Generalized Minimal Residual (GMRes) method *

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Contents

*This is a memorandum to write down what a forgetful author studied a long time ago. Surely it contains many mistakes. Excuse me. It is appreciated if you let me know if you have any comments or suggestions.

1 Summary

GMRes method It is an iterative method which can solve a linear system with a asymmetric (non-Hermitian) coefficient matrix proposed by Y. Saad et al. GMRes method is a method of finding a solution $\mathbf{x}_k$ that minimizes the square norm $J(\mathbf{x}) = ||\mathbf{b} - \mathbf{Ax}||_2$ of residuals from all vectors $\mathbf{x}_k$ belonging to the subspace $x_0 + \mathcal{K}_k$ in the k th iteration. In other words,

GMRes method

$find\ \mathbf{x} \in x_0 + \mathcal{K}_k\ \ that\ minimize\ ||\mathbf{b} - \mathbf{Ax}||_2$

Here $\mathcal{K}_k$ is the k-dimensional Krylov subspace $\mathcal{K}_k = span\{\mathbf{r}_0, \mathbf{Ar}_0, \mathbf{A}^2\mathbf{r}_0, \cdots, \mathbf{A}^{k-1}\mathbf{r}_0\}$.

2 Basic procedure

For the sake of simplicity, first explain how to solve after m times iteration. In this method, first, m orthonormal bases are created, and a solution that minimizes the residual from the orthogonal basis is obtained. Since the magnitude of the residual is found after the iteration of the m solution, if the residuals become sufficiently small, it is not possible to terminate the iteration halfway. The method of finding out how much the residual is different for each iteration will be described later. Let $\mathbf{V}_m$ be the matrix in which the orthonormal basis $\mathbf{v}_1, \ldots, \mathbf{v}_m$ of Krylov subspace $\mathcal{K}_m$ orthonormalized using the Arnoldi method is arranged and let $\mathbf{H}_m$ matrix the coefficients in orthogonalizing Gram-Shumit. $\mathbf{H}_m$ is a Hessenberg matrix of $m+1\times m$ that satisfies $\mathbf{H}_m = 0\ for\ i > j+1$.

2.1 Expression of residuals using Hessenberg matrix

Since $\mathbf{v}_1, \ldots, \mathbf{v}_m$ was the basis of Krylov subspace $\mathcal{K}_m$, the vector $\mathbf{x}$ belonging to $\mathbf{x}_0 + \mathcal{K}_m$ can be expressed as follows.

$$\mathbf{x} = \mathbf{x}_0 + y_1\mathbf{v}_1 + y_2\mathbf{v}_2 + \cdots + y_m\mathbf{v}_m = \mathbf{x}_0 + \mathbf{V}_m\mathbf{y} \tag{1}$$

Here, $\mathbf{y}$ is a vector as follows.

$$\mathbf{y}^T = (y_1, y_2, \ldots, y_m) \tag{2}$$

We use these to calculate the residual $\mathbf{r}$ for the vector $\mathbf{x}$. $\beta = ||\mathbf{r}_0||_2$, $\mathbf{e}_1^T = (\overbrace{1, 0, \ldots, 0}^{m+1})$ and the residual $\mathbf{r}$

$$
\begin{aligned}
\mathbf{r} &= \mathbf{b} - \mathbf{A}\mathbf{x} && (3)\\
&= \mathbf{b} - A(\mathbf{x}_0 + \mathbf{V}_m\mathbf{y}) && (4)\\
&= \mathbf{r}_0 - \mathbf{A}\mathbf{V}_m\mathbf{y} && (5)\\
&= \beta\mathbf{v}_1 - \mathbf{V}_m\bar{\mathbf{H}}_m\mathbf{y} && (6)\\
&= \mathbf{V}_m(\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y}) && (7)
\end{aligned}
$$

. However, since it is $\mathbf{v}_1 = \mathbf{r}_0/||\mathbf{r}_0||_2$, it becomes $\mathbf{r}_0 = \beta\mathbf{v}_1$, and also it becomes $\mathbf{A}\mathbf{V}_m = \mathbf{V}_m\bar{\mathbf{H}}_m$ because of the nature of Arnoldi method When using these, the square norm J of the residual to be minimized is

$$
J(\mathbf{y}) = ||\mathbf{b} - \mathbf{A}\mathbf{x}||_2 = ||\mathbf{V}_m(\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y})||_2 = ||(\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y})||_2 \tag{8}
$$

. Here we used that $\mathbf{v}_1, \ldots, \mathbf{v}_m$ is an orthonormal basis. Eventually, the GMRes method can be said to be the same as searching for the vector $\mathbf{y}$ that minimizes $||(\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y})||_2$.

