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A Geometric View of Krylov Subspace Methods on Singular Systems

Ken Hayami[*†] and Masaaki Sugihara[‡]

Abstract

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

Brown and Walker [3] gave some conditions concerning $\mathcal{R}(A)$ and $\mathcal{N}(A)$ for the Generalized Minimal Residual (GMRES) method to converge to a least squares solution without breakdown for singular systems.

In this paper, we provide a geometrical view of Krylov subspace methods applied to singular systems by decomposing the algorithm into components of $\mathcal{R}(A)$ and its orthogonal complement $\mathcal{R}(A)^\perp$. Taking coordinates along $\mathcal{R}(A)$ and $\mathcal{R}(A)^\perp$ will provide an interpretation of the conditions given in [3], at the same time giving new proofs for the conditions.

We will apply the approach to the GMRES and GMRES(k) methods as well as the Generalized Conjugate Residual (GCR(k)) method, deriving conditions for convergence for inconsistent and consistent singular systems, for each method.

Finally, we give examples arising in the finite difference discretization of two-point boundary value problems of an ordinary differential equation as an illustration of the convergence conditions.

Key words: Krylov subspace method – GMRES method – GCR(k) method – singular systems – least squares problems – geometric interpretation – decomposition of algorithms

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

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1 Introduction

Consider the system of linear equation

$$A\boldsymbol{x} = \boldsymbol{b}, \tag{1.1}$$

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

When A is nonsymmetric, there are Krylov subspace type iterative solvers for (1.1) based on biorthogonality, such as the Bi-CG method [12] and its modified versions such as the CGS [34], Bi-CGSTAB [38], QMR [16] and TFQMR [14] methods. There are also methods based on minimizing the residual $\boldsymbol{r} = \boldsymbol{b} - A\boldsymbol{x}$, such as the Generalized Minimum Residual (GMRES) method [28] and the Generalized Conjugate Residual (GCR) method [10]. When the coefficient matrix A is nonsingular, the behaviour of these methods is fairly well understood [10, 28].

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, 26, 20]. Such systems also arise when using redundant interpolation functions in the finite element method [35]. The computation of stationary probability vectors of stochastic matrices in the analysis of Markov chains also gives rise to singular systems [37, 15, 5].

For such singular systems, the system (1.1) does not always have solutions, so it is generally more appropriate to consider the least squares problem $\min_{\boldsymbol{x}\in\mathbf{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|_2$.

The analysis of linear stationary iterative methods on singular systems can be found, for instance, in [36, 6]. Work on semi-iterative methods for such systems was done in [9, 17, 32].

As for the analysis of Krylov subspace methods for singular systems, there are the works of [23, 37, 22, 13] for the conjugate gradient (CG) method, [15, 42] for methods based on biorthogonality such as the QMR and TFQMR. For residual minimization type methods, we refer to [1, 18, 19] for the conjugate residual (CR) method, [43] for the Orthomin(k) method, [30, 31] for GCR and [3, 33, 21, 4, 31, 29] for GMRES.

When the system is singular, CG and methods based on biorthogonality may diverge [43], and one has to modify the system in order to guarantee convergence[22, 41]. On the other hand, for methods based on minimizing the residual, by principle, the residual is expected to decrease monotonically without such modifications [1, 43].

Brown and Walker [3] gave some conditions concerning $\mathcal{R}(A)$ and $\mathcal{N}(A)$ for GMRES to converge without breakdown to the least squares solutions for singular systems.

In this paper, we provide a geometrical view of Krylov subspace methods applied to singular systems by decomposing the algorithm into the $\mathcal{R}(A)$ component and the $\mathcal{R}(A)^\perp$ component. This will clarify the meaning of the convergence conditions given in Brown and Walker[3] and also give different proofs of the convergence theorems based on this interpretation.

We will apply the approach to the GMRES and GMRES(k) methods as well as the Generalized Conjugate Residual (GCR(k)) method.

The rest of the paper is organized as follows: In Section 2, we analyse the convergence of GMRES and GMRES(k) on singular systems, by introducing an orthonormal basis for decomposing vector variables into the $\mathcal{R}(A)$ component and the $\mathcal{R}(A)^{\perp}$ component. In Section 3, we analyse GCR(k) on singular systems using the same framework. Finally, in Section 4, we give examples coming from the discretization of two-point boundary value problems of an ordinary differential equation to illustrate the convergence conditions.

In this paper, exact arithmetic (i.e., no rounding errors) will be assumed.

The following notations will be used.

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

$V^{\perp}$: 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 $\boldsymbol{v} \in \mathbf{R}^n$ such that $X\boldsymbol{v} = \mathbf{0}$,

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

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

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

2 Convergence analysis of GMRES on singular systems

2.1 GMRES

Consider the least squares problem

$$\min_{\boldsymbol{x}\in\mathbf{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|_2 \tag{2.1}$$

where $A \in \mathbf{R}^{n\times n}$ may be singular and $\boldsymbol{b} \in \mathbf{R}^n$.

We first consider applying the following GMRES [28] to this system.

GMRES

Choose $\boldsymbol{x}_0$.
$\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$
$\boldsymbol{v}_1 = \boldsymbol{r}_0/||\boldsymbol{r}_0||_2$
For $j = 1, 2, \cdots$ until satisfied do
  $h_{i,j} = (\boldsymbol{v}_i, A\boldsymbol{v}_j) \quad (i = 1, 2, \cdots, j)$
  $\hat{\boldsymbol{v}}_{j+1} = A\boldsymbol{v}_j - \sum_{i=1}^{j} h_{i,j}\boldsymbol{v}_i$
  $h_{j+1,j} = ||\hat{\boldsymbol{v}}_{j+1}||_2$. If $h_{j+1,j} = 0$, goto $*$.
  $\boldsymbol{v}_{j+1} = \hat{\boldsymbol{v}}_{j+1}/h_{j+1,j}$
End do

$* \, k := j$
Form the approximate solution
$\boldsymbol{x}_k = \boldsymbol{x}_0 + [\boldsymbol{v}_1, \cdots, \boldsymbol{v}_k]\boldsymbol{y}_k$
where $\boldsymbol{y} = \boldsymbol{y}_k$ minimizes $||\boldsymbol{r}_k||_2 = ||\beta \boldsymbol{e}_1 - \overline{H}_k \boldsymbol{y}||_2$.

Here, $\overline{H}_k = [h_{i,j}] \in \mathbf{R}^{(k+1)\times k}$, $\beta = ||\boldsymbol{r}_0||_2$ and $\boldsymbol{e}_1 = [1, 0, \cdots, 0]^{\mathrm{T}}$. The method minimizes the residual norm $\|\boldsymbol{r}_k\|_2$, over the search space $\boldsymbol{x}_k = \boldsymbol{x}_0 + \langle \boldsymbol{v}_1, \cdots, \boldsymbol{v}_k \rangle$, where $\langle \boldsymbol{v}_1, \cdots, \boldsymbol{v}_k \rangle = \langle \boldsymbol{r}_0, A\boldsymbol{r}_0, \cdots, A^{k-1}\boldsymbol{r}_0 \rangle$, and $(\boldsymbol{v}_i, \boldsymbol{v}_j) = 0 \quad (i \neq j)$. The GMRES is said to break down when $h_{j+1,j} = 0$.

When A is nonsingular, the iterates of GMRES converges to the solution for all $\boldsymbol{b}, \boldsymbol{x}_0 \in \mathbf{R}^n$ within at most n steps in exact arithmetic [28].

For the general case when A may be singular, Brown and Walker showed the following [3].

Theorem 2.1 *GMRES determines a least-squares solution of (1.1) without breakdown for all* $\boldsymbol{b}$ *and* $\boldsymbol{x}_0$ *if and only if* $\mathcal{N}(A) = \mathcal{N}(A^T)$.

Theorem 2.2 *Suppose (1.1) is consistent (i.e.,* $\boldsymbol{b} \in \mathcal{R}(A)$*). If* $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$*, then GMRES determines a solution without breakdown.*

2.2 A geometrical framework

In this section we will begin by giving geometric interpretations to the conditions $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$ and $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$. This is done by decomposing the space $\mathbf{R}^n$ into $\mathcal{R}(A)$ and $\mathcal{R}(A)^{\perp}$.

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

$$\boldsymbol{q}_1, \dots, \boldsymbol{q}_r : \text{orthonormal basis of } \mathcal{R}(A), \tag{2.2}$$

$$\boldsymbol{q}_{r+1}, \dots, \boldsymbol{q}_n : \text{orthonormal basis of } \mathcal{R}(A)^{\perp}, \tag{2.3}$$

$$Q_1 := [\,\boldsymbol{q}_1, \dots, \boldsymbol{q}_r] \in \mathbf{R}^{n\times r}, \tag{2.4}$$

$$Q_2 := [\,\boldsymbol{q}_{r+1}, \dots, \boldsymbol{q}_n] \in \mathbf{R}^{n\times(n-r)}, \tag{2.5}$$

so that,

$$Q := [\,Q_1, Q_2] \in \mathbf{R}^{n\times n} \tag{2.6}$$

is an orthogonal matrix satisfying

$$Q^{\mathrm{T}}Q = QQ^{\mathrm{T}} = \mathrm{I}_n, \tag{2.7}$$

where I_n is the identity matrix of order n.

Orthogonal transformation of the coefficient matrix A using Q gives

$$\tilde{A} := Q^{\mathrm{T}}AQ = \begin{bmatrix} {Q_1}^{\mathrm{T}}AQ_1 & {Q_1}^{\mathrm{T}}AQ_2 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ 0 & 0 \end{bmatrix}, \tag{2.8}$$

since ${Q_2}^{\mathrm{T}}AQ = 0$. Here, $A_{11} := {Q_1}^{\mathrm{T}}AQ_1$ and $A_{12} := {Q_1}^{\mathrm{T}}AQ_2$.

