Enhancing Convergence in Singular Linear Systems: A Study on New Techniques and Drazin Inverse Solutions

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We examine the expansion of the GMRES algorithm and present the methodologies of DGMRES and LDGMRES for the resolution of the equation Ax=b, in which A denotes a singular matrix. DGMRES is a computational method created to determine the Drazin-inverse solution of either consistent or inconsistent linear systems of the form Ax = b, where A ∈ C^(n×n) is a singular and generally non-Hermitian matrix with an arbitrary index. Typically, this strategy involves restarting, which may hinder convergence and result in stagnation within the DGMRES procedure. By drawing from "the LGMRES and GMRES-E methodologies, we suggest two innovative tactics to improve the convergence of restarted DGMRES by introducing approximate error vectors or approximate eigenvectors (related to a subset of the smallest eigenvalues) to the Krylov subspace. We elaborate on the execution of these methods and offer numerical examples to showcase the efficacy of these approaches."

Keywords: Drazin inverse solution", Krylov subspace, GMRES, convergence.

1. Introduction

Consider the following linear system

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

where A is a real square matrix of size $n \times n$ and b is a real vector of size n is consistent, if it includes at least one solution, otherwise it said to be inconsistent [1]. For example,

the system

$$\begin{cases} x + 2y = 1 \\ x - y = 2 \end{cases}$$

is a consistent system,

but the system

$$\begin{cases} x + y = 1 \\ x + y = 2 \end{cases}$$

is inconsistent, because it has no solution.

The matrix coefficient A in the system (1.1) is said to be singular, if

det $A = 0$,

The matrix A is nonsingular [3,5], if

det $A \neq 0$,

If the matrix A is nonsingular, then, there exists the inverse of A. Moreover, if the system (1.1) is also consistent, then it has unique solution

$x = A^{-1}b$.

1.1 Hermitian matrix

The square matrix A is Hemitian, if [7]

$A^H = A$, where $A^H = \bar{A}^T$,

with $\bar{A}$ as conjugate of A and A^T is the transpose of A.

If A is a real matrix, then $A^H = A^T$.

In other words, a real matrix A is Hermitian, whenever, $A^T = A$.

For example, the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & -1 & 4 \\ 3 & 4 & 0 \end{bmatrix}$$

Is Hermitian matrix

1.2 Eigenvalue and Eigenvector

For any square matrix A of size $m \times m$, if there exist a scalar value λ and a nonzero vector x such that [13,2]

$Ax = \lambda x$, (1.2)

then λ and x are called eigenvalue and eigenvector of A

For example, if $A = I$ an identity matrix, then we will obviously have $Ix = 1x$, that is, "$\lambda = 1$ is an eigenvalue of A and any vector in $\mathbb{R}^m$ is an eigenvector of A. One not that" (1) implies that

$(A - \lambda I)x = 0$, (1.3)

The equation (1.2) has non-trivial solution, if $A - \lambda I$ is a singular matrix. In other words, if

$\det(A - \lambda I) = 0$, (1.4)

the equation (1.3) includes non-trivial solution [6].

If A is of size 3 × 3,

$$"A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}"$$

we will have

$$\det(A - \lambda I) = \det\left(\begin{bmatrix} a_{11}-\lambda & a_{12} & a_{13} \\ a_{21} & a_{22}-\lambda & a_{23} \\ a_{31} & a_{32} & a_{33}-\lambda \end{bmatrix}\right)$$

$$= (a_{11}-\lambda)\det\left(\begin{bmatrix} a_{22}-\lambda & a_{23} \\ a_{32} & a_{33}-\lambda \end{bmatrix}\right) -$$

$$(a_{12})\det\left(\begin{bmatrix} a_{21} & a_{23} \\ a_{31} & a_{33}-\lambda \end{bmatrix}\right) + (a_{13})\det\left(\begin{bmatrix} a_{21} & a_{22}-\lambda \\ a_{31} & a_{32} \end{bmatrix}\right)$$

