_j^i \mathbf{p}_j^2$$

end

$$\mathbf{x}_0^1 := \mathbf{x}_{k+1}^1$$

$$\mathbf{x}_0^2 := \mathbf{x}_{k+1}^2$$

Go to *.

(19)

Note that \mathbf{r}_i^2 , the $\mathcal{R}(A)^\perp$ component of the residual vector is always equal to the least squares residual \mathbf{b}^2 of (8) (cf. (17), (18)).

3.3 Convergence theorem for arbitrary \mathbf{b}

Using the decomposition obtained above, we will first derive the convergence theorem for arbitrary \mathbf{b} , i.e. when \mathbf{b} may not necessarily be in $\mathcal{R}(A)$.

First note that, for the case when $\mathcal{R}(A) \perp \mathcal{N}(A)$, we have $A_{12} = 0$ from Theorem 4. Hence, (17) becomes

$$\begin{aligned} \mathbf{r}^1 &= \mathbf{b}^1 - A_{11}\mathbf{x}^1 \\ \mathbf{r}^2 &= \mathbf{b}^2. \end{aligned} \quad (20)$$

Note also that, from Corollary 1, A_{11} is nonsingular. Hence, from (18) and (20), a least squares solution of (8) is given by $\mathbf{x}^1 = A_{11}^{-1}\mathbf{b}^1$.

Now, for the case $\mathcal{R}(A) \perp \mathcal{N}(A)$, the above decomposed GCR(k) algorithm (19) can be simplified as follows.

Decomposed GCR(k) algorithm (Case $\mathcal{R}(A) \perp \mathcal{N}(A)$)

Choose initial approximate solution \mathbf{x}_0 .

<u>$\mathcal{R}(A)$ component</u>	<u>$\mathcal{R}(A)^\perp$ component</u>
--	--

$\mathbf{b}^1 := Q_1^\top \mathbf{b}$	$\mathbf{b}^2 := Q_2^\top \mathbf{b}$
$\mathbf{x}_0^1 := Q_1^\top \mathbf{x}_0$	$\mathbf{x}_0^2 := Q_2^\top \mathbf{x}_0$
$* \mathbf{r}_0^1 := \mathbf{b}^1 - A_{11} \mathbf{x}_0^1$	$\mathbf{r}_0^2 := \mathbf{b}^2$
$\mathbf{p}_0^1 := \mathbf{r}_0^1$	$\mathbf{p}_0^2 := \mathbf{r}_0^2 = \mathbf{b}^2$

For $i = 0, 1, \dots, k$ until convergence do

begin

$$\alpha_i := \frac{(\mathbf{r}_i^1, A_{11} \mathbf{p}_i^1)}{(A_{11} \mathbf{p}_i^1, A_{11} \mathbf{p}_i^1)}$$

$\mathbf{x}_{i+1}^1 := \mathbf{x}_i^1 + \alpha_i \mathbf{p}_i^1$	$\mathbf{x}_{i+1}^2 := \mathbf{x}_i^2 + \alpha_i \mathbf{p}_i^2$
--	--

$\mathbf{r}_{i+1}^1 := \mathbf{r}_i^1 - \alpha_i A_{11} \mathbf{p}_i^1$	$\mathbf{r}_{i+1}^2 := \mathbf{r}_i^2 = \mathbf{b}^2$
---	---

$$\beta_i^j := -\frac{(A_{11} \mathbf{r}_{i+1}^1, A_{11} \mathbf{p}_j^1)}{(A_{11} \mathbf{p}_j^1, A_{11} \mathbf{p}_j^1)} \quad (0 \leq j \leq i)$$

$\mathbf{p}_{i+1}^1 := \mathbf{r}_{i+1}^1 + \sum_{j=0}^i \beta_j^i \mathbf{p}_j^1$	$\mathbf{p}_{i+1}^2 := \mathbf{r}_{i+1}^2 + \sum_{j=0}^i \beta_j^i \mathbf{p}_j^2$
--	--

end

$\mathbf{x}_0^1 := \mathbf{x}_{k+1}^1$	$\mathbf{x}_0^2 := \mathbf{x}_{k+1}^2$
--	--

Go to * .

(21)

Note that the $\mathcal{R}(A)$ component of the above algorithm is equivalent to the GCR(k) algorithm applied to the system of linear equations

$$A_{11} \mathbf{x}^1 = \mathbf{b}^1. \tag{22}$$

Hence, the convergence of the residual of the decomposed GCR(k) algorithm (21) is determined by the convergence of the residual \mathbf{r}^1 for the GCR(k) method applied to the

system (22). Hence, from Theorem 1, we obtain the following lemma concerning the convergence of the residual of the decomposed GCR(k) method (21).

Lemma 8 *If $A_{12} = 0$, and the symmetric part $M(A_{11})$ of $A_{11} := Q_1^T A Q_1$ is definite, either of the following holds for the decomposed GCR(k) algorithm (21).*

1. *There exists $l \geq 0$ such that $\mathbf{p}_i^1 \neq \mathbf{0}$ ($0 \leq i < l$) and $\mathbf{r}_i^1 = \mathbf{0}$. Further,*

$$\frac{\|\mathbf{r}_{i+1}^1\|_2^2}{\|\mathbf{r}_i^1\|_2^2} \leq 1 - \frac{\{\lambda_{\min}(M(A_{11}))\}^2}{\lambda_{\max}(A_{11}^T A_{11})} \quad (23)$$

holds for $0 \leq i < l$.

2. *For all $i \geq 0$, $\mathbf{p}_i^1 \neq \mathbf{0}$, $\mathbf{r}_i^1 \neq \mathbf{0}$, and (23) hold.*

From Lemmas 3 and 8, we derive the following theorem. The proof is similar to that of Theorem 3.3 in [1] for the CR method.

Theorem 5

For the least squares problem $\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$, $A \in \mathbf{R}^{n \times n}$, the necessary and sufficient condition for the GCR(k) method to converge to a least squares solution without breakdown for arbitrary $\mathbf{b} \in \mathbf{R}^n$ and initial approximate solution $\mathbf{x}_0 \in \mathbf{R}^n$ is that, $A_{12} := Q_1^T A Q_2 = \mathbf{0}$ and the symmetric part $M(A_{11})$ of $A_{11} := Q_1^T A Q_1$ is definite.

Remark Here, by the term “the GCR(k) method to converge to a least squares solution”, we mean \mathbf{r}^1 (the $\mathcal{R}(A)$ component of the residual \mathbf{r}) to converge to $\mathbf{0}$, or equivalently, the residual \mathbf{r} to converge to $Q_2 \mathbf{b}^2$, the $\mathcal{R}(A)^\perp$ component of \mathbf{b} .