In the following, we clarify some properties concerning the sub-matrices A_{11} and A_{12} in (2.8).

Theorem 2.3 A_{11} : *nonsingular* $\iff \mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$.

Proof.
$\mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$
$\Updownarrow$
$\mathcal{R}(\tilde{A}) \cap \mathcal{N}(\tilde{A}) = \{\mathbf{0}\}$
$\Updownarrow$

$$\mathcal{R}\left(\left[\begin{array}{cc} A_{11} & A_{12} \\ 0 & 0 \end{array}\right]\right) \cap \mathcal{N}\left(\left[\begin{array}{cc} A_{11} & A_{12} \\ 0 & 0 \end{array}\right]\right) = \left\{ \left(\begin{array}{c} \boldsymbol{x}_1 \\ \mathbf{0} \end{array} \right) \middle| \boldsymbol{x}_1 \in \mathcal{N}(A_{11}) \right\} = \{\mathbf{0}\}$$

$\Updownarrow$
A_{11} : nonsingular. $\square$

Lemma 2.4 $A_{12} = 0 \Longrightarrow A_{11}$: *nonsingular*

Proof.
Since $\mathrm{rank}\tilde{A} = \mathrm{rank}\left[\begin{array}{cc} A_{11} & 0 \\ 0 & 0 \end{array}\right] = \mathrm{rank}A = r$ and $A_{11} \in \mathbf{R}^{r\times r}$, A_{11} is nonsingular. $\square$

Theorem 2.5 $A_{12} = 0 \iff \mathcal{R}(A) = \mathcal{R}(A^T) \iff \mathcal{N}(A) = \mathcal{N}(A^T)$.

Proof.
The first equivalence is shown as follows.
$\mathcal{R}(A) = \mathcal{R}(A^{\mathrm{T}})$
$\Updownarrow$
$\mathcal{R}(\tilde{A}) = \mathcal{R}(\tilde{A}^{\mathrm{T}})$
$\Updownarrow$
$\mathcal{R}\left(\left[\begin{array}{cc} A_{11} & A_{12} \\ 0 & 0 \end{array}\right]\right) = \mathcal{R}\left(\left[\begin{array}{cc} {A_{11}}^{\mathrm{T}} & 0 \\ {A_{12}}^{\mathrm{T}} & 0 \end{array}\right]\right)$
$\Updownarrow$
$A_{12} = 0$, where Lemma 2.4 was used for the last equivalence.

The second equivalence of the theorem follows immediately from the well-known relation $\mathcal{R}(A)^{\perp} = \mathcal{N}(A^{\mathrm{T}})$. $\square$

Examples of matrices A for which $A_{12} = 0$ hold are nonsingular, normal and symmetric matrices, respectively.

Now we will consider decomposing iterative algorithms into the $\mathcal{R}(A)$ and $\mathcal{R}(A)^{\perp}$ components as in [1]. In order to do so, we will use the transformation

$$\tilde{\boldsymbol{v}} := Q^{\mathrm{T}}\boldsymbol{v} = [Q_1, Q_2]^{\mathrm{T}}\boldsymbol{v} = \left[\begin{array}{c} {Q_1}^{\mathrm{T}}\boldsymbol{v} \\ {Q_2}^{\mathrm{T}}\boldsymbol{v} \end{array}\right] = \left[\begin{array}{c} \boldsymbol{v}^1 \\ \boldsymbol{v}^2 \end{array}\right],$$

$$\boldsymbol{v} = Q\tilde{\boldsymbol{v}} = [Q_1, Q_2]\left[\begin{array}{c} \boldsymbol{v}^1 \\ \boldsymbol{v}^2 \end{array}\right] = Q_1\boldsymbol{v}^1 + Q_2\boldsymbol{v}^2,$$

cf. (2.2)-(2.7), to decompose a vector variable $\boldsymbol{v}$ in the algorithm. Here, $\boldsymbol{v}^1$ corresponds to the $\mathcal{R}(A)$ component $Q_1\boldsymbol{v}^1$ of $\boldsymbol{v}$, and $\boldsymbol{v}^2$ corresponds to the $\mathcal{R}(A)^\perp$ component $Q_2\boldsymbol{v}^2$ of $\boldsymbol{v}$.

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

$$\tilde{\boldsymbol{r}} := Q^{\mathrm{T}}\boldsymbol{r} = Q^{\mathrm{T}}\boldsymbol{b} - Q^{\mathrm{T}}AQ(Q^{\mathrm{T}}\boldsymbol{x}),$$

or

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

i.e.,

$$\begin{aligned} \boldsymbol{r}^1 &= \boldsymbol{b}^1 - A_{11}\boldsymbol{x}^1 - A_{12}\boldsymbol{x}^2 \\ \boldsymbol{r}^2 &= \boldsymbol{b}^2. \end{aligned} \tag{2.9}$$

Hence, in the least squares problem (2.1), we have

$$\|\boldsymbol{b} - A\boldsymbol{x}\|_2{}^2 = \|\boldsymbol{r}\|_2{}^2 = ||\tilde{\boldsymbol{r}}||_2{}^2 = \|\boldsymbol{r}^1\|_2{}^2 + \|\boldsymbol{b}^2\|_2{}^2. \tag{2.10}$$

2.3 Decomposition of GMRES

Based on the above geometric framework, we will analyze GMRES for the case when A is singular, by decomposing it into the $\mathcal{R}(A)$ component and the $\mathcal{R}(A)^\perp$ component as follows.

Decomposed GMRES (general case)

$\mathcal{R}(A)$ component	$\mathcal{R}(A)^\perp$ component
$\boldsymbol{b}^1 = Q_1{}^{\mathrm{T}}\boldsymbol{b}$	$\boldsymbol{b}^2 = Q_2{}^{\mathrm{T}}\boldsymbol{b}$
Choose $\boldsymbol{x}_0$	
$\boldsymbol{x}_0^1 = Q_1{}^{\mathrm{T}}\boldsymbol{x}_0$	$\boldsymbol{x}_0^2 = Q_2{}^{\mathrm{T}}\boldsymbol{x}_0$
$\boldsymbol{r}_0^1 = \boldsymbol{b}^1 - A_{11}\boldsymbol{x}_0^1 - A_{12}\boldsymbol{x}_0^2$ $\|\|\boldsymbol{r}_0\|\|_2 = \sqrt{\|\|\boldsymbol{r}_0^1\|\|_2{}^2 + \|\|\boldsymbol{b}^2\|\|_2{}^2}$	$\boldsymbol{r}_0^2 = \boldsymbol{b}^2$
$\boldsymbol{v}_1^1 = \boldsymbol{r}_0^1/\|\|\boldsymbol{r}_0\|\|_2$	$\boldsymbol{v}_1^2 = \boldsymbol{b}^2/\|\|\boldsymbol{r}_0\|\|_2$

For $j = 1, 2, \cdots$ until satisfied do

$$h_{i,j} = (\boldsymbol{v}_i^1, A_{11}\boldsymbol{v}_j^1 + A_{12}\boldsymbol{v}_j^2) \quad (i = 1, 2, \cdots, j)$$

$$\hat{\boldsymbol{v}}_{j+1}^1 = A_{11}\boldsymbol{v}_j^1 + A_{12}\boldsymbol{v}_j^2 - \sum_{i=1}^{j} h_{i,j}\boldsymbol{v}_i^1 \qquad \hat{\boldsymbol{v}}_{j+1}^2 = -\sum_{i=1}^{j} h_{i,j}\boldsymbol{v}_i^2$$

$$h_{j+1,j} = \sqrt{||\hat{\boldsymbol{v}}_{j+1}^1||_2{}^2 + ||\hat{\boldsymbol{v}}_{j+1}^2||_2{}^2}. \quad \text{If } h_{j+1,j} = 0, \text{ goto } * .$$

$$\boldsymbol{v}^1_{j+1} = \hat{\boldsymbol{v}}^1_{j+1}/h_{j+1,j} \qquad \boldsymbol{v}^2_{j+1} = \hat{\boldsymbol{v}}^2_{j+1}/h_{j+1,j}$$

End do

$* \, k := j$

Form the approximate solution

$$\boldsymbol{x}^1_k = \boldsymbol{x}^1_0 + [\boldsymbol{v}^1_1, \cdots, \boldsymbol{v}^1_k] \, \boldsymbol{y}_k \qquad \boldsymbol{x}^2_k = \boldsymbol{x}^2_0 + [\boldsymbol{v}^2_1, \cdots, \boldsymbol{v}^2_k] \, \boldsymbol{y}_k$$

where $\boldsymbol{y} = \boldsymbol{y}_k$ minimizes $||\boldsymbol{r}_k||_2 = ||\beta \boldsymbol{e}_1 - \overline{H}_k \boldsymbol{y}||_2$.

In Theorem 2.5 we gave a geometric interpretation: $A_{12} = 0$ to Brown and Walker's condition: $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$. Now it is important to notice that if $A_{12} = 0$ holds, the decomposed GMRES further simplifies as follows.