$$" = (a_{11}-\lambda)((a_{22}-\lambda)(a_{33}-\lambda) - a_{23}a_{32}) - a_{12}(a_{21}(a_{33}-\lambda) - a_{23}a_{31}) +"$$

$$a_{13}(a_{21}a_{32} - a_{31}(a_{22}-\lambda))$$

$$= -\lambda^3 + (a_{11} + a_{22} + a_{33})\lambda^2 +$$

$$(-a_{11}a_{22} - a_{11}a_{33} - a_{22}a_{33} + a_{23}a_{32} + a_{12}a_{21} + a_{13}a_{31})\lambda +$$

$$(-a_{11}a_{22}a_{33} - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{13}a_{31}a_{22}).$$

It is seen that det $(A - \lambda I)$ is a polynomial of degree 3 and so it has 3 roots. So, in general for $m \times m$ matrix A, we have

$$\det(A - \lambda I) = (-1)^m((\lambda - \lambda_1)(\lambda - \lambda_2)\cdots(\lambda - \lambda_m)), \quad (1.5)$$

where $\lambda_1, \lambda_2, \cdots, \lambda_m$ are roots of det $(A - \lambda I)$ and also are eigenvalues of A.

1.3 Definition Two square matrices of A and B are similar, if there exists a nonsingular matrix P such that $B = P^{-1}AP$ [4,6].

1.4 Definition Positive definite and positive semi definite A square matrix A of size $m \times m$ is positive definite if for any nonzero $x \in \mathbb{C}^m$ [10]

$x^HAx > 0$,

Semi-positive definite if for any nonzero

$x \in \mathbb{C}^m$ $x^HAx \geq 0$,

Symmetric positive definite, if $A^H = A$,

and for any nonzero $x \in \mathbb{C}^m$

$x^HAx > 0$,

Symmetric semi-positive definite, if

$A^H = A$,

and for any nonzero $x \in \mathbb{C}^m$

$x^H A x \geq 0$.

For example, the matrix

$$A = \begin{bmatrix} 5 & 1 \\ 1 & 4 \end{bmatrix}$$

is symmetric positive definite, because

$A^H = A^T = A$, and for any nonzero $x \in \mathbb{C}^2$

$$x^H A x = [\bar{x}_1, \bar{x}_2] \begin{bmatrix} 5 & 1 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = [\bar{x}_1, \bar{x}_2] \begin{bmatrix} 5x_1 + x_2 \\ 5x_1 + 4x_2 \end{bmatrix}$$

$$= 5x_1\bar{x}_1 + x_2\bar{x}_1 + x_1\bar{x}_2 + 4x_2\bar{x}_2$$

On the other hand, we have

$$|\mathbf{x_1} + \mathbf{x_2}|^2 = (\mathbf{x_1} + \mathbf{x_2})\overline{(\mathbf{x_1} + \mathbf{x_2})} = (\mathbf{x_1} + \mathbf{x_2})(\bar{\mathbf{x}}_1 + \bar{\mathbf{x}}_2)$$

$$= \boldsymbol{x_1\bar{x}_1 + x_2\bar{x}_1 + x_1\bar{x}_2 + x_2\bar{x}_2}$$

Then,

$$\boldsymbol{x^H A x = |x_1 + x_2|^2 + 4x_1\bar{x}_1 + 3x_2\bar{x}_2 = |x_1 + x_2|^2 + 4|x_1|^2 + 3|x_2|^2 > 0}$$

2. Drazin inverse

Drazin inverse is in fact a generalization of the inverse of a square matrix. It is extended to the case that a square matrix has no custom inverse. Before that we need to define the index of a matrix [5,9,11].

2.1 Index of a matrix

For a square matrix A, the index of A, denoted by $ind(A)$, is the smallest nonnegative integer number k such that [8]

$rank(A^{k+1}) = rank(A^k)$,

where $rank(A)$ shows the rank of the matrix A.