Proof. We will show the necessity of the condition by contraposition, i.e. we will show that if $M(A_{11})$ is not definite or if $A_{12} \neq \mathbf{0}$, then, there exists a \mathbf{b} such that the GCR(k) method breaks down before reaching a least squares solution.

(Case 1) The case when $M(A_{11})$ is not definite.

If we suppose that $M(A_{11})$ is not definite, then from Lemma 3, there exists $\mathbf{v} \neq \mathbf{0}$ such that $(\mathbf{v}, A_{11}\mathbf{v}) = 0$. Thus, for such \mathbf{v} , let

$$\mathbf{b} = Q \begin{bmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \end{bmatrix}, \quad \begin{bmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \end{bmatrix} = \begin{bmatrix} \mathbf{v} + Q_1^T A \mathbf{x}_0 \\ \mathbf{0} \end{bmatrix}.$$

Then,

$$\begin{aligned} \mathbf{r}_0^1 &= Q_1^T \mathbf{r}_0 = Q_1^T (\mathbf{b} - A \mathbf{x}_0) = \mathbf{b}^1 - Q_1^T A \mathbf{x}_0 = \mathbf{v} \neq \mathbf{0}, \\ \mathbf{r}_0^2 &= \mathbf{b}^2 = \mathbf{0}. \end{aligned}$$

Hence, \mathbf{x}_0 is not a least squares solution, and

$$\begin{aligned} (\mathbf{r}_0, A \mathbf{p}_0) &= (\mathbf{r}_0, A \mathbf{r}_0) = \mathbf{r}_0^T A \mathbf{r}_0 = (Q \tilde{\mathbf{r}}_0)^T A Q \tilde{\mathbf{r}}_0 \\ &= \begin{bmatrix} \mathbf{r}_0^{1T} & \mathbf{r}_0^{2T} \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{r}_0^1 \\ \mathbf{r}_0^2 \end{bmatrix} = (\mathbf{r}_0^1, A_{11} \mathbf{r}_0^1) = (\mathbf{v}, A_{11} \mathbf{v}) = 0. \end{aligned}$$

If $(A\mathbf{p}_0, A\mathbf{p}_0) = 0$, the GCR(k) method of (3) breaks down at step $i = 0$ before reaching a least squares solution.

On the other hand, if $(A\mathbf{p}_0, A\mathbf{p}_0) \neq 0$, then, $\alpha_0 = \frac{(\mathbf{r}_0, A\mathbf{p}_0)}{(A\mathbf{p}_0, A\mathbf{p}_0)} = 0$.

Hence, $\mathbf{x}_1 = \mathbf{x}_0$, $\mathbf{r}_1 = \mathbf{r}_0 = \mathbf{p}_0$, so that \mathbf{x}_1 is not a least squares solution. Further, $\beta_0^0 = -\frac{(A\mathbf{r}_1, A\mathbf{p}_0)}{(A\mathbf{p}_0, A\mathbf{p}_0)} = -\frac{(A\mathbf{p}_0, A\mathbf{p}_0)}{(A\mathbf{p}_0, A\mathbf{p}_0)} = -1$, and $\mathbf{p}_1 = \mathbf{r}_1 + \beta_0^0 \mathbf{p}_0 = \mathbf{p}_0 - \mathbf{p}_0 = \mathbf{0}$.

Hence, for $k \geq 1$, the denominator $(A\mathbf{p}_1, A\mathbf{p}_1)$ of α_1 becomes zero, and the GCR(k) method breaks down at step $i = 1$ before reaching a least squares solution.

For $k = 0$, new $\mathbf{x}_0 := \text{old } \mathbf{x}_1 = \text{old } \mathbf{x}_0$, so that the process repeats without ever giving a least squares solution.

(Case 2) The case when $M(A_{11})$ is definite and $A_{12} \neq 0$.

From $A_{12} \neq 0$, there exist i and j such that $(A_{12})_{i,j} \neq 0$. Hence, let $\mathbf{v}_1 = (v_{1,1}, \dots, v_{1,k}, \dots, v_{1,r})^T$ where $v_{1,k} = \delta_{ik}$, and $\mathbf{v}_2 = (v_{2,1}, \dots, v_{2,k}, \dots, v_{2,n-r})^T$ where $v_{2,k} = \delta_{jk}$. Then, $\mathbf{v}_1^T A_{12} \mathbf{v}_2 = (A_{12})_{i,j} \neq 0$. Hence, there exist $\mathbf{v}_1 \neq \mathbf{0}$ and $\mathbf{v}_2 \neq \mathbf{0}$, such that $(\mathbf{v}_1, A_{12} \mathbf{v}_2) \neq 0$.

Thus, for such \mathbf{v}_1 and \mathbf{v}_2 , let

$$\mathbf{b} = Q \begin{bmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \end{bmatrix}, \quad \begin{bmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \end{bmatrix} = \begin{bmatrix} \mathbf{v}_1 + Q_1^T A \mathbf{x}_0 \\ \epsilon \mathbf{v}_2 \end{bmatrix}.$$

Then,

$$\begin{aligned} \mathbf{r}_0^1 &= Q_1^T \mathbf{r}_0 = Q_1^T (\mathbf{b} - A \mathbf{x}_0) = \mathbf{b}^1 - Q_1^T A \mathbf{x}_0 = \mathbf{v}_1 \neq \mathbf{0}, \\ \mathbf{r}_0^2 &= Q_2^T \mathbf{r}_0 = Q_2^T (\mathbf{b} - A \mathbf{x}_0) = \mathbf{b}^2 = \epsilon \mathbf{v}_2. \end{aligned}$$

Hence, \mathbf{x}_0 is not a least squares solution.

If we let $\epsilon = -\frac{(\mathbf{v}_1, A_{11} \mathbf{v}_1)}{(\mathbf{v}_1, A_{12} \mathbf{v}_2)}$, then,

$$(\mathbf{r}_0, A\mathbf{p}_0) = (\mathbf{r}_0^1, A_{11} \mathbf{r}_0^1) + (\mathbf{r}_0^2, A_{12} \mathbf{r}_0^2) = (\mathbf{v}_1, A_{11} \mathbf{v}_1) + \epsilon (\mathbf{v}_1, A_{12} \mathbf{v}_2) = 0.$$

Now, if $A\mathbf{p}_0 = A\mathbf{r}_0 = \mathbf{0}$, the GCR(k) method of (3) breaks down at step $i = 0$ before reaching a least squares solution.