Decomposed GMRES (Case $\mathcal{N}(A) = \mathcal{N}(A^{\mathbf{T}})$)

$\mathcal{R}(A)$ component | $\mathcal{R}(A)^{\perp}$ component

$$\boldsymbol{b}^1 = {Q_1}^{\mathrm{T}} \boldsymbol{b} \qquad \boldsymbol{b}^2 = {Q_2}^{\mathrm{T}} \boldsymbol{b}$$

Choose $\boldsymbol{x}_0$

$$\boldsymbol{x}^1_0 = {Q_1}^{\mathrm{T}} \boldsymbol{x}_0 \qquad \boldsymbol{x}^2_0 = {Q_2}^{\mathrm{T}} \boldsymbol{x}_0$$

$$\boldsymbol{r}^1_0 = \boldsymbol{b}^1 - A_{11} \boldsymbol{x}^1_0 \qquad \boldsymbol{r}^2_0 = \boldsymbol{b}^2$$

$$||\boldsymbol{r}_0||_2 = \sqrt{{||\boldsymbol{r}^1_0||_2}^2 + {||\boldsymbol{b}^2||_2}^2}$$

$$\boldsymbol{v}^1_1 = \boldsymbol{r}^1_0 / ||\boldsymbol{r}_0||_2 \qquad \boldsymbol{v}^2_1 = \boldsymbol{b}^2 / ||\boldsymbol{r}_0||_2$$

For $j = 1, 2, \cdots$ until satisfied do

$$h_{i,j} = (\boldsymbol{v}^1_i, A_{11} \boldsymbol{v}^1_j) \quad (i = 1, 2, \cdots, j)$$

$$\hat{\boldsymbol{v}}^1_{j+1} = A_{11} \boldsymbol{v}^1_j - \sum_{i=1}^{j} h_{i,j} \boldsymbol{v}^1_i \qquad \hat{\boldsymbol{v}}^2_{j+1} = - \sum_{i=1}^{j} h_{i,j} \boldsymbol{v}^2_i$$

$$h_{j+1,j} = \sqrt{{||\hat{\boldsymbol{v}}^1_{j+1}||_2}^2 + {||\hat{\boldsymbol{v}}^2_{j+1}||_2}^2}. \quad \text{If } h_{j+1,j} = 0, \text{ goto } * .$$

$$\boldsymbol{v}^1_{j+1} = \hat{\boldsymbol{v}}^1_{j+1}/h_{j+1,j} \qquad \boldsymbol{v}^2_{j+1} = \hat{\boldsymbol{v}}^2_{j+1}/h_{j+1,j}$$

End do

$* \, k := j$

Form the approximate solution

$$\boldsymbol{x}_k^1 = \boldsymbol{x}_0^1 + [\boldsymbol{v}_1^1, \cdots, \boldsymbol{v}_k^1]\,\boldsymbol{y}_k \qquad \boldsymbol{x}_k^2 = \boldsymbol{x}_0^2 + [\boldsymbol{v}_1^2, \cdots, \boldsymbol{v}_k^2]\,\boldsymbol{y}_k$$

where $\boldsymbol{y} = \boldsymbol{y}_k$ minimizes $||\boldsymbol{r}_k||_2 = ||\beta \boldsymbol{e}_1 - \overline{H}_k \boldsymbol{y}||_2$.

Note here that the $\mathcal{R}(A)$ component of GMRES is essentially equivalent to GMRES applied to $A_{11}\boldsymbol{x}^1 = \boldsymbol{b}^1$, except for the scaling factors for $\boldsymbol{v}_j^1$. Note also that, from Lemma 2.4, $A_{12} = 0$ implies that A_{11} is nonsingular. Hence, arguments similar to [28] for GMRES on nonsingular systems imply that GMRES gives a least-squares solution for all $\boldsymbol{b}$ and $\boldsymbol{x}_0$.

2.4 Convergence theorem for arbitrary $\boldsymbol{b}$

Thus, for the general case where $\boldsymbol{b} \in \mathcal{R}(A)$ does not necessarily hold, we have the following.

Theorem 2.6
GMRES determines a least-squares solution of (2.1) for all $\boldsymbol{b}, \boldsymbol{x}_0 \in \mathbf{R}^n$ *if and only if* $A_{12} = 0$.

Proof. The sufficiency of the condition was shown above. The necessity follows since if we assume that $A_{12} \neq 0$, then there exists a $\boldsymbol{b}$ such that the algorithm breaks down at step $j = 1$ without giving a least squares solution. The details are given below.

Assume $A_{12} \neq 0$. Then there exist $\boldsymbol{s}^1 \neq \boldsymbol{0}$ such that $A_{11}\boldsymbol{s}^1 + A_{12}\boldsymbol{s}^2 = \boldsymbol{0}$ where $\boldsymbol{s}^1 \in \mathbf{R}^r$ and $\boldsymbol{s}^2 \in \mathbf{R}^{n-r}$.

This can be shown as follows.

If A_{11} is singular, there exist $\boldsymbol{s}^1 \neq \boldsymbol{0}$ such that $A_{11}\boldsymbol{s}^1 = \boldsymbol{0}$, so let $\boldsymbol{s}^2 = \boldsymbol{0}$.

If A_{11} is nonsingular, consider the following. Since $A_{12} \neq 0$, there exists $(A_{12})_{i,j} \neq 0$, so that $A_{12}\boldsymbol{e}_j \neq \boldsymbol{0}$, where $\boldsymbol{e}_j \in \mathbf{R}^{n-r}$ is the j-th unit vector. Let $\boldsymbol{s}^2 = \boldsymbol{e}_j \neq \boldsymbol{0}$, so that $A_{12}\boldsymbol{s}^2 \neq \boldsymbol{0}$. Then let $\boldsymbol{s}^1 = -{A_{11}}^{-1}A_{12}\boldsymbol{s}^2 \neq \boldsymbol{0}$. Thus we have $A_{11}\boldsymbol{s}^1 + A_{12}\boldsymbol{s}^2 = \boldsymbol{0}$, where $\boldsymbol{s}^1 \neq \boldsymbol{0}$.

Thus, let $\boldsymbol{b}^1 = \boldsymbol{s}^1 + A_{11}\boldsymbol{x}_0^1 + A_{12}\boldsymbol{x}_0^2$ and $\boldsymbol{b}^2 = \boldsymbol{s}^2$ in the decomposed GMRES (general case). Then, $\boldsymbol{r}_0^1 = \boldsymbol{s}^1 \neq \boldsymbol{0}, \boldsymbol{r}_0^2 = \boldsymbol{s}^2$, and $\boldsymbol{v}_1^1 = \boldsymbol{s}^1/\|\boldsymbol{s}\|_2, \boldsymbol{v}_1^2 = \boldsymbol{s}^2/\|\boldsymbol{s}\|_2$, where $\|\boldsymbol{s}\|_2 = \sqrt{{\|\boldsymbol{s}^1\|_2}^2 + {\|\boldsymbol{s}^2\|_2}^2}$, and we have $A_{11}\boldsymbol{v}_1^1 + A_{12}\boldsymbol{v}_1^2 = \boldsymbol{0}$.

Hence, at step $j = 1$, $h_{1,1} = (\boldsymbol{v}_1^1, A_{11}\boldsymbol{v}_1^1 + A_{12}\boldsymbol{v}_1^2) = 0, \hat{\boldsymbol{v}}_2^1 = \boldsymbol{0}, \hat{\boldsymbol{v}}_2^2 = \boldsymbol{0}, h_{2,1} = \sqrt{{\|\hat{\boldsymbol{v}}_2^1\|_2}^2 + {\|\hat{\boldsymbol{v}}_2^2\|_2}^2} = 0$, so that the algorithm terminates.

However, for $k = 1$, $\boldsymbol{x}_1^1 = \boldsymbol{x}_0^1 + y_1\boldsymbol{v}_1^1 = \boldsymbol{x}_0^1 + \frac{y_1}{\|\boldsymbol{s}\|_2}\boldsymbol{s}^1$, $\boldsymbol{x}_1^2 = \boldsymbol{x}_0^2 + y_1\boldsymbol{v}_1^2 = \boldsymbol{x}_0^1 + \frac{y_1}{\|\boldsymbol{s}\|_2}\boldsymbol{s}^2$. Thus, (2.9) gives $\boldsymbol{r}_1^1 = \boldsymbol{b}^1 - A_{11}\boldsymbol{x}_1^1 - A_{12}\boldsymbol{x}_1^2 = \boldsymbol{b}^1 - A_{11}\boldsymbol{x}_0^1 - A_{12}\boldsymbol{x}_0^2 - \frac{y_1}{\|\boldsymbol{s}\|_2}(A_{11}\boldsymbol{s}^1 + A_{12}\boldsymbol{s}^2) = \boldsymbol{r}_0^1 = \boldsymbol{s}^1 \neq \boldsymbol{0}$. Hence, ${Q_1}^{\mathrm{T}}\boldsymbol{r}_1 = \boldsymbol{r}_1^1 \neq \boldsymbol{0}$, so that $A^{\mathrm{T}}\boldsymbol{r}_1 \neq \boldsymbol{0}$, which means that $\boldsymbol{x}_1$ is not a least squares solution. $\square$

Figure 2.4 summarizes the above arguments. Especially, it is interesting to note that convergence without breakdown is equivalent to simple decomposition of the algorithm.

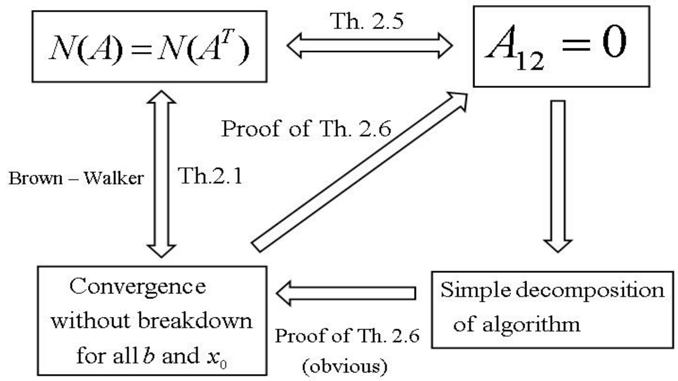

Figure 1: The relation between convergence without breakdown and simple decomposition of the algorithm.

Concerning where the approximate solution $\boldsymbol{x}_i$ converges, we have the following.

Theorem 2.7 *If $\mathcal{N}(A) = \mathcal{N}(A^T)$, the following hold for GMRES.*

The $\mathcal{R}(A)$ component of $\boldsymbol{x}_i$: $\boldsymbol{x}_i^1$ converges to ${A_{11}}^{-1}\boldsymbol{b}^1$.