Example. For any identity matrix I,

$I^1 = I^0 = I$,

and so, $rank(I^1) = rank(I^0)$.

Therefore, $ind(A) = 0$.

Example Consider the following matrix:

$$\boldsymbol{A} = \begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{3} \\ \mathbf{5} & \mathbf{2} & \mathbf{6} \\ \mathbf{-2} & \mathbf{-1} & \mathbf{-3} \end{bmatrix}$$

It is seen that

$rank\ (A^4) = rank(A^3)$.

So, $ind(A) = 3$.

2.2 Drazin-inverse matrix [2]

Let A be a real or complex square matrix of dimension $n \times n$ with $ind(A) = k$.

The matrix A^D is called the Drazin inverse of A, if it satisfies the following three conditions:

1- $A \times A^D = A^D \times A$,

2- $A^D \times A \times A^D = A^D$,

3- $A^k \times A^D \times A = A^k$.

2.3 Nilpotent of a matrix [12]

A square matrix N is nilpotent of order k, if

$N^k = 0,$ (2.1)

where k is the smallest positive integer number satisfying (2-1).

Example: For the matrix

$$\boldsymbol{A} = \begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{3} \\ \mathbf{5} & \mathbf{2} & \mathbf{6} \\ -\mathbf{2} & -\mathbf{1} & -\mathbf{3} \end{bmatrix},$$

we have $N^3 = 0$, So, N is nilpotent of order 3.

Now, we are ready to directly compute the Drazine inverse of a square matrix. In fact, one way is to compute the Jordan canonical form of A. In other words, if

$$\mathrm{A} = \mathrm{P}\begin{bmatrix} \mathrm{C} & 0 \\ 0 & \mathrm{N} \end{bmatrix}\mathrm{P}^{-1}, \qquad (2,2)$$

in which

P is a nonsingular matrix,

C is a nonsingular matrix,

$Rank(C) = Rank(A^k)$, where k is the index of A,

N is nilpotent of order k.

In this case, the Drazin inverse A^D is directly given by

$$\mathrm{A} = \mathrm{P}\begin{bmatrix} \mathrm{C}^{-1} & 0 \\ 0 & 0 \end{bmatrix}\mathrm{P}^{-1},$$

If $ind(A) = 1$, then $N = 0$ in (2.2).

Example Compute the Drazin inverse A^D of the following matrix:

$$A = \begin{bmatrix} 2 & -3 & -5 \\ -1 & 4 & 5 \\ 1 & -3 & -4 \end{bmatrix} \quad ,$$

It is readily seen that $ind(A) = 2$ and also the eigenvalues of A are $\lambda_1 = 1$ with geometric multiplicity of $\sigma = 2$ and $\lambda_2 = 0$ with geometric multiplicity $\sigma = 1$. The Jordan canonical form of A is given as follows:

$$A = \begin{bmatrix} 0 & -1 & 1 \\ \frac{5}{3} & -\frac{1}{3} & -1 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & -1 & 1 \\ \frac{5}{3} & -\frac{1}{3} & -1 \\ -1 & 0 & 1 \end{bmatrix}^{-1} \quad ,$$

and so

$$A^D = \begin{bmatrix} 0 & -1 & 1 \\ \frac{5}{3} & -\frac{1}{3} & -1 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & -1 & 1 \\ \frac{5}{3} & -\frac{1}{3} & -1 \\ -1 & 0 & 1 \end{bmatrix}^{-1} ,$$

Because the inverse of

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Is the same matrix.

How to generate a real Singular matrix?