On the other hand, if $A\mathbf{p}_0 \neq \mathbf{0}$, then, $\alpha_0 = \frac{(\mathbf{r}_0, A\mathbf{p}_0)}{(A\mathbf{p}_0, A\mathbf{p}_0)} = 0$. Hence, $\mathbf{r}_1 = \mathbf{r}_0 = \mathbf{p}_0$, so

that \mathbf{x}_1 is not a least squares solution. Further, $\beta_0^0 = -\frac{(A\mathbf{r}_1, A\mathbf{p}_0)}{(A\mathbf{p}_0, A\mathbf{p}_0)} = -1$,

$\mathbf{p}_1 = \mathbf{r}_1 + \beta_0^0 \mathbf{p}_0 = \mathbf{p}_0 - \mathbf{p}_0 = \mathbf{0}$.

Hence, for $k \geq 1$, the denominator $(A\mathbf{p}_1, A\mathbf{p}_1)$ of α_1 becomes zero, and the GCR(k) method breaks down at step $i = 1$ before reaching a least squares solution.

For $k = 0$, new $\mathbf{x}_0 := \text{old } \mathbf{x}_1 = \text{old } \mathbf{x}_0$, so that the process repeats without ever giving a least squares solution.

Thus, we have shown the necessity of the condition.

The sufficiency of the condition follows from Lemma 8. \square

In order to rephrase the condition in Theorem 5 in terms of the original matrix A , note the following.

Lemma 9 $M(A_{11})$ is definite $\iff M(A)$ is definite in $\mathcal{R}(A)$.

Proof. Note

$$\begin{aligned} (\mathbf{y}^1, M(A_{11})\mathbf{y}^1) &= (\mathbf{y}^1, A_{11}\mathbf{y}^1) = \mathbf{y}^{1T} Q_1^T A Q_1 \mathbf{y}^1 \\ &= (Q_1 \mathbf{y}^1, A Q_1 \mathbf{y}^1) = (Q_1 \mathbf{y}^1, M(A) Q_1 \mathbf{y}^1). \end{aligned}$$

Hence,

$$\begin{aligned} M(A_{11}) \text{ is positive-definite} &\iff (\mathbf{y}^1, M(A_{11})\mathbf{y}^1) > 0 \text{ for all } \mathbf{y}^1 \neq \mathbf{0} \\ &\iff (Q_1 \mathbf{y}^1, M(A) Q_1 \mathbf{y}^1) > 0 \text{ for all } \mathbf{y}^1 \neq \mathbf{0} \\ &\iff (\mathbf{y}, M(A)\mathbf{y}) > 0 \text{ for all } \mathbf{y} \in \mathcal{R}(A); \mathbf{y} \neq \mathbf{0} \\ &\iff M(A) \text{ is positive-definite in } \mathcal{R}(A). \end{aligned}$$

(Similarly for the negative-definite case.) \square

Lemma 10 If $\mathcal{R}(A) \perp \mathcal{N}(A)$, then,

$M(A_{11})$ is definite \iff “ $M(A)$ is semidefinite, and $\text{rank } M(A) = \text{rank } A$ ”.

Proof. If $\mathcal{R}(A) \perp \mathcal{N}(A)$, then from Theorem 4, (16) holds, so that

$$Q^T A^T Q = \begin{bmatrix} A_{11}^T & 0 \\ 0 & 0 \end{bmatrix},$$

and

$$Q^T M(A) Q = \begin{bmatrix} M(A_{11}) & 0 \\ 0 & 0 \end{bmatrix}. \quad (24)$$

Thus,

$$Q^T \{M(A) - \lambda I\} Q = Q^T M(A) Q - \lambda I,$$

so that

$$\begin{aligned} \det Q^T \det \{M(A) - \lambda I\} \det Q \\ = \det \{Q^T M(A) Q - \lambda I\} = \det \begin{bmatrix} M(A_{11}) - \lambda I_r & 0 \\ 0 & -\lambda I_{n-r} \end{bmatrix}. \end{aligned} \quad (25)$$

Since $M(A)^T = M(A)$, there exists a nonsingular matrix S such that $S^{-1}M(A)S = \text{diag}[\lambda_1, \dots, \lambda_n]$, where the right hand side is the diagonal matrix with diagonal elements $\lambda_1, \dots, \lambda_n$.

Hence, $\text{rank } M(A)$ = the number of nonzero eigenvalues of $M(A)$. Thus, $M(A_{11})$: definite \iff “ $M(A)$: semidefinite, $\text{rank } M(A) = \text{rank } M(A_{11}) = r = \text{rank } A$ ”. \square

Remark Example 2 shows that the equivalence in Lemma 10 does not necessarily hold when $\mathcal{R}(A) \perp \mathcal{N}(A)$ does not hold. In this case, $M(A_{11})$ is definite, but $M(A)$ is not semidefinite, and $\text{rank } M(A) \neq \text{rank } A$.

Thus, we have the following.

Theorem 6

For the least squares problem $\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$, $A \in \mathbf{R}^{n \times n}$, the following are equivalent.

- (C1) The GCR(k) method converges to a least squares solution without breakdown for arbitrary $\mathbf{b} \in \mathbf{R}^n$ and initial approximate solution $\mathbf{x}_0 \in \mathbf{R}^n$.
- (C2) $A_{12} := Q_1^T A Q_2 = 0$, and the symmetric part $M(A_{11})$ of $A_{11} := Q_1^T A Q_1$ is definite.
- (C3) $\mathcal{R}(A) \perp \mathcal{N}(A)$, the symmetric part $M(A)$ of A is semi-definite, $\text{rank } M(A) = \text{rank } A$.
- (C4) $\mathcal{R}(A) \perp \mathcal{N}(A)$ and $M(A)$ is definite in $\mathcal{R}(A)$.

Remark 1 The above theorem is a natural extension of Theorem 2 for the nonsingular case, since if A is nonsingular, $\mathcal{R}(A) = \mathbf{R}^n$, $\mathcal{N}(A) = \{\mathbf{0}\}$, so that $\mathcal{R}(A) \perp \mathcal{N}(A)$.

Remark 2 If the condition of the above theorem is satisfied, the (full) GCR method ($k = \infty$) will give a least squares solution of (8) within $r = \text{rank } A$ iterations. This is because the $\mathcal{R}(A)$ component of the algorithm is equivalent to the method applied to $A_{11}\mathbf{x}^1 = \mathbf{b}^1$ in \mathbf{R}^r , where A_{11} is definite (cf. (21)).