Moreover, if $\boldsymbol{b} \in \mathcal{R}(A)$ (i.e., if $\boldsymbol{b}^2 = \boldsymbol{0}$), then the $\mathcal{R}(A)^\perp$ component of $\boldsymbol{x}_i$: $\boldsymbol{x}_i^2 \equiv \boldsymbol{x}_0^2$, so that $\boldsymbol{x}_i$ converges to $Q_1 {A_{11}}^{-1} {Q_1}^T \boldsymbol{b} + Q_2 {Q_2}^T \boldsymbol{x}_0$.

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

Remark In the general case when $\boldsymbol{b} \notin \mathcal{R}(A)$, we cannot say anything about where the $\mathcal{R}(A)^\perp$ component of $\boldsymbol{x}_i$ converges to.

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

In the consistent case $\boldsymbol{b} \in \mathcal{R}(A)$, we have $\boldsymbol{b}^2 = {Q_2}^{\mathrm{T}} \boldsymbol{b} = \boldsymbol{0}$. Hence, the decomposed GMRES simplifies as follows.

Decomposed GMRES (Case $\boldsymbol{b} \in \mathcal{R}(A)$)

$\mathcal{R}(A)$ component	$\mathcal{R}(A)^\perp$ component
$\boldsymbol{b}^1 = {Q_1}^{\mathrm{T}} \boldsymbol{b}$	$\boldsymbol{b}^2 = \boldsymbol{0}$
Choose $\boldsymbol{x}_0$	
$\boldsymbol{x}_0^1 = {Q_1}^{\mathrm{T}} \boldsymbol{x}_0$	$\boldsymbol{x}_0^2 = {Q_2}^{\mathrm{T}} \boldsymbol{x}_0$
$\boldsymbol{r}_0^1 = \boldsymbol{b}^1 - A_{11}\boldsymbol{x}_0^1 - A_{12}\boldsymbol{x}_0^2$	$\boldsymbol{r}_0^2 = \boldsymbol{0}$
$\lvert\lvert \boldsymbol{r}_0 \rvert\rvert_2 = \lvert\lvert \boldsymbol{r}_0^1 \rvert\rvert_2$	

$\boldsymbol{v}_1^1 = \boldsymbol{r}_0^1/||\boldsymbol{r}_0||_2 \qquad \boldsymbol{v}_1^2 = \boldsymbol{0}$

For $j = 1, 2, \cdots$ until satisfied do

$$h_{i,j} = (\boldsymbol{v}_i^1, A_{11}\boldsymbol{v}_j^1) \quad (i = 1, 2, \cdots, j)$$

$$\hat{\boldsymbol{v}}_{j+1}^1 = A_{11}\boldsymbol{v}_j^1 - \sum_{i=1}^{j} h_{i,j}\boldsymbol{v}_i^1 \qquad \hat{\boldsymbol{v}}_{j+1}^2 = \boldsymbol{0}$$

$h_{j+1,j} = ||\hat{\boldsymbol{v}}_{j+1}^1||_2$. If $h_{j+1,j} = 0$, goto $*$.

$$\boldsymbol{v}_{j+1}^1 = \hat{\boldsymbol{v}}_{j+1}^1/h_{j+1,j} \qquad \boldsymbol{v}_{j+1}^2 = \boldsymbol{0}$$

End do

$* \, k := j$

Form the approximate solution

$$\boldsymbol{x}_k^1 = \boldsymbol{x}_0^1 + [\boldsymbol{v}_1^1, \cdots, \boldsymbol{v}_k^1]\,\boldsymbol{y}_k \qquad \boldsymbol{x}_k^2 = \boldsymbol{x}_0^2$$

where $\boldsymbol{y} = \boldsymbol{y}_k$ minimizes $||\boldsymbol{r}_k||_2 = ||\beta\boldsymbol{e}_1 - \overline{H}_k\boldsymbol{y}||_2$.

Note that in the above, the $\mathcal{R}(A)$ component of the GMRES is equivalent to GMRES applied to $A_{11}\boldsymbol{x}^1 = \boldsymbol{b}^1$. Thus, we have the following.

Theorem 2.8
GMRES determines a solution for all $\boldsymbol{b} \in \mathcal{R}(A), \boldsymbol{x}_0 \in \mathbf{R}^n$ if and only if $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\boldsymbol{0}\}$.

Proof. The sufficiency is shown as follows. Assume $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\boldsymbol{0}\}$. From Theorem 2.3, $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\boldsymbol{0}\} \Leftrightarrow A_{11}$: nonsingular. Hence, arguments in [28] for nonsingular systems imply that GMRES gives a solution for arbitrary $\boldsymbol{b} \in \mathcal{R}(A)$ and $\boldsymbol{x}_0$.

Next we show the necessity. Assume $\mathcal{R}(A) \cap \mathcal{N}(A) \neq \{\boldsymbol{0}\}$, i.e., A_{11} : singular. Hence, there exists $\boldsymbol{s}^1 \neq \boldsymbol{0}$ such that $A_{11}\boldsymbol{s}^1 = \boldsymbol{0}$. Thus, let $\boldsymbol{b}^1 = \boldsymbol{s}^1 + A_{11}\boldsymbol{x}_0^1 + A_{12}\boldsymbol{x}_0^2$. Then, in the above decomposed GMRES for the case $\boldsymbol{b} \in \mathcal{R}(A)$, $\boldsymbol{r}_0^1 := \boldsymbol{s}^1$, $\quad \boldsymbol{v}_1^1 = \boldsymbol{s}^1/||\boldsymbol{s}^1||_2 \neq \boldsymbol{0}$.

In step $j = 1$, since $A_{11}\boldsymbol{s}_1^1 = \boldsymbol{0}, h_{1,1} = (\boldsymbol{v}_1^1, A_{11}\boldsymbol{v}_1^1) = 0, \hat{\boldsymbol{v}}_2^1 = A_{11}\boldsymbol{v}_1^1 - h_{1,1}\boldsymbol{v}_1^1 = \boldsymbol{0}$ and $h_{2,1} = ||\hat{\boldsymbol{v}}_2^1||_2 = 0$, so that the algorithm terminates.

However, for $k = 1$, $\boldsymbol{x}_1^1 = \boldsymbol{x}_0^1 + y_1\boldsymbol{v}_1^1 = \boldsymbol{x}_0^1 + \frac{y_1}{\|\boldsymbol{s}^1\|_2}\boldsymbol{s}^1$, $\boldsymbol{x}_1^2 = \boldsymbol{x}_0^2$. Thus, (2.9) gives $\boldsymbol{r}_1^1 = \boldsymbol{b}^1 - A_{11}\boldsymbol{x}_1^1 - A_{12}\boldsymbol{x}_1^2 = \boldsymbol{b}^1 - A_{11}(\boldsymbol{x}_0^1 + \frac{y_1}{\|\boldsymbol{s}^1\|_2}\boldsymbol{s}^1) - A_{12}\boldsymbol{x}_0^2 = \boldsymbol{r}_0^1 - \frac{y_1}{\|\boldsymbol{s}^1\|_2}A_{11}\boldsymbol{s}^1 = \boldsymbol{r}_0^1 = \boldsymbol{s}^1 \neq \boldsymbol{0}$. Hence, $\boldsymbol{x}^1$ is not a solution. $\square$

Remark Theorem 2.2 (Theorem 2.6 in Brown and Walker [3]) claims only the sufficiency of the condition.

Concerning where the approximate solution $\boldsymbol{x}_i$ converges, we have the following. Note that $\boldsymbol{r}_i^1 = \boldsymbol{b}^1 - A_{11}\boldsymbol{x}_0^1 - A_{12}\boldsymbol{x}_0^2$.

Theorem 2.9
If $\boldsymbol{b} \in \mathcal{R}(A)$ and $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\boldsymbol{0}\}$, the following hold for GMRES.

$\boldsymbol{x}_i^1$ converges to ${A_{11}}^{-1}(\boldsymbol{b}^1 - A_{12}\boldsymbol{x}_0^2)$ and $\boldsymbol{x}_i^2 = \boldsymbol{x}_0^2$, so that $\boldsymbol{x}_i$ converges to $Q_1{A_{11}}^{-1}(\boldsymbol{b}_1 - A_{12}\boldsymbol{x}_0^2) + Q_2\boldsymbol{x}_0^2$.

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

Remark From the proofs of the above theorems, it is clear that GMRES will converge to the least squares solution within $r = \mathrm{rank}A$ iterations, when the condition for convergence is fulfilled.

2.6 GMRES(k)

The restarted GMRES (GMRES(k)) method [28, 27] sets $\boldsymbol{x}_0 = \boldsymbol{x}_k$ at every k iterations in order to save memory and computational work. GMRES(k) also never breaks down for nonsingular systems, but they may stagnate without converging to the solution. For GMRES(k), we have the following. (See, e.g. Saad [27].)

Theorem 2.10 *GMRES(k) converges to the solution for all $\boldsymbol{b}, \boldsymbol{x}_0 \in \mathbf{R}^n$ if A is definite.*

Here, definite means either positive definite or negative definite. For $k = 1$, the definiteness of A is also a necessary condition for convergence, so that GMRES(1) may stagnate and not converge to the exact solution for some $\boldsymbol{b}$ and $\boldsymbol{x}_0$ if A is not definite.

For singular systems, note the following.