In this section, we produce a real matrix with positive index. In fact, we produce a singular matrix that is applicable to derive the Drazin inverse of such a matrix. For this sake, we consider the following problem that is Poisson's equation with Neumann condition [5,8]:

$$\begin{cases} -\Delta u = f \text{, in } \varphi = (0,1) \times (0,1) \\ \frac{\partial u}{\partial n} = 0, \qquad \text{on } \partial\varphi, \end{cases} \qquad (2.3)$$

Where The Laplacian operator Δ is defined by

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \ ,$$

$\partial\varphi$ denoted the boundary of φ,

The Neumann boundary condition is defined by

$$\frac{\partial u}{\partial n} = \langle \nabla u, n \rangle,$$

where n is the outward normal vector. In order to discretize the problem (2.3), we consider the uniform mesh φ_h as follows:

$$\varphi_h = \{(ih, jh) \ : \ 0 \le i, j \le M\},$$

where $(xi, yj) = (ih, jh)$ and M is a positive integer number. The parameter h is called step length and it is defined by

$h = \frac{1}{M},$

By Taylor expansion, the terms of Laplacian operator Δ can be given by

$$\frac{\partial^2 u}{\partial x^2}(x_i, y_i) = \text{"}\frac{u_{i-1,j} - 2u_{i,j+}2u_{i+1,j}}{h^2} + \vartheta(h^2),\text{"}$$

and

$$\text{"}\frac{\partial^2 u}{\partial x^2}(x_i, y_i) = \frac{u_{i,j-1} - 2u_{i,j+}2u_{i,j+1}}{h^2} + \vartheta(h^2),\text{"}$$

Hence, a discretization of Poisson's equation can be given by

$$-\left(\frac{u_{i-1,j} - 2u_{i,j+}2u_{i+1,j}}{h^2} + \frac{u_{i,j-1} - 2u_{i,j+}2u_{i,j+1}}{h^2}\right) = f_{i,j}, \qquad (2,4)$$

where $f_{i,j} = f(x_i, y_i)$. The equation (2.4) can be rewritten by

$$\frac{u_{i-1,j} - 2u_{i,j+}2u_{i+1,j}}{h^2} + \frac{u_{i,j-1} - 2u_{i,j+}2u_{i,j+1}}{h^2} = -f_{i,j} \ , 1 \le i, j \le M - 1 \qquad (2,5)$$

As Figure 2.1 shows, the scheme (2.5) is a 5-point stencil of finite difference scheme as follows [4]:

$$\begin{bmatrix} & \frac{1}{h^2} & \\ \frac{1}{h^2} & -\frac{1}{h^2} & \frac{1}{h^2} \\ & \frac{1}{h^2} & \end{bmatrix}$$

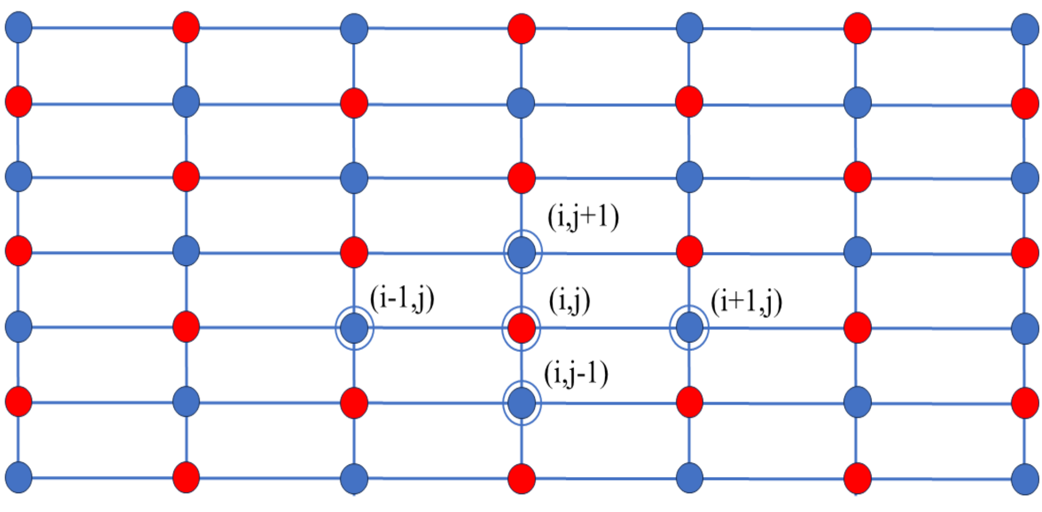

Figure 2.1. A schematic of the mesh points on unit square.