Remark 3 In [3], it is shown that $\mathcal{R}(A) \perp \mathcal{N}(A)$ is the necessary and sufficient condition for the GMRES method to converge to a least squares solution without breakdown for arbitrary $\mathbf{b} \in \mathbf{R}^n$ and initial approximate solution $\mathbf{x}_0 \in \mathbf{R}^n$. The GCR and GCR(k) methods require the extra condition: “ $M(A)$ is definite in $\mathcal{R}(A)$ ” in order to avoid breakdowns unique to the methods.

Remark 4 In order to judge whether the method has converged to a least squares solution for inconsistent systems (i.e. when $\mathbf{b} \notin \mathcal{R}(A)$), one could monitor the norm of $A^T \mathbf{r}$. This observation is based on the following lemma.

Lemma 11 $\mathbf{r}^1 := Q_1^T \mathbf{r} = \mathbf{0} \iff A^T \mathbf{r} = \mathbf{0}$.

Proof. Let $A := [\mathbf{a}_1, \dots, \mathbf{a}_n]$.

$$\begin{aligned} \mathbf{r}^1 := Q_1^T \mathbf{r} = \mathbf{0} &\iff \mathcal{R}(A) \perp \mathbf{r} \\ &\iff \langle \mathbf{a}_1, \dots, \mathbf{a}_n \rangle \perp \mathbf{r} \\ &\iff \begin{bmatrix} \mathbf{a}_1^T \\ \vdots \\ \mathbf{a}_n^T \end{bmatrix} \mathbf{r} = A^T \mathbf{r} = \mathbf{0}. \end{aligned}$$

□

Finally, we consider where the approximate solution \mathbf{x}_i converges when the GCR(k) method converges according to Theorem 6.

Lemma 12 Let $\mathcal{R}(A) \perp \mathcal{N}(A)$. Then, the following hold for the GCR(k) method.

If \mathbf{r}_i^1 converges to $\mathbf{0}$ (least squares solution), \mathbf{x}_i^1 converges to $A_{11}^{-1} \mathbf{b}^1$.

Moreover, if $\mathbf{b} \in \mathcal{R}(A)$, $\mathbf{x}_i^2 = \mathbf{x}_0^2$, so that \mathbf{x}_i converges to $Q_1 A_{11}^{-1} \mathbf{b}^1 + Q_2 \mathbf{x}_0^2$.

Further, if $\mathbf{x}_0^2 = \mathbf{0}$ (i.e. $\mathbf{x}_0 \in \mathcal{R}(A)$), \mathbf{x}_i converges to $Q_1 A_{11}^{-1} \mathbf{b}^1$, which is the pseudo-inverse solution (the least squares solution with minimum Euclidean norm).

Proof. If $\mathcal{R}(A) \perp \mathcal{N}(A)$, the $\mathcal{R}(A)$ component of decomposed GCR(k) algorithm (21) can be regarded as the GCR(k) method applied to $A_{11}\mathbf{x}^1 = \mathbf{b}^1$, where A_{11} is nonsingular from Corollary 1. Hence, if the $\mathcal{R}(A)$ component of the residual converges to $\mathbf{0}$, \mathbf{x}_i^1 converges to $A_{11}^{-1}\mathbf{b}^1$.

Moreover, if $\mathbf{b} \in \mathcal{R}(A)$, $\mathbf{b}^2 = \mathbf{0}$ in the $\mathcal{R}(A)^\perp$ component of the decomposed GCR(k) algorithm (21), so that $\mathbf{p}_i^2 \equiv \mathbf{0}$ ($i \geq 0$), and hence, $\mathbf{x}_i^2 \equiv \mathbf{x}_0^2$ ($i \geq 0$).

Hence, $\mathbf{x}_i = Q_1\mathbf{x}_i^1 + Q_2\mathbf{x}_i^2$ converges to $Q_1A_{11}^{-1}\mathbf{b}^1 + Q_2\mathbf{x}_0^2$.

Further, if $\mathbf{x}_0^2 = \mathbf{0}$, $\mathbf{x}_i^2 \equiv \mathbf{x}_0^2 = \mathbf{0}$ ($i \geq 0$), so that \mathbf{x}_i converges to $Q_1A_{11}^{-1}\mathbf{b}^1$. Now, since $\|\mathbf{x}\|_2^2 = \mathbf{x}^\top\mathbf{x} = \|\mathbf{x}^1\|_2^2 + \|\mathbf{x}^2\|_2^2$, if we denote the converged solution by \mathbf{x}_* , $\|\mathbf{x}_*\|_2^2 = \|A_{11}^{-1}\mathbf{b}^1\|_2^2 + \|\mathbf{x}_0^2\|_2^2$, and $\mathbf{x}_0^2 = \mathbf{0}$ gives the pseudo-inverse solution. \square

Remark 1 Hence, if $\mathcal{R}(A) \perp \mathcal{N}(A)$, A is definite in $\mathcal{R}(A)$, and $\mathbf{b} \in \mathcal{R}(A)$, we can obtain the pseudo-inverse solution by setting $\mathbf{x}_0 = \mathbf{0}$.

Remark 2 Even if $\mathcal{R}(A) \perp \mathcal{N}(A)$ holds, if \mathbf{b} is not in $\mathcal{R}(A)$ (inconsistent case), $\mathbf{b}^2 \neq \mathbf{0}$ in the decomposed GCR(k) algorithm of (21), so that it is not obvious where \mathbf{x}_i^2 , and hence \mathbf{x}_i will end up.

3.4 Convergence theorem for the case $\mathbf{b} \in \mathcal{R}(A)$

Next, we will consider the case when the system is consistent, that is when $\mathbf{b} \in \mathcal{R}(A)$. In this case, $\mathbf{b}^2 := Q_2^\top\mathbf{b} = \mathbf{0}$ holds. Hence, the decomposed GCR(k) algorithm of (19) can be simplified as follows.