Lemma 2.11 *$M(A_{11})$ is definite $\Longleftrightarrow$ $M(A)$ is definite in $\mathcal{R}(A)$.*

Proof. Note $(\boldsymbol{y}^1, M(A_{11})\boldsymbol{y}^1) = (\boldsymbol{y}^1, A_{11}\boldsymbol{y}^1) = {\boldsymbol{y}^1}^{\mathrm{T}}{Q_1}^{\mathrm{T}}AQ_1\boldsymbol{y}^1$
$= (Q_1\boldsymbol{y}^1, AQ_1\boldsymbol{y}^1) = (Q_1\boldsymbol{y}^1, M(A)Q_1\boldsymbol{y}^1)$. Hence,

$M(A_{11})$ is positive-definite
$\Longleftrightarrow (\boldsymbol{y}^1, M(A_{11})\boldsymbol{y}^1) > 0$ for all $\boldsymbol{y}^1 \neq \boldsymbol{0}$
$\Longleftrightarrow (Q_1\boldsymbol{y}^1, M(A)Q_1\boldsymbol{y}^1) > 0$ for all $\boldsymbol{y}^1 \neq \boldsymbol{0}$
$\Longleftrightarrow (\boldsymbol{y}, M(A)\boldsymbol{y}) > 0$ for all $\boldsymbol{y} \in \mathcal{R}(A)$; $\boldsymbol{y} \neq \boldsymbol{0}$
$\Longleftrightarrow M(A)$ is positive-definite in $\mathcal{R}(A)$.

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

Hence, we have the following.

Theorem 2.12 *GMRES(k) converges to a least squares solution for all $\boldsymbol{b}, \boldsymbol{x}_0 \in \mathbf{R}^n$ if $\mathcal{N}(A) = \mathcal{N}(A^T)$ and $M(A)$ is definite in $\mathcal{R}(A)$.*

We also have the following.

Lemma 2.13 *If $M(A)$ is definite, then A is nonsingular.*

Thus, if $M(A_{11})$ is definite, A_{11} is nonsingular, which is equivalent to $\mathcal{R}(A) \cap \mathcal{N}(A) = \{0\}$. Hence, we also have the following.

Theorem 2.14 *GMRES(k) converges to a solution for all $\boldsymbol{b} \in \mathcal{R}(A), \boldsymbol{x}_0 \in \mathbf{R}^n$ if $M(A)$ is definite in $\mathcal{R}(A)$.*

In the following, we derive a different interpretation of the definiteness of $M(A_{11})$ in terms of A.

Lemma 2.15 *Let $S \in \mathbf{R}^{n\times n}, S^T = S, T \in \mathbf{R}^{n\times n}, \mathrm{rank}T = r$. Let $\boldsymbol{q}_1, \dots, \boldsymbol{q}_r$ be a basis of $\mathcal{R}(T)$, and $Q_1 = [\boldsymbol{q}_1, \dots, \boldsymbol{q}_r] \in \mathbf{R}^{n\times r}$. Let the inertia of $S_{11} := {Q_1}^T S Q_1 \in \mathbf{R}^{r\times r}$ be (π, ν, ζ). Then, the inertia of $T^T S T$ is $(\pi, \nu, \zeta + n - r)$.*

Proof. There is a permutation matrix $P \in \mathbf{R}^{n\times n}$ such that $TP = [Q, 0]R$, where $R \in \mathbf{R}^{n\times n}$ is nonsingular. Hence, we have

$$T^{\mathrm{T}} S T = P R^{\mathrm{T}} \begin{bmatrix} {Q_1}^{\mathrm{T}} \\ 0 \end{bmatrix} S [Q_1 0] R P^{\mathrm{T}} = P R^{\mathrm{T}} \begin{bmatrix} S_{11} & 0 \\ 0 & 0 \end{bmatrix} R P^{\mathrm{T}}.$$

Hence, from Sylvester's law of inertia, the inertia of $T^{\mathrm{T}} S T$ is the same as that of $\begin{bmatrix} S_{11} & 0 \\ 0 & 0 \end{bmatrix}$.
□

From Lemma 2.15, we have the following.

Theorem 2.16 *$M(A_{11})$ is definite $\Longleftrightarrow$ $A^T M(A) A$ is semidefinite and its rank is $r = \mathrm{rank}A$.*

Proof.
$M(A_{11})$ is positive definite.
$\Longleftrightarrow$ ${Q_1}^{\mathrm{T}} M(A) Q_1$ is positive definite.
$\Longleftrightarrow$ The inertia of ${Q_1}^{\mathrm{T}} M(A) Q_1$ is $(r, 0, 0)$.
$\Longleftrightarrow$ The inertia of $A^{\mathrm{T}} M(A) A$ is $(r, 0, n - r)$.
$\Longleftrightarrow$ $A^{\mathrm{T}} M(A) A$ is positive semidefinite and its rank is r.

Here, we have put $S = M(A)$ and $T = A$ in Lemma 2.15. Similarly for the negative definite case. □

3 Convergence analysis of GCR(k) on singular systems

Next, we analyse GCR(k) using the same geometric framework.

3.1 GCR(k) on nonsingular systems

First, we briefly review the convergence of GCR(k) for nonsingular systems according to [11, 10, 25, 1].

For the system of linear equations

$$A\boldsymbol{x} = \boldsymbol{b}, \tag{3.1}$$

where $A \in \mathbf{R}^{n\times n}$ is nonsingular but not necessarily symmetric,
$\boldsymbol{b} \in \mathbf{R}^n$ is the right hand side, and $\boldsymbol{x} \in \mathbf{R}^n$ is the solution, GCR(k) [10] is given as follows.

GCR(k)

Choose $\boldsymbol{x}_0$

$*$ $\boldsymbol{r}_0 := \boldsymbol{b} - A\boldsymbol{x}_0$
$\boldsymbol{p}_0 := \boldsymbol{r}_0$
For $i = 0, 1, \ldots, k$ until the residual ($\boldsymbol{r}$) converges, do
begin

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

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

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

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

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

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

(3.2)

The method is a Krylov subspace method which minimizes the residual norm $||\boldsymbol{r}_i||_2$ over $\boldsymbol{x}_i = \boldsymbol{x}_0 + \langle \boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{i-1}\boldsymbol{r}_0\rangle$, satisfying the orthogonality $(A\boldsymbol{p}_l, A\boldsymbol{p}_m) = 0$ $(l < m)$, 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 without restarts may be considered as GCR(∞).

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

If the (full) GCR does not break down, it determines the solution of (3.1) in at most n iterations [10].

When A is nonsingular, the sufficient condition for the residual vector of GCR(k) to converge to $\mathbf{0}$ is given by the following theorem [10, 25].

Theorem 3.1 *If $M(A)$ is definite, either of the following holds for GCR(k) ($k \ge 0$).*

1. *There exists $l \ge 0$, such that $\boldsymbol{p}_i \ne \mathbf{0}$ $(0 \le i < l)$ and $\boldsymbol{r}_l = \mathbf{0}$. Further,*

$$\frac{{\|\boldsymbol{r}_{i+1}\|_2}^2}{{\|\boldsymbol{r}_i\|_2}^2} \le 1 - \frac{\{\lambda_{\min}(M(A))\}^2}{\lambda_{\max}(A^T A)} \tag{3.3}$$

holds for $0 \le i < l$.

2. For all $i \geq 0$, $\boldsymbol{p}_i \neq \boldsymbol{0}$, $\boldsymbol{r}_i \neq \boldsymbol{0}$ and (3.3) hold.

Next, note the following lemma.

Lemma 3.2 *If $M(A)$ is not definite, there exists $\boldsymbol{v} \neq \boldsymbol{0}$ such that $(\boldsymbol{v}, A\boldsymbol{v}) = 0$.*

Theorem 3.1 and Lemma 3.2 give the following theorem which gives the necessary and sufficient condition for GCR(k) to converge without breakdown [1].

Theorem 3.3 *Let $A \in \mathbf{R}^{n\times n}$ be nonsingular. Then, GCR(k) converges to the solution of $A\boldsymbol{x} = \boldsymbol{b}$ without breakdown for all $\boldsymbol{b}, \boldsymbol{x}_0 \in \mathbf{R}^n$ if and only if $M(A)$ is definite.*

GCR is a simple implementation of the Krylov subspace method for nonsymmetric matrices. GCR requires more memory and computation compared to GMRES. However, GCR may have some advantages in the context of variable preconditioning [39, 7, 8, 24].

Although GCR is "mathematically equivalent" to GMRES [28], GCR has breakdowns unique to the method, which may occur when the system is indefinite, as shown in the theorem above, where as GMRES never breaks down for nonsingular systems. This character is reflected in the singular case, as will be shown in the following section.

3.2 GCR(k) on singular systems

In this section, we will consider the convergence of GCR(k) when it is applied to singular systems.

The quantities in the GCR(k) algorithm (3.2) can be expressed as follows.

First,

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

Next,

$$\begin{aligned}(A\boldsymbol{p}, A\boldsymbol{p}) &= (AQ\tilde{\boldsymbol{p}}, AQ\tilde{\boldsymbol{p}}) = \tilde{\boldsymbol{p}}^{\mathrm{T}} Q^{\mathrm{T}} A^{\mathrm{T}} AQ\tilde{\boldsymbol{p}} \\ &= \tilde{\boldsymbol{p}}^{\mathrm{T}} Q^{\mathrm{T}} A^{\mathrm{T}} QQ^{\mathrm{T}} AQ\tilde{\boldsymbol{p}} = (\tilde{A}\tilde{\boldsymbol{p}}, \tilde{A}\tilde{\boldsymbol{p}}),\end{aligned}$$

where,

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

so that

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

Further,

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

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

Decomposed GCR(k) (general case)

Choose initial approximate solution $\boldsymbol{x}_0$.

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

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

begin

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

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

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

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

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

end

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

Go to $*$.

(3.4)

Note that $\boldsymbol{r}_i^2$, the $\mathcal{R}(A)^\perp$ component of the residual vector is always equal to the least squares residual $\boldsymbol{b}^2$ of (2.1) (cf. (2.9), (2.10)).

3.2.1 Convergence theorem for arbitrary $\boldsymbol{b}$

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

First note that, for the case when $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$, we have $A_{12} = 0$ from Theorem 2.5. Hence, (2.9) becomes

$$\begin{aligned} \boldsymbol{r}^1 &= \boldsymbol{b}^1 - A_{11}\boldsymbol{x}^1 \\ \boldsymbol{r}^2 &= \boldsymbol{b}^2. \end{aligned} \tag{3.5}$$

Note also that, from Lemma 2.4, A_{11} is nonsingular. Hence, from (2.10) and (3.5), a least squares solution of (2.1) is given by $\boldsymbol{x}^1 = {A_{11}}^{-1}\boldsymbol{b}^1$.