2.1.1 GMRes method (Hessenberg matrix)

begin enumerate item *make* $\mathbf{V}_m$ $\bar{\mathbf{H}}_m$ *with Arnoldi method* item *find* $\mathbf{y}_m \in \mathcal{R}^m$ *that minimize* $||(\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y})||_2$ item $\mathbf{x}_m = \mathbf{x}_0 + \mathbf{V}_m\mathbf{y}_m$ end enumerate

2.2 Expression of residual using upper triangular matrix

By repeating the operation of Givens rotation on the Hessenberg matrix, it can be transformed into an upper triangular matrix. Since the rotation operation does not change the norm, minimizing the norm of the residual after the rotation is the same as minimizing the norm of the residual before rotation.

2.2.1 example when m = 4

For the sake of clarity, we explain the transformation to the upper triangular matrix by taking the Hessenberg matrix $\bar{\mathbf{H}}_4$ in the case of $m = 4$ as an example.

$$
\bar{\mathbf{H}}_4 = \begin{pmatrix} h_{11} & h_{12} & h_{13} & h_{14} \\ h_{21} & h_{22} & h_{23} & h_{24} \\ & h_{32} & h_{33} & h_{34} \\ & & h_{43} & h_{44} \\ & & & h_{54} \end{pmatrix} \tag{9}
$$

Think of 5×5's matrix Ω_1 like

$$\Omega_1 = \begin{pmatrix} c_1 & s_1 & & & \\ -s_1 & c_1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \tag{10}$$

However, $s_1 = \frac{h_{21}}{\sqrt{h_{11}^2+h_{21}^2}}$, $c_1 = \frac{h_{11}}{\sqrt{h_{11}^2+h_{21}^2}}$ If this matrix Ω_1 is multiplied from the left of $\bar{\mathbf{H}}_4$ and $\bar{\mathbf{H}}_4^{(1)}$

$$\mathbf{H}_4^{(1)} = \Omega_1 \bar{\mathbf{H}}_4 = \begin{pmatrix} h_{11}^{(1)} & h_{12}^{(1)} & h_{13}^{(1)} & h_{14}^{(1)} \\ & h_{22}^{(1)} & h_{23}^{(1)} & h_{24}^{(1)} \\ & h_{32} & h_{33} & h_{34} \\ & & h_{43} & h_{44} \\ & & & h_{54} \end{pmatrix} \tag{11}$$

You can delete the $(2, 1)$ component. Likewise, consider the following 5×5 matrix Ω_2

$$\Omega_1 = \begin{pmatrix} 1 & & & & \\ & c_2 & s_2 & & \\ & -s_2 & c_2 & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \tag{12}$$

However, $s_2 = \frac{h_{32}}{\sqrt{\left(h_{22}^{(1)}\right)^2+h_{32}^2}}$, $c_2 = \frac{h_{22}^{(1)}}{\sqrt{\left(h_{22}^{(1)}\right)^2+h_{32}^2}}$ Let Ω_2 from the left of $\bar{\mathbf{H}}_4^{(1)}$ be $\bar{\mathbf{H}}_4^{(2)}$

$$\mathbf{H}_4^{(2)} = \Omega_2 \bar{\mathbf{H}}_4^{(1)} = \Omega_2 \Omega_1 \bar{\mathbf{H}}_4 = \begin{pmatrix} h_{11}^{(1)} & h_{12}^{(1)} & h_{13}^{(1)} & h_{14}^{(1)} \\ & h_{22}^{(2)} & h_{23}^{(2)} & h_{24}^{(2)} \\ & & h_{33}^{(2)} & h_{34}^{(2)} \\ & & h_{43} & h_{44} \\ & & & h_{54} \end{pmatrix} \tag{13}$$

You can delete the $(3, 2)$ component. By repeating this operation it is possible to convert the Hessenberg matrix $\bar{\mathbf{H}}_4$ into the upper triangular matrix $\bar{\mathbf{R}}_4$.

$$
\bar{\mathbf{R}}_4 = \bar{\mathbf{H}}^{(4)} = \overbrace{\Omega_4\Omega_3\Omega_2\Omega_1}^{Q_4} \bar{\mathbf{H}}_4 = Q_4\bar{\mathbf{H}}_4 = \begin{pmatrix} h_{11}^{(1)} & h_{12}^{(1)} & h_{13}^{(1)} & h_{14}^{(1)} \\ & h_{22}^{(2)} & h_{23}^{(2)} & h_{24}^{(2)} \\ & & h_{33}^{(3)} & h_{34}^{(3)} \\ & & & h_{44}^{(4)} \\ & & & 0 \end{pmatrix} \tag{14}
$$

Here we have $Q_4 = \Omega_4\Omega_3\Omega_2\Omega_1$.