Decomposed GCR(k) algorithm (Case $\mathbf{b} \in \mathcal{R}(A)$)

$\mathcal{R}(A)$ component	$\mathcal{R}(A)^\perp$ component
Choose initial approximate solution \mathbf{x}_0 .	
$\mathbf{b}^1 := Q_1^\top\mathbf{b}$	$\mathbf{b}^2 := \mathbf{0}$
$\mathbf{x}_0^1 := Q_1^\top\mathbf{x}_0$	$\mathbf{x}_0^2 := Q_2^\top\mathbf{x}_0$
$* \mathbf{r}_0^1 := \mathbf{b}^1 - A_{11}\mathbf{x}_0^1 - A_{12}\mathbf{x}_0^2$	$\mathbf{r}_0^2 := \mathbf{b}^2 = \mathbf{0}$
$\mathbf{p}_0^1 := \mathbf{r}_0^1$	$\mathbf{p}_0^2 := \mathbf{r}_0^2 = \mathbf{0}$
For $i = 0, 1, \dots, k$ until convergence do	
begin	
$\alpha_i := \frac{(\mathbf{r}_i^1, A_{11}\mathbf{p}_i^1)}{(A_{11}\mathbf{p}_i^1, A_{11}\mathbf{p}_i^1)}$	
$\mathbf{x}_{i+1}^1 := \mathbf{x}_i^1 + \alpha_i\mathbf{p}_i^1$	$\mathbf{x}_{i+1}^2 := \mathbf{x}_i^2 = \mathbf{x}_0^2$

$$\mathbf{r}_{i+1}^1 := \mathbf{r}_i^1 - \alpha_i A_{11} \mathbf{p}_i^1 \quad \mathbf{r}_{i+1}^2 := \mathbf{r}_i^2 = \mathbf{0}$$

$$\beta_i^j := -\frac{(A_{11} \mathbf{r}_{i+1}^1, A_{11} \mathbf{p}_j^1)}{(A_{11} \mathbf{p}_j^1, A_{11} \mathbf{p}_j^1)} \quad (0 \leq j \leq i)$$

$$\mathbf{p}_{i+1}^1 := \mathbf{r}_{i+1}^1 + \sum_{j=0}^i \beta_j^i \mathbf{p}_j^1 \quad \mathbf{p}_{i+1}^2 := \mathbf{r}_{i+1}^2 = \mathbf{0}$$

end

$$\mathbf{x}_0^1 := \mathbf{x}_{k+1}^1 \quad \mathbf{x}_0^2 := \mathbf{x}_{k+1}^2$$

Go to * .

(26)

Note that \mathbf{x}_0^2 remains unchanged in the above algorithm.

Then, we have the following theorem.

Theorem 7

For the least squares problem $\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$, $A \in \mathbf{R}^{n \times n}$, the following are equivalent.

(C1) The GCR(k) method converges to an exact solution without breakdown

for arbitrary $\mathbf{b} \in \mathcal{R}(A)$ and initial approximate solution $\mathbf{x}_0 \in \mathbf{R}^n$.

(C2) The symmetric part $M(A_{11})$ of $A_{11} := Q_1^T A Q_1$ is definite.

(C3) The symmetric part $M(A)$ of A is definite in $\mathcal{R}(A)$.

Proof.

(C2 \implies C1) : For $\mathbf{b} \in \mathcal{R}(A)$, the $\mathcal{R}(A)$ component of the decomposed GCR(k) algorithm of (26) is equivalent to the GCR(k) method applied to the system

$A_{11} \mathbf{x}^1 = \mathbf{b}^1 - A_{12} \mathbf{x}_0^2$. Hence, from Theorem 2, if $M(A_{11})$ is definite, \mathbf{r}_i^1 , the $\mathcal{R}(A)$ component of the residual, will converge to $\mathbf{0}$ without breakdown. Since \mathbf{r}_i^2 , the $\mathcal{R}(A)^\perp$ component of the residual, is always $\mathbf{0}$, the method converges to an exact solution without breakdown for arbitrary $\mathbf{b} \in \mathcal{R}(A)$ and $\mathbf{x}_0 \in \mathbf{R}^n$.

(C1 \implies C2) : We will prove by contraposition, i.e. we will show that if $M(A_{11})$ is not definite, there exists a $\mathbf{b} \in \mathcal{R}(A)$ such that the GCR(k) method breaks down before reaching an exact solution.

Assume that $M(A_{11})$ is not definite. Then, from Lemma 3, there exists $\mathbf{v}^1 \neq \mathbf{0}$ such that $(\mathbf{v}^1, A_{11} \mathbf{v}^1) = 0$. Let $\mathbf{b} := Q_1 \mathbf{b}^1 + Q_2 \mathbf{b}^2 = Q_1 \mathbf{b}^1$ where $\mathbf{b}^1 := \mathbf{v}^1 + A_{11} \mathbf{x}_0^1 + A_{12} \mathbf{x}_0^2$. Then, $\mathbf{p}_0^1 := \mathbf{r}_0^1 = \mathbf{v}^1 \neq \mathbf{0}$, so that \mathbf{x}_0 is not an exact solution.

Then, at step $i = 0$, if $A_{11} \mathbf{p}_0^1 = A_{11} \mathbf{v}^1 = \mathbf{0}$, breakdown occurs when computing α_0 . But, $\mathbf{r}_0^1 = \mathbf{v}^1 \neq \mathbf{0}$, so that $\mathbf{r}_0 \neq \mathbf{0}$, i.e. \mathbf{x}_0 is not an exact solution.

On the other hand, if $A_{11} \mathbf{p}_0^1 = A_{11} \mathbf{v}^1 \neq \mathbf{0}$, then $(\mathbf{r}_0^1, A_{11} \mathbf{p}_0^1) = (\mathbf{v}^1, A_{11} \mathbf{v}^1) = 0$, so that $\alpha_0 = 0$, and $\mathbf{x}_1^1 = \mathbf{x}_0^1$, $\mathbf{r}_1^1 = \mathbf{r}_0^1 = \mathbf{v}^1 \neq \mathbf{0}$. Hence, \mathbf{x}_1 is not an exact solution. Further,

$$\beta_0^0 = -\frac{(A_{11} \mathbf{r}_1^1, A_{11} \mathbf{p}_0^1)}{(A_{11} \mathbf{p}_0^1, A_{11} \mathbf{p}_0^1)} = -\frac{(A_{11} \mathbf{v}^1, A_{11} \mathbf{v}^1)}{(A_{11} \mathbf{v}^1, A_{11} \mathbf{v}^1)} = -1, \text{ and } \mathbf{p}_1^1 = \mathbf{r}_1^1 + \beta_0^0 \mathbf{p}_0^1 = \mathbf{v}^1 - \mathbf{v}^1 = \mathbf{0}.$$

Hence, for $k \geq 1$, $\mathbf{p}_1^1 = \mathbf{0}$, so that breakdown occurs at step $i = 1$, when computing α_1 , even though \mathbf{x}_1 is not an exact solution.

For $k = 0$, new $\mathbf{x}_1 = \text{old } \mathbf{x}_0$, so the process repeats without ever giving an exact solution.