Now, for the case $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$, the above decomposed GCR(k) (3.4) can be simplified as follows.

Decomposed GCR(k) (Case $\mathcal{N}(A) = \mathcal{N}(A^{\mathbf{T}})$)

Choose initial approximate solution $\boldsymbol{x}_0$.

$\mathcal{R}(A)$ component	$\mathcal{R}(A)^{\perp}$ component
$\boldsymbol{b}^1 := {Q_1}^{\mathrm{T}}\boldsymbol{b}$	$\boldsymbol{b}^2 := {Q_2}^{\mathrm{T}}\boldsymbol{b}$
$\boldsymbol{x}_0^1 := {Q_1}^{\mathrm{T}}\boldsymbol{x}_0$	$\boldsymbol{x}_0^2 := {Q_2}^{\mathrm{T}}\boldsymbol{x}_0$
$*\ \boldsymbol{r}_0^1 := \boldsymbol{b}^1 - A_{11}\boldsymbol{x}_0^1$	$\boldsymbol{r}_0^2 := \boldsymbol{b}^2$
$\boldsymbol{p}_0^1 := \boldsymbol{r}_0^1$	$\boldsymbol{p}_0^2 := \boldsymbol{r}_0^2 = \boldsymbol{b}^2$

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

begin

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

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

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

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

end

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

Go to $*$.

(3.6)

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

$$A_{11}\boldsymbol{x}^1 = \boldsymbol{b}^1. \tag{3.7}$$

Hence, the convergence of the residual of the decomposed GCR(k) (3.6) is determined by the convergence of the residual $\boldsymbol{r}^1$ for GCR(k) applied to the system (3.7). Hence, from Theorem 3.1, we obtain the following lemma concerning the convergence of the residual of the decomposed GCR(k) (3.6).

Lemma 3.4
If $A_{12} = 0$ and $M(A_{11})$ is definite, either of the following holds for the decomposed GCR(k) algorithm (3.6).

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

$$\frac{{\|\boldsymbol{r}_{i+1}^1\|_2}^2}{{\|\boldsymbol{r}_i^1\|_2}^2} \leq 1 - \frac{\{\lambda_{\min}(M(A_{11}))\}^2}{\lambda_{\max}(A_{11}^T A_{11})} \tag{3.8}$$

holds for $0 \leq i < l$.

2. *For all $i \geq 0$, $\boldsymbol{p}_i^1 \neq \mathbf{0}$, $\boldsymbol{r}_i^1 \neq \mathbf{0}$, and* (3.8) *hold.*

From Lemmas 3.2 and 3.4, we derive the following theorem. The proof is similar to that of Theorem 3.3 in [1] for CR.

Theorem 3.5
For the least squares problem $\min_{\boldsymbol{x}\in\mathbf{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|_2$, $A \in \mathbf{R}^{n\times n}$, the necessary and sufficient condition for GCR(k) to converge to a least squares solution without breakdown for all $\boldsymbol{b}, \boldsymbol{x}_0 \in \mathbf{R}^n$ is that $A_{12} = 0$ and $M(A_{11})$ is definite.

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

Proof.
The sufficiency of the condition follows from Lemma 3.4.
The necessity of the condition is shown by contraposition, i.e., it is shown that if $M(A_{11})$ is not definite or if $A_{12} \neq 0$, then, there exists a $\boldsymbol{b}$ such that GCR(k) 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 3.2, there exists $\boldsymbol{v} \neq \mathbf{0}$ such that $(\boldsymbol{v}, A_{11}\boldsymbol{v}) = 0$. Thus, for such $\boldsymbol{v}$, let

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

Then,

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

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

$$\begin{aligned} (\boldsymbol{r}_0, A\boldsymbol{p}_0) &= (\boldsymbol{r}_0, A\boldsymbol{r}_0) = {\boldsymbol{r}_0}^{\mathrm{T}}A\boldsymbol{r}_0 = (Q\tilde{\boldsymbol{r}}_0)^{\mathrm{T}}AQ\tilde{\boldsymbol{r}}_0 \\ &= \left[{\boldsymbol{r}_0^1}^{\mathrm{T}}, {\boldsymbol{r}_0^2}^{\mathrm{T}}\right] \begin{bmatrix} A_{11} & A_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{r}_0^1 \\ \boldsymbol{r}_0^2 \end{bmatrix} = (\boldsymbol{r}_0^1, A_{11}\boldsymbol{r}_0^1) = (\boldsymbol{v}, A_{11}\boldsymbol{v}) = 0. \end{aligned}$$

If $(A\boldsymbol{p}_0, A\boldsymbol{p}_0) = 0$, GCR($k$) of (3.2) breaks down at step $i = 0$ before reaching a least squares solution.

On the other hand, if $(A\boldsymbol{p}_0, A\boldsymbol{p}_0) \neq 0$, then, $\alpha_0 = \dfrac{(\boldsymbol{r}_0, A\boldsymbol{p}_0)}{(A\boldsymbol{p}_0, A\boldsymbol{p}_0)} = 0$.
Hence, $\boldsymbol{x}_1 = \boldsymbol{x}_0$, $\boldsymbol{r}_1 = \boldsymbol{r}_0 = \boldsymbol{p}_0$, so that $\boldsymbol{x}_1$ is not a least squares solution. Further, $\beta_0^0 = -\dfrac{(A\boldsymbol{r}_1, A\boldsymbol{p}_0)}{(A\boldsymbol{p}_0, A\boldsymbol{p}_0)} = -\dfrac{(A\boldsymbol{p}_0, A\boldsymbol{p}_0)}{(A\boldsymbol{p}_0, A\boldsymbol{p}_0)} = -1$, and $\boldsymbol{p}_1 = \boldsymbol{r}_1 + \beta_0^0\,\boldsymbol{p}_0 = \boldsymbol{p}_0 - \boldsymbol{p}_0 = \boldsymbol{0}$.

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

For $k = 0$, new $\boldsymbol{x}_0 :=$ old $\boldsymbol{x}_1 =$ old $\boldsymbol{x}_0$, 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 $\boldsymbol{v}_1 = (v_{1,1}, \ldots, v_{1,k}, \ldots, v_{1,r})^{\mathrm{T}}$ where $v_{1,k} = \delta_{ik}$, and
$\boldsymbol{v}_2 = (v_{2,1}, \ldots, v_{2,k}, \ldots, v_{2,n-r})^{\mathrm{T}}$ where $v_{2,k} = \delta_{jk}$.
Then, $\boldsymbol{v}_1^{\mathrm{T}}A_{12}\boldsymbol{v}_2 = (A_{12})_{i,j} \neq 0$. Hence, there exist $\boldsymbol{v}_1 \neq \boldsymbol{0}$ and $\boldsymbol{v}_2 \neq \boldsymbol{0}$, such that $(\boldsymbol{v}_1, A_{12}\boldsymbol{v}_2) \neq 0$.

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

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

Then,

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

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

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

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

Now, if $A\boldsymbol{p}_0 = A\boldsymbol{r}_0 = \boldsymbol{0}$, GCR($k$) of (3.2) breaks down at step $i = 0$ before reaching a least squares solution.

On the other hand, if $A\boldsymbol{p}_0 \neq \boldsymbol{0}$, then, $\alpha_0 = \dfrac{(\boldsymbol{r}_0, A\boldsymbol{p}_0)}{(A\boldsymbol{p}_0, A\boldsymbol{p}_0)} = 0$. Hence, $\boldsymbol{r}_1 = \boldsymbol{r}_0 = \boldsymbol{p}_0$, so that $\boldsymbol{x}_1$ is not a least squares solution. Further, $\beta_0^0 = -\dfrac{(A\boldsymbol{r}_1, A\boldsymbol{p}_0)}{(A\boldsymbol{p}_0, A\boldsymbol{p}_0)} = -1$, $\boldsymbol{p}_1 = \boldsymbol{r}_1 + \beta_0^0\boldsymbol{p}_0 = \boldsymbol{p}_0 - \boldsymbol{p}_0 = \boldsymbol{0}$.

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

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

Thus, we have shown the necessity of the condition. $\square$

In order to rephrase the condition in Theorem 3.5 in terms of the original matrix A, note the following.

Lemma 3.6 *If* $\mathcal{N}(A) = \mathcal{N}(A^T)$, *then,*
$M(A_{11})$ *is definite*
$\Longleftrightarrow$ "*$M(A)$ is semidefinite, and* $\operatorname{rank} M(A) = \operatorname{rank} A$" .

Proof. If $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$, Theorem 2.5 gives

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

Thus, we have

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

so that

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

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

Hence, $\operatorname{rank} M(A) =$ the number of nonzero eigenvalues of $M(A)$. Thus,
$M(A_{11})$: definite
$\Longleftrightarrow$ "$M(A)$: semidefinite, $\operatorname{rank} M(A) = \operatorname{rank} M(A_{11}) = r = \operatorname{rank} A$". $\square$

Thus, also noting Lemma 2.11, we have the following.

Theorem 3.7
For the least squares problem $\min\limits_{\boldsymbol{x} \in \mathbf{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|_2,\ A \in \mathbf{R}^{n \times n}$, *the following are equivalent.*
(C1) *GCR(k) converges to a least squares solution*
without breakdown for arbitrary $\boldsymbol{b}, \boldsymbol{x}_0 \in \mathbf{R}^n$.
(C2) $A_{12} = 0$ *and* $M(A_{11})$ *is definite.*
(C3) $\mathcal{N}(A) = \mathcal{N}(A^T), M(A)$ *is semi-definite and* $\operatorname{rank} M(A) = \operatorname{rank} A$.
(C4) $\mathcal{N}(A) = \mathcal{N}(A^T)$ *and* $M(A)$ *is definite in* $\mathcal{R}(A)$.