2.2.2 General case

I mentioned the conversion of Hessenberg matrix to upper triangular matrix specifically in the case of $m = 4$. A general case will be described here. Consider the following matrix Ω_i

$$
\Omega_i = \begin{pmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & s_i & & & \\ & & & -s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{pmatrix} \begin{array}{l} \\ \\ \\ \leftarrow \mathit{row}\ i \\ \leftarrow \mathit{row}\ i+1 \\ \\ \\ \\ \end{array} \tag{15}
$$

However, $s_i = \frac{h_{i+1,i}}{\sqrt{\left(h_{ii}^{(i-1)}\right)^2 + h_{i+1,i}^2}}$, $c_i = \frac{h_{ii}^{(i-1)}}{\sqrt{\left(h_{ii}^{(1)}\right)^2 + h_{i+1,i}^2}}$ Considering the following matrix Q_m multiplied by Ω

$$
Q_m = \Omega_m\Omega_{m-1}\ldots\Omega_1 \tag{16}
$$

The conversion to the upper triangular matrix $\bar{R}_m$ is as follows.

$$
\bar{R}_m = \bar{\mathbf{H}}_m^{(m)} = Q_m\bar{\mathbf{H}}_m \tag{17}
$$

$$
\bar{\mathbf{g}}_m = Q_m(\beta\mathbf{e}_1) = (\gamma_1, \ldots, \gamma_{m+1})^T \tag{18}
$$

Using these, the residual $\mathbf{r}$ can be transformed as follows.

$$
\begin{aligned}
\mathbf{r} &= \mathbf{b} - \mathbf{A}\mathbf{x} && (19)\\
&= \mathbf{V}_m(\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y}) && (20)\\
&= \mathbf{V}_m Q_m^T Q_m(\beta\mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y}) && (21)\\
&= \mathbf{V}_m Q_m^T(\bar{\mathbf{g}}_m - \bar{R}_m\mathbf{y}) && (22)
\end{aligned}
$$

Using these, the square norm J of the residual to be minimized is

$$J(\mathbf{y}) = ||\mathbf{b} - \mathbf{A}\mathbf{x}||_2 = ||\mathbf{V}_m Q_m^T(\bar{\mathbf{g}}_m - \bar{R}_m\mathbf{y})||_2 = ||\bar{\mathbf{g}}_m - \bar{R}_m\mathbf{y}||_2 \quad (23)$$

become that way. However, we used that $\mathbf{V}_m Q_m^T$ is unitary. Using these, the algorithm of the GMRes method is as follows.

2.2.3 GMRes method (upper triangular matrix)

1. *make* $\mathbf{V}_m$ $\bar{\mathbf{H}}_m$ *with Arnoldi method*
2. *make* $\bar{\mathbf{g}}_m$ $\bar{R}_m$ *from* $\mathbf{H}_m$
3. *find* $\mathbf{y}_m \in \mathcal{R}^m$ *that minimize* $||\bar{\mathbf{g}}_m - \bar{R}_m\mathbf{y}||_2$
4. $\mathbf{x}_m = \mathbf{x}_0 + \mathbf{V}_m\mathbf{y}_m$

2.3 Method for finding the minimum value of residual norm using upper triangular matrix

This section describes a method for finding the value of $\mathbf{y}_m$ which minimizes the residual from the upper triangular matrix $\bar{\mathbf{R}}_m$. Let $\mathbf{g}_m$ be a vector of magnitude m excluding the $m+1$th component of $\bar{\mathbf{g}}_m$. Also assume that $\mathbf{R}_m$ is a square matrix with $m+1$ th row removed from $\bar{\mathbf{R}}_m$. the $\bar{\mathbf{R}}_m$ The zth row of the weth row has all components 0

$$||\mathbf{b} - A\mathbf{x}||_2 = ||\bar{\mathbf{g}}_m - \bar{R}_m\mathbf{y}||_2 = ||\mathbf{g}_m - R_m\mathbf{y} + \gamma_{m+1}\mathbf{e}_{m+1}||_2 \quad (24)$$

Is satisfied. Using that $\mathbf{g}_m - R_m\mathbf{y}$ and $\mathbf{e}_{m+1}$ are orthogonal to each other

$$||\mathbf{g}_m - R_m\mathbf{y} + \gamma_{m+1}\mathbf{e}_{m+1}||_2 \geq ||\gamma_{m+1}\mathbf{e}_{m+1}||_2 = |\gamma_{m+1}| \quad (25)$$

Is satisfied. Equality sign is the time of $\mathbf{y} = R_m^{-1}\mathbf{g}_m$. From the above, the vector $\mathbf{y}_m$ that minimizes the residual norm can be obtained as follows.

$$\mathbf{y}_m = R_m^{-1}\mathbf{g}_m \quad (26)$$

At this time, the minimum value