Hence, if $M(A_{11})$ is not definite, for any \mathbf{x}_0 , there exists $\mathbf{b} := Q_1 \mathbf{b}^1 \in \mathcal{R}(A)$ such that the GCR(k) method does not converge to an exact solution.

(C2 \iff C3) is a consequence of Lemma 9. \square

Remark 1 The above theorem is also a natural extension of Theorem 2 for the nonsingular case, since if A is nonsingular, $\mathcal{R}(A) = \mathbf{R}^n$.

Remark 2 If the condition of the above theorem is satisfied and $\mathbf{b} \in \mathcal{R}(A)$, the GCR method without restarts will give a solution to (8) within $r = \text{rank} A$ iterations, since the $\mathcal{R}(A)$ component of the algorithm is equivalent to the method applied to $A_{11} \mathbf{x}^1 = \mathbf{b}^1 - A_{12} \mathbf{x}_0^2$ in \mathbf{R}^r , where A_{11} is definite.

Remark 3 Note here that, if $M(A_{11})$ is definite, then, A_{11} is nonsingular from Lemma 1, and $\mathcal{R}(A) \cap \mathcal{N}(A) = \mathbf{0}$ holds from Theorem 3.

Since, $\mathbf{r}_i^1 = \mathbf{b}^1 - A_{12} \mathbf{x}_0^2 - A_{11} \mathbf{x}_i^1$, we have the following.

Lemma 13 *If $\mathbf{b} \in \mathcal{R}(A)$ and $M(A)$ is definite in $\mathcal{R}(A)$, the following hold for the GCR(k) method.*

\mathbf{x}_i^1 converges to $A_{11}^{-1}(\mathbf{b}^1 - A_{12} \mathbf{x}_0^2)$ and $\mathbf{x}_i^2 = \mathbf{x}_0^2$, so that \mathbf{x}_i converges to $Q_1 A_{11}^{-1}(\mathbf{b}^1 - A_{12} \mathbf{x}_0^2) + Q_2 \mathbf{x}_0^2$.

Further, if $\mathbf{x}_0^2 = \mathbf{0}$, (i.e. $\mathbf{x}_0 \in \mathcal{R}(A)$), \mathbf{x}_i^1 converges to $A_{11}^{-1} \mathbf{b}^1$ and $\mathbf{x}_i^2 = \mathbf{0}$, so that \mathbf{x}_i converges to the pseudo-inverse solution $Q_1 A_{11}^{-1} \mathbf{b}^1$.

3.5 Examples

Finally, we analyze the convergence of the GCR(k) method for the following examples taken from [1].

Consider the two point boundary value problem of the ordinary differential equation

$$\frac{d^2 u}{dx^2} + \beta \frac{du}{dx} = f(x) \quad (0 < x < 1)$$

with boundary conditions

1. periodic boundary condition: $u(0) = u(1)$

or

2. Neumann boundary condition: $\left. \frac{du}{dx} \right|_{x=0} = \left. \frac{du}{dx} \right|_{x=1} = 0$.

As discretization of this problem, we discretize the interval $[0, 1]$ into $(n - 1)$ sub-intervals of the same width, and approximate the derivative by centered finite difference. Let the width of the sub-intervals be $h = \frac{1}{n - 1}$, and $x_i := (i - 1)h$ ($i = 1, \dots, n$). Let u_i be the approximation of $u(x_i)$, and $f_i := f(x_i)$. Further, let $\alpha_{\pm} := 1 \pm \frac{\beta h}{2}$. Hence, $\alpha_+ + \alpha_- = 2$.

3.5.1 Periodic boundary condition

If we approximate the boundary condition by $u_0 = u_n$, $u_{n+1} = u_1$, the system of linear equation $A\mathbf{u} = \mathbf{f}$ is given by

$$\frac{1}{h^2} \begin{bmatrix} -2 & \alpha_+ & & \alpha_- \\ \alpha_- & -2 & \alpha_+ & \\ & \ddots & \ddots & \ddots \\ \mathbf{0} & & \alpha_- & -2 & \alpha_+ \\ \alpha_+ & & & \alpha_- & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n \end{bmatrix}. \quad (27)$$

Here, the coefficient matrix A is a nonsymmetric $n \times n$ matrix, except for the case $\beta = 0$. Since, $\text{rank}A = n - 1$, A is singular. Hence, from the dimension theorem, $\dim(\mathcal{N}(A)) = 1$, and if we define $\mathbf{e} = (1, 1, \dots, 1)^T$, $A\mathbf{e} = \mathbf{0}$, and $\mathcal{N}(A) = \langle \mathbf{e} \rangle$.

On the other hand, let $A = (a_{ij})$. Then, we have

$$(A\mathbf{u}, \mathbf{e}) = \sum_{i=1}^n \sum_{j=1}^n a_{ij}u_j = \sum_{j=1}^n \left(\sum_{i=1}^n a_{ij} \right) u_j = 0 \quad \forall \mathbf{u} \in \mathbf{R}^n,$$

so that $\mathbf{e} \perp \mathcal{R}(A)$, or $\mathbf{e} \in \mathcal{R}(A)^\perp$. Further, since $\dim \mathcal{R}(A)^\perp = \dim \mathcal{N}(A) = 1$, we have $\mathcal{R}(A)^\perp = \mathcal{N}(A) = \langle \mathbf{e} \rangle$.

Since

$$M(A) := \frac{A + A^T}{2} = \frac{1}{h^2} \begin{bmatrix} -2 & 1 & & 1 \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ \mathbf{0} & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{bmatrix},$$

from Gerschgorin's theorem, the eigenvalues of $M(A)$ lie with in the closed interval $[-4, 0]$. Thus, $M(A)$ is negative semi-definite. Note also that $\text{rank} M(A) = \text{rank}A = n - 1$.

Hence, from Theorem 6, when one applies the GCR(k) method to the system of linear equations (27) arising from the case of periodic boundary condition, the method will converge to a least squares solution without breakdown for arbitrary initial approximate solution.

Since

$$\mathbf{f} \in \mathcal{R}(A) = (\mathcal{N}(A))^\perp \iff \mathbf{f} \perp \mathcal{N}(A) = \langle \mathbf{e} \rangle \iff (\mathbf{f}, \mathbf{e}) = \sum_{i=1}^n f_i = 0,$$

if $\sum_{i=1}^n f_i = 0$, we have $\mathbf{f} \in \mathcal{R}(A)$. In this case, from Theorem 12, the approximate solution will converge to the least squares solution $Q_1 A_{11}^{-1} Q_1^T \mathbf{f} + Q_2 Q_2^T \mathbf{x}_0$.