Remark 1 The above theorem is a natural extension of Theorem 3.3 for the nonsingular case, since if A is nonsingular, $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}}) = \{\mathbf{0}\}$.

Remark 2 If the condition of the above theorem is satisfied, the (full) GCR method

($k = \infty$) will give a least squares solution of (2.1) within $r = \mathrm{rank} A$ iterations. This is because the $\mathcal{R}(A)$ component of the algorithm is equivalent to the method applied to $A_{11}\boldsymbol{x}^1 = \boldsymbol{b}^1$ in $\mathbf{R}^r$, where A_{11} is definite (cf. (3.6)).

Remark 3 As shown in subsection 2.4, and also in [3], $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$ is the necessary and sufficient condition for GMRES to converge to a least squares solution without breakdown for arbitrary $\boldsymbol{b} \in \mathbf{R}^n$ and initial approximate solution $\boldsymbol{x}_0 \in \mathbf{R}^n$. GCR and GCR($k$) 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 $\boldsymbol{b} \notin \mathcal{R}(A)$), one could monitor the norm of $A^{\mathrm{T}}\boldsymbol{r}$. This observation is based on the following lemma.

Lemma 3.8 $\boldsymbol{r}^1 := {Q_1}^T\boldsymbol{r} = \mathbf{0} \Longleftrightarrow A^T\boldsymbol{r} = \mathbf{0}$.

Concerning where the approximate solution $\boldsymbol{x}_i$ converges, we have the following.

Theorem 3.9 *If $\mathcal{N}(A) = \mathcal{N}(A^T)$, the following hold for GCR(k).*
If $\boldsymbol{r}_i^1$ converges to $\mathbf{0}$ (least squares solution), $\boldsymbol{x}_i^1$ converges to ${A_{11}}^{-1}\boldsymbol{b}^1$.
Moreover, if $\boldsymbol{b} \in \mathcal{R}(A), \boldsymbol{x}_i^2 = \boldsymbol{x}_0^2$, so that $\boldsymbol{x}_i$ converges to $Q_1{A_{11}}^{-1}\boldsymbol{b}^1 + Q_2\boldsymbol{x}_0^2$.
Further, if $\boldsymbol{x}_0^2 = \mathbf{0}$ (i.e., $\boldsymbol{x}_0 \in \mathcal{R}(A)$), $\boldsymbol{x}_i$ converges to $Q_1{A_{11}}^{-1}\boldsymbol{b}^1$, which is the pseudo-inverse solution (the least squares solution with minimum Euclidean norm).

Proof. If $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$, the $\mathcal{R}(A)$ component of the decomposed GCR(k) (3.6) can be regarded as GCR(k) applied to $A_{11}\boldsymbol{x}^1 = \boldsymbol{b}^1$, where A_{11} is nonsingular from Lemma 2.4. Hence, if the $\mathcal{R}(A)$ component of the residual converges to $\mathbf{0}$, $\boldsymbol{x}_i^1$ converges to ${A_{11}}^{-1}\boldsymbol{b}^1$.

Moreover, if $\boldsymbol{b} \in \mathcal{R}(A)$, $\boldsymbol{b}^2 = \mathbf{0}$ in the $\mathcal{R}(A)^{\perp}$ component of the decomposed GCR(k) (3.6), so that $\boldsymbol{p}_i^2 \equiv \mathbf{0}\,(i \geq 0)$, and hence, $\boldsymbol{x}_i^2 \equiv \boldsymbol{x}_0^2\,(i \geq 0)$. Hence, $\boldsymbol{x}_i = Q_1\boldsymbol{x}_i^1 + Q_2\boldsymbol{x}_i^2$ converges to $Q_1{A_{11}}^{-1}\boldsymbol{b}^1 + Q_2\boldsymbol{x}_0^2$.

Further, if $\boldsymbol{x}_0^2 = \mathbf{0}$, $\boldsymbol{x}_i^2 \equiv \boldsymbol{x}_0^2 = \mathbf{0}\,(i \geq 0)$, so that $\boldsymbol{x}_i$ converges to $Q_1{A_{11}}^{-1}\boldsymbol{b}^1$. Now, since $\|\boldsymbol{x}\|_2^2 = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{x} = \|\boldsymbol{x}^1\|_2^2 + \|\boldsymbol{x}^2\|_2^2$, if we denote the converged solution by $\boldsymbol{x}_*$, $\|\boldsymbol{x}_*\|_2^2 = \|{A_{11}}^{-1}\boldsymbol{b}^1\|_2^2 + \|\boldsymbol{x}_0^2\|_2^2$, and $\boldsymbol{x}_0^2 = \mathbf{0}$ gives the pseudo-inverse solution. □

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

Remark 2 Even if $\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$ holds, if $\boldsymbol{b}$ is not in $\mathcal{R}(A)$ (inconsistent case), $\boldsymbol{b}^2 \neq \mathbf{0}$ in the decomposed GCR(k) (3.6), so that it is not obvious where $\boldsymbol{x}_i^2$, and hence $\boldsymbol{x}_i$ will end up.

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

Next, we will consider the case when the system is consistent, that is when $\boldsymbol{b} \in \mathcal{R}(A)$. In this case, $\boldsymbol{b}^2 = Q_2^{\mathrm{T}}\boldsymbol{b} = \mathbf{0}$ holds. Hence, the decomposed GCR(k) (3.4) can be simplified as follows.

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

$\mathcal{R}(A)$ component	$\mathcal{R}(A)^{\perp}$ component
Choose initial approximate solution $\boldsymbol{x}_0$.	
$\boldsymbol{b}^1 = {Q_1}^{\mathrm{T}}\boldsymbol{b}$	$\boldsymbol{b}^2 = \mathbf{0}$
$\boldsymbol{x}_0^1 = {Q_1}^{\mathrm{T}}\boldsymbol{x}_0$	$\boldsymbol{x}_0^2 = {Q_2}^{\mathrm{T}}\boldsymbol{x}_0$
$*\ \boldsymbol{r}_0^1 = \boldsymbol{b}^1 - A_{11}\boldsymbol{x}_0^1 - A_{12}\boldsymbol{x}_0^2$	$\boldsymbol{r}_0^2 = \boldsymbol{b}^2 = \mathbf{0}$
$\boldsymbol{p}_0^1 = \boldsymbol{r}_0^1$	$\boldsymbol{p}_0^2 = \boldsymbol{r}_0^2 = \mathbf{0}$
For $i = 0, 1, \ldots, k$ until convergence do	
begin	
$\alpha_i = \dfrac{(\boldsymbol{r}_i^1,\, A_{11}\boldsymbol{p}_i^1)}{(A_{11}\boldsymbol{p}_i^1,\, A_{11}\boldsymbol{p}_i^1)}$	
$\boldsymbol{x}_{i+1}^1 = \boldsymbol{x}_i^1 + \alpha_i \boldsymbol{p}_i^1$	$\boldsymbol{x}_{i+1}^2 = \boldsymbol{x}_i^2 = \boldsymbol{x}_0^2$
$\boldsymbol{r}_{i+1}^1 = \boldsymbol{r}_i^1 - \alpha_i A_{11}\boldsymbol{p}_i^1$	$\boldsymbol{r}_{i+1}^2 = \boldsymbol{r}_i^2 = \mathbf{0}$
$\beta_i^j = -\dfrac{(A_{11}\boldsymbol{r}_{i+1}^1,\, A_{11}\boldsymbol{p}_j^1)}{(A_{11}\boldsymbol{p}_j^1,\, A_{11}\boldsymbol{p}_j^1)} \quad (0 \le j \le i)$	
$\boldsymbol{p}_{i+1}^1 = \boldsymbol{r}_{i+1}^1 + \sum_{j=0}^{i} \beta_j^i \boldsymbol{p}_j^1$	$\boldsymbol{p}_{i+1}^2 = \boldsymbol{r}_{i+1}^2 = \mathbf{0}$
end	
$\boldsymbol{x}_0^1 = \boldsymbol{x}_{k+1}^1$	$\boldsymbol{x}_0^2 = \boldsymbol{x}_{k+1}^2$
Go to $*$.	

(3.9)

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

Then, we have the following theorem.

Theorem 3.10
For the least squares problem $\min_{\boldsymbol{x}\in\mathbf{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|_2,\ A \in \mathbf{R}^{n\times n}$, *the following are equivalent.*

(C1) *GCR(k) converges to a solution without breakdown for all* $\boldsymbol{b} \in \mathcal{R}(A), \boldsymbol{x}_0 \in \mathbf{R}^n$.

(C2) *$M(A_{11})$ is definite.*
(C3) *$M(A)$ is definite in $\mathcal{R}(A)$.*

Proof.

(C2 $\Longrightarrow$ C1) : For $\boldsymbol{b} \in \mathcal{R}(A)$, the $\mathcal{R}(A)$ component of the decomposed GCR(k) (3.9) is equivalent to GCR(k) applied to the system $A_{11}\boldsymbol{x}^1 = \boldsymbol{b}^1 - A_{12}\boldsymbol{x}_0^2$. Hence, from Theorem 3.3, if $M(A_{11})$ is definite, $\boldsymbol{r}_i^1$, the $\mathcal{R}(A)$ component of the residual, will converge to $\mathbf{0}$ without breakdown. Since $\boldsymbol{r}_i^2$, the $\mathcal{R}(A)^\perp$ component of the residual, is always $\mathbf{0}$, the method converges to a solution without breakdown for arbitrary $\boldsymbol{b} \in \mathcal{R}(A)$ and $\boldsymbol{x}_0 \in \mathbf{R}^n$.