In order to apply the boundary condition, let the Neumann boundary condition is on the boundary $x = 0$. At point $(0, y_j)$, we have (see Figure 2.2)

$$0 = \frac{\partial u}{\partial x}(x_0, y_i) \times (-1), \qquad (2,6)$$

We use the central difference of first order derivative for (2.6) as follows:

$$0 = \frac{u_{1,j} - u_{-1,j}}{2h}, \qquad (2,7)$$

that implies

$$u_{1,j} = u_{-1,j} \quad , \quad j = 1,2, \cdots , M. \qquad (2,8)$$

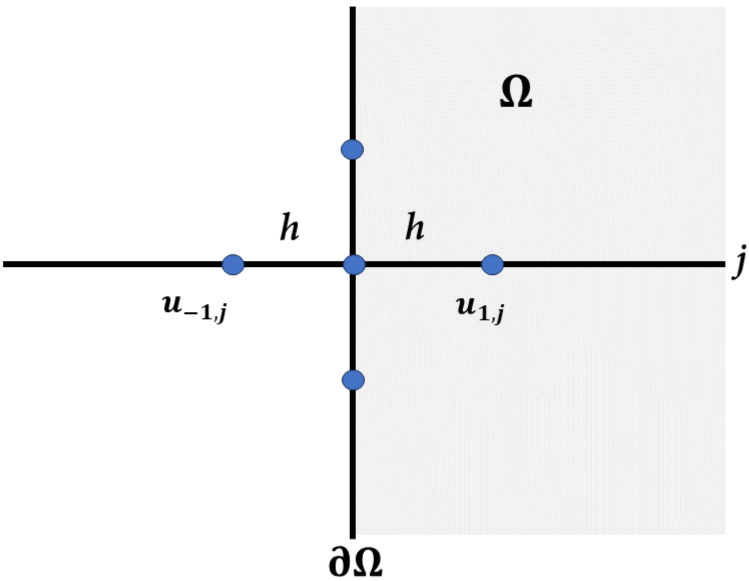

Figure 2.2. The mesh points on the lines $\boldsymbol{x} = \mathbf{0}$ and $y = \frac{j}{M}$.

Now, by (2.5), we have

$$u_{i,j+1} + u_{i,j-1} + u_{i-1,j} - 4u_{i,j} + u_{i+1,j} = -h^2 f_{i,j} , \qquad 1 \le i,j \le M \qquad (2.9)$$

For $i = 0$, by (2.8) and (2.9), we have the following extra equations:

$$u_{o,j+1} + u_{0,j-1} - 4u_{0,j} + 2u_{1,j} = -h^2 f_{i,j} \quad . \qquad (2.10)$$

Now, by (2.9) and (2.10), the structure of the matrix coefficient is as follows:

$$A_h = \begin{bmatrix}
2 & -1 & & \cdot & -1 & & & \cdot & & & \\
-1 & 3 & -1 & \cdot & & -1 & & \cdot & & & \\
 & -1 & 2 & & & & -1 & & & & \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
-1 & & & \cdot & 3 & -1 & & \cdot & -1 & & \\
 & -1 & & & -1 & 4 & -1 & & & -1 & \\
 & & -1 & \cdot & & -1 & 3 & \cdot & & & -1 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & \cdot & -1 & & & \cdot & 2 & -1 & \\
 & & & & & -1 & & & -1 & 3 & -1 \\
 & & & \cdot & & & -1 & \cdot & & -1 & 2
\end{bmatrix}$$

The matrix A_h is a singular matrix.

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