If further, $\mathbf{x}_0 \in \mathcal{R}(A)$, the approximate solution will converge to the pseudo-inverse solution (the least squares solution with minimum Euclidean norm) $Q_1 A_{11}^{-1} Q_1^T \mathbf{f}$.

3.5.2 Neumann boundary condition

In this case, if we approximate the boundary condition by $-u_1 + u_2 = 0$, $u_{n-1} - u_n = 0$, the system of linear equation $A\mathbf{u} = \mathbf{f}$ obtained by discretization is

$$\frac{1}{h^2} \begin{bmatrix} -1 & 1 & & & \mathbf{0} \\ \alpha_- & -2 & \alpha_+ & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_- & -2 & \alpha_+ \\ \mathbf{0} & & & 1 & -1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} 0 \\ f_2 \\ \vdots \\ f_{n-1} \\ 0 \end{bmatrix}.$$

In this case, A is a nonsymmetric $n \times n$ matrix except when $\beta = 0$. Since $\text{rank} A = n-1$, A is singular. Hence, $\dim(\mathcal{N}(A)) = 1$, and from $A\mathbf{e} = \mathbf{0}$, we have $\mathcal{N}(A) = \langle \mathbf{e} \rangle$.

On the other hand, if we let $\mathbf{y} = \left(1, \frac{1}{\alpha_-}, \frac{\alpha_+}{\alpha_-^2}, \dots, \frac{\alpha_+^{n-3}}{\alpha_-^{n-2}}, \frac{\alpha_+^{n-2}}{\alpha_-^{n-2}}\right)^T$, from $\mathbf{y}^T A = \mathbf{0}^T$, we have $\mathbf{y}^T A\mathbf{x} = (\mathbf{y}, A\mathbf{x}) = 0$ for all $\mathbf{x} \in \mathbf{R}^n$. Hence, $\mathbf{y} \in \mathcal{R}(A)^\perp$. By the way, from $\dim \mathcal{R}(A)^\perp = \dim \mathcal{N}(A) = 1$, we have $\mathcal{R}(A)^\perp = \langle \mathbf{y} \rangle$.

Hence, unless $\beta = 0$, we have $\mathcal{R}(A)^\perp \neq \langle \mathbf{e} \rangle = \mathcal{N}(A)$, that is, $\mathcal{R}(A)^\perp \neq \mathcal{N}(A)$.

However, $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$ holds. This is because $\mathcal{N}(A) = \langle \mathbf{e} \rangle$, $\mathcal{R}(A) = \langle \mathbf{y} \rangle^\perp$, so that $\mathcal{N}(A) \cap \mathcal{R}(A) = \{\mathbf{0}\} \iff \langle \mathbf{e} \rangle \subset \mathcal{R}(A)$ does not hold $\iff \mathbf{e} \perp \mathbf{y}$ does not hold $\iff (\mathbf{e}, \mathbf{y}) \neq 0$. This holds because, $\alpha_\pm = 1 \pm \frac{\beta h}{2} > 0$ gives

$$(\mathbf{e}, \mathbf{y}) = 1 + \frac{1}{\alpha_-} + \frac{\alpha_+}{\alpha_-^2} + \dots + \frac{\alpha_+^{n-3}}{\alpha_-^{n-2}} + \frac{\alpha_+^{n-2}}{\alpha_-^{n-2}} > 1.$$

Here, if we choose f_2, \dots, f_{n-1} such that $\mathbf{f} \perp \mathbf{y}$, which is equivalent to

$$(\mathbf{f}, \mathbf{y}) = \frac{1}{\alpha_-} f_2 + \frac{\alpha_+}{\alpha_-^2} f_3 + \dots + \frac{\alpha_+^{i-2}}{\alpha_-^{i-1}} f_i + \dots + \frac{\alpha_+^{n-3}}{\alpha_-^{n-2}} f_{n-1} = 0,$$

we have $\mathbf{f} \in \mathcal{R}(A)$.

However, it is difficult to show the definiteness of $M(A_{11})$, which is the necessary and sufficient condition for the GCR(k) method to converge to an exact solution without breakdown (condition (C2) of Theorem 7), for arbitrary n .

For the case $n = 3$,

$$A = \begin{bmatrix} -4 & 4 & 0 \\ 4 - \beta & -8 & 4 + \beta \\ 0 & 4 & -4 \end{bmatrix}.$$

From $\mathcal{R}(A) = \langle \mathbf{y} \rangle^\perp$, and $\mathbf{y} = (4 - \beta, 4, 4 + \beta)^T$, for instance, we may take $\mathbf{q}_1 = c_1(4, \beta - 4, 0)^T$, $\mathbf{q}_2 = c_2[(4 - \beta)(4 + \beta), 4(4 + \beta), -(4 - \beta)^2 - 16]^T$, where c_1 and c_2 are normalization constants. Hence, we obtain $A_{11} = Q_1^T A Q_1$ where $Q_1 = [\mathbf{q}_1, \mathbf{q}_2]$, and $M(A_{11}) = (m_{ij})$. Then, we can show that $m_{11} < 0$ and $\det M(A_{11}) > 0$, so that $M(A_{11})$ is negative definite.

4 Concluding remark

In this paper, we used the idea of decomposing the algorithm into the range space and its orthogonal complement in order to analyse the behaviour of the GCR(k) method on singular systems. This idea can also be applied to the analysis of other iterative methods on singular systems. In a forthcoming paper, we will apply it to the GMRES method.