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

Assume that $M(A_{11})$ is not definite. Then, from Lemma 3.2, there exists $\boldsymbol{v}^1 \neq \mathbf{0}$ such that $(\boldsymbol{v}^1, A_{11}\boldsymbol{v}^1) = 0$. Let $\boldsymbol{b} = Q_1\boldsymbol{b}^1 + Q_2\boldsymbol{b}^2 = Q_1\boldsymbol{b}^1$ where $\boldsymbol{b}^1 = \boldsymbol{v}^1 + A_{11}\boldsymbol{x}_0^1 + A_{12}\boldsymbol{x}_0^2$. Then, $\boldsymbol{p}_0^1 = \boldsymbol{r}_0^1 = \boldsymbol{v}^1 \neq \mathbf{0}$.

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

On the other hand, if $A_{11}\boldsymbol{p}_0^1 = A_{11}\boldsymbol{v}^1 \neq \mathbf{0}$, then
$(\boldsymbol{r}_0^1, A_{11}\boldsymbol{p}_0^1) = (\boldsymbol{v}^1, A_{11}\boldsymbol{v}^1) = 0$, so that $\alpha_0 = 0$, and $\boldsymbol{x}_1^1 = \boldsymbol{x}_0^1$,
$\boldsymbol{r}_1^1 = \boldsymbol{r}_0^1 = \boldsymbol{v}^1$, $\beta_0^0 = -\dfrac{(A_{11}\boldsymbol{r}_1^1, A_{11}\boldsymbol{p}_0^1)}{(A_{11}\boldsymbol{p}_0^1, A_{11}\boldsymbol{p}_0^1)} = -\dfrac{(A_{11}\boldsymbol{v}, A_{11}\boldsymbol{v})}{(A_{11}\boldsymbol{v}^1, A_{11}\boldsymbol{v}^1)} = -1$, and $\boldsymbol{p}_1^1 = \boldsymbol{r}_1^1 + \beta_0^0\boldsymbol{p}_0^1 = \boldsymbol{v}^1 - \boldsymbol{v}^1 = \mathbf{0}$.

When $k = 0$, new $\boldsymbol{x}_0^1$ = old $\boldsymbol{x}_1^1$ = old $\boldsymbol{x}_0^1$, new $\boldsymbol{x}_0^2$ = old $\boldsymbol{x}_1^2$ = old $\boldsymbol{x}_0^2$, $\boldsymbol{r}_0^1 = \boldsymbol{v}^1 \neq \mathbf{0}$. Hence, the new $\boldsymbol{x}_0$ is not a solution, and this repeats for ever.

When $k \geq 1, \boldsymbol{p}_1^1 = \mathbf{0}$, so that breakdown occurs at step $i = 1$, when computing α_1, even though $\boldsymbol{r}_1^1 = \boldsymbol{v}^1 \neq \mathbf{0}$.

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

(C2 $\Longleftrightarrow$ C3) is a consequence of Lemma 2.11. $\square$

Remark 1 The above theorem is also a natural extension of Theorem 3.1 for the nonsingular case, since if A is nonsingular, $\boldsymbol{b} \in \mathcal{R}(A) = \mathbf{R}^n$.

Remark 2 If the condition of the above theorem is satisfied and $\boldsymbol{b} \in \mathcal{R}(A)$, GCR without restarts will give a solution to (2.1) with in $r = \mathrm{rank}A$ iterations, since the $\mathcal{R}(A)$ component of the algorithm is equivalent to the method applied to $A_{11}\boldsymbol{x}^1 = \boldsymbol{b}^1 - A_{12}\boldsymbol{x}_0^2$ 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 2.13, and $\mathcal{R}(A) \cap \mathcal{N}(A) = \{\mathbf{0}\}$ holds from Theorem 2.3, which was the condition for GMRES in Theorem 2.8.

Concerning where the approximate solution converges, we have the following. Note that $\boldsymbol{r}_i^1 = \boldsymbol{b}^1 - A_{12}\boldsymbol{x}_0^2 - A_{11}\boldsymbol{x}_i^1$.

Theorem 3.11 *If $\boldsymbol{b} \in \mathcal{R}(A)$ and $M(A)$ is definite in $\mathcal{R}(A)$, the following hold for GCR(k).*

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

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

4 Examples

Finally, we analyse the convergence of GMRES, GMRES(k) and GCR(k) for the following examples taken from [1].

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

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \beta\frac{\mathrm{d}u}{\mathrm{d}x} = f(x) \qquad (0 < x < 1)$$

with boundary conditions

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

or

2. Neumann boundary condition: $\left.\frac{\mathrm{d}u}{\mathrm{d}x}\right|_{x=0} = \left.\frac{\mathrm{d}u}{\mathrm{d}x}\right|_{x=1} = 0.$

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 $h = \dfrac{1}{n-1}$, and $x_i := (i-1)h \ (i = 1, \ldots, n)$. Let u_i be the approximation of $u(x_i)$, and $f_i := f(x_i)$. Further, let $\alpha_\pm := 1 \pm \dfrac{\beta h}{2}$. Hence, $\alpha_+ + \alpha_- = 2$.

4.1 Periodic boundary condition

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

$$\frac{1}{h^2}\begin{bmatrix} -2 & \alpha_+ & & & \alpha_- \\ \alpha_- & -2 & \alpha_+ & & \text{\Large 0} \\ & \ddots & \ddots & \ddots & \\ \text{\Large 0} & & \alpha_- & -2 & \alpha_+ \\ \alpha_+ & & & \alpha_- & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n \end{bmatrix}. \tag{4.1}$$

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

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

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

so that $\boldsymbol{e} \perp \mathcal{R}(A)$, or $\boldsymbol{e} \in \mathcal{R}(A)^{\perp}$. Besides, since $\dim \mathcal{R}(A)^{\perp} = \dim \mathcal{N}(A) = 1$, we have $\mathcal{R}(A)^{\perp} = \mathcal{N}(A) = \langle \boldsymbol{e} \rangle$, i.e., $\mathcal{R}(A) \perp \mathcal{N}(A)$ ($\mathcal{N}(A) = \mathcal{N}(A^{\mathrm{T}})$). Hence, from Theorem 2.6, when one applies GMRES to the system of linear equations (4.1) arising from the case of periodic boundary condition, the method will converge to a least squares solution without breakdown for arbitrary initial approximate solution $\boldsymbol{x}_0$.

Further, since

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

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 $\operatorname{rank} M(A) = \operatorname{rank} A = n - 1$.

Hence, from Lemma 2.12, Lemma 3.6 and Theorem 3.7, when one applies GMRES(k) or GCR(k) to the system of linear equations (4.1), the methods will converge to a least squares solution without breakdown for arbitrary $\boldsymbol{x}_0$.

Since $\boldsymbol{f} \in \mathcal{R}(A) = (\mathcal{N}(A))^{\perp} \iff \boldsymbol{f} \perp \mathcal{N}(A) = \langle \boldsymbol{e} \rangle \iff (\boldsymbol{f}, \boldsymbol{e}) = \sum_{i=1}^{n} f_i = 0$, if $\sum_{i=1}^{n} f_i = 0$, we have $\boldsymbol{f} \in R(A)$. In this case, from Lemma 3.9 and 2.9, the approximate solution of both methods will converge to the least squares solution $Q_1 {A_{11}}^{-1} Q_1^{\mathrm{T}} \boldsymbol{f} + Q_2 Q_2^{\mathrm{T}} \boldsymbol{x}_0$.

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

4.2 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 $A\boldsymbol{u} = \boldsymbol{f}$ obtained by discretization is

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

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

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

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

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

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

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

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

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

Hence, GMRES determines a solution for all $\boldsymbol{f} \in \mathcal{R}(A), \boldsymbol{x}_0 \in \mathbf{R}^n$.

As for the definiteness of $M(A_{11})$, which is a sufficient condition for GMRES(k), and the necessary and sufficient condition for GCR(k) to converge to a solution without breakdown for all $\boldsymbol{f} \in \mathcal{R}(A)$, (condition (C2) of Theorem 3.10), we could show the following, using Theorem 2.16.

For $n = 2, 3, M(A_{11})$ is definite. However, for $n = 4, M(A_{11})$ is not always definite, depending on the value of β. The details are as follows.

Let $a := \frac{\beta h}{4}$. Then, $\alpha_+ = 1 + 2a$ and $\alpha_- = 1 - 2a$. Redefine A as Ah^2. Let $S := A^{\mathrm{T}} M(A) A$ (cf. Theorem 2.16), s_i be the i-th leading principal minor of S, and $r = \mathrm{rank} A$.

For $n = 2, A^{\mathrm{T}} = A = M(A), r = 1, s_1 < 0, s_2 = \det S = 0$, so that S is negative semidefinite and $\mathrm{rank} S = 1 = r$, so that $M(A_{11})$ is negative definite.

For $n = 3, r = 2, s_1 = -12(a - \frac{7}{12})^2 - \frac{11}{12} < 0, s_2 = 20a^2 + 9 > 0, s_3 = \det S = 0$, so that S is negative semidefinite and $\mathrm{rank} S = 2 = r$, so that $M(A_{11})$ is negative definite.

For $n = 4, r = 3, s_1 = -12(a - \frac{7}{12})^2 - \frac{11}{12} < 0, s_2 = 60a^4 - 148a^3 + 151a^2 - 60a + 14 > 0, s_4 = \det S = 0, \mathrm{rank} S = 3 = r$, and $s_3 = 4(32a^6 - 80a^4 - 55a^2 - 4)$. Hence, for $-a_* \leq a \leq a_*$ where $a_* \approx 1.752, s_3 \leq 0$, so that S is negative semidefinite and $M(A_{11})$ is negative definite, but for $a < -a_*$ or $a > a_*, s_3 > 0$, so that S is not negative semidefinite and $M(A_{11})$ is not negative definite. Hence, when the convection term is too strong, the condition does not hold.

5 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 GMRES, GMRES(k) and GCR(k) methods on singular systems. The idea is a useful geometric framework for analyzing the behaviour of iterative methods on singular systems.

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