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References

- [1] Abe, K., Ogata, H., Sugihara, M., Zhang, S-L., Mitsui, T.: Convergence theory of the CR method for linear singular systems. *Trans. Japan Soc. Ind. Appl. Math.* **9**, 1–13 (1999) (in Japanese)
- [2] Biro, O., Preis, K., Richter, K.R.: On the use of the magnetic vector potential in the nodal and edge finite element analysis of 3-D magnetostatic problems. *IEEE Trans. Magn.* **32**, 651–654 (1996)
- [3] Brown, P., Walker, H.F.: GMRES on (nearly) singular systems. *SIAM J. Matrix Anal. Appl.* **18**, 37–51 (1997)
- [4] Calvetti, D., Lewis, B., Reichel, L.: GMRES-type methods for inconsistent systems. *Linear Algebra Appl.* **316**, 157–169 (2000)
- [5] Dayar, T., Stewart, W.J.: Comparison of partitioning techniques for two-level iterative solvers on large, sparse Markov chains. *SIAM J. Sci. Comput.* **21**, 1691–1705 (2000)
- [6] Dax, A.: The convergence of linear stationary iterative processes for solving singular unstructured systems of linear equations. *SIAM Rev.* **32**, 611–635 (1990)
- [7] Eiermann, M., Marek, I., Niethammer, W.: On the solution of singular linear systems of algebraic equations by semiiterative methods. *Numer. Math.* **53**, 265–283 (1988)
- [8] Eisenstat, S.C., Elman, H.C., Schultz, M.H.: Variational iterative methods for non-symmetric systems of linear equations. *SIAM J. Numer. Anal.* **20**, 345–357 (1983)
- [9] Fletcher, R.: Conjugate gradient methods for indefinite systems. In: G. Watson (ed.), *Numerical Analysis Dundee 1975*, Lecture Notes in Mathematics, vol. 506, Springer-Verlag, Berlin, 1976, pp. 73–89
- [10] Fischer, B., Hanke, M., Hochbruch, M.: A note on conjugate-gradient type methods for indefinite and/or inconsistent linear systems. *Numer. Algorithms* **11**, 181–189 (1996)

- [11] Freund, R.W.: A transpose-free quasi-minimal residual algorithm for non-Hermitian linear systems. *SIAM J. Sci. Comput.* **14**, 425–448 (1993)
- [12] Freund, R.W., Hochbruck, M.: On the use of two QMR algorithms for solving singular systems and applications in Markov chain modeling. *Numer. Linear Algebra Appl.* **1**, 403–420 (1994)
- [13] Freund, R.W., Nachtigal, N.M.: QMR: a quasi-minimal residual method for non-Hermitian linear systems. *Numer. Math.* **60**, 315–339 (1991)
- [14] Hanke, M., Hochbruck, M.: A Chebyshev-like semiiteration for inconsistent linear systems. *Electr. Trans. Numer. Anal.* **1**, 89–103 (1993)
- [15] Hayami, K.: On the behaviour of the conjugate residual method for singular systems. In: Z.-C. Shi, H. Kawarada (eds.), *Proc. of Fifth China-Japan Seminar on Numerical Mathematics*, Shanghai, 2000, Science Press, Beijing/New York, 2002, pp. 117–126
- [16] Hayami, K.: On the convergence of the conjugate residual method for singular systems. *Trans. Japan Soc. Ind. Appl. Math.*, **13**, 1–33 (2003) (in Japanese)
- [17] Igarashi, H.: On the reconstruction of magnetic source in cylindrical permanent magnets. In: M. Tanaka, G.S. Dulikravich (eds.), *Inverse Problems in Engineering Mechanics II*, Elsevier, 2000, pp. 467–476
- [18] Ipsen, I.C.F., Meyer, C.D.: The idea behind Krylov methods. *Am. Math. Mon.*, **105**, 889–899 (1998)
- [19] Kaasschieter, E.F.: Preconditioned conjugate gradients for solving singular systems. *J. Comput. Appl. Math.* **24**, 265–275 (1988)
- [20] Kammerer, W.J., Nashed, M.Z.: On the convergence of the conjugate gradient method for singular linear operator equations. *SIAM J. Numer. Anal.* **9**, 165–181 (1972)
- [21] Mori, M., Sugihara, M., Murota, K.: *Linear Computation*. Iwanami-shoten, Tokyo, 1994 (in Japanese)
- [22] Ren, Z.: Influence of the R.H.S. on the convergence behaviour of the curl-curl equation. *IEEE Trans. Magn.* **32**, 655–658 (1996)
- [23] Saad, Y., Schultz, M.H.: GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM J. Sci. Stat. Comput.* **7**, 856–869 (1986)
- [24] Sidi, A.: A unified approach to Krylov subspace methods for the Drazin-inverse solution of singular nonsymmetric linear systems. *Linear Algebra Appl.* **298**, 99–113 (1999)
- [25] Sidi, A.: DGMRES: A GMRES-type algorithm for Drazin-inverse solution of singular nonsymmetric linear systems. *Linear Algebra Appl.* **335**, 189–204 (2001)

- [26] Sidi, A.: Orthogonal polynomials and semi-iterative methods for the Drazin-inverse solution of singular linear systems. *Numer. Math.* **93**, 563–581 (2003)
- [27] Sleijpen, G.L.G., van der Vorst, H.A.: A Jacobi-Davidson iteration method for linear eigenvalue problems. *SIAM J. Matrix Anal. Appl.* **17**, 401–425 (1996)
- [28] Smoch, L.: Some results about GMRES in the singular case. *Numer. Algorithms* **22**, 193–212 (1999)
- [29] Sonneveld, P.: CGS: a fast Lanczos-type solver for nonsymmetric linear systems. *SIAM J. Sci. Stat. Comput.* **10**, 36–52 (1989)
- [30] Strouboulis, T., Babuška, I., Copps, K.: The design and analysis of the generalized finite element method. *Comput. Methods Appl. Mech. Eng.* **181**, 43–69 (2000)
- [31] Tanabe, K.: Characterization of linear stationary processes for solving singular system of linear equations. *Numer. Math.* **22**, 349–359 (1974)
- [32] Tanabe, K.: The conjugate gradient method for computing all the extremal stationary probability vectors of a stochastic matrix. *Ann. Inst. Stat. Math.* **37** Part B, 173–187 (1985)
- [33] van der Vorst, H.A.: Bi-CGSTAB: A more smoothly converging variant of CG-S for the solution of nonsymmetric linear systems. *SIAM J. Sci. Statist. Comput.* **13**, 631–644 (1992)
- [34] Vinsome, P.K.W.: Orthomin, an iterative method for solving sparse sets of simultaneous linear equations. In: *Proc. Fourth Symp. on Reservoir Simulation, Soc. of Petroleum Engineers of AIME*, 1976, pp. 149–159
- [35] Washio, T., Doi, S.: A solution of Neumann problem on curvilinear coordinate systems. In: *Matrix Analysis and Parallel Computing, Proc. of PCG'94*, March, 1994, Keio Univ., pp. 75–87
- [36] Wei, Y., Wu, H.: Convergence properties of Krylov subspace methods for singular linear systems with arbitrary index. *J. Comput. Appl. Math.* **114**, 305–318 (2000)
- [37] Zhang, S.-L., Oyanagi, Y., Sugihara, M.: Necessary and sufficient conditions for the convergence of Orthomin(k) on inconsistent linear systems. *Numer. Math.* **87**, 391–405 (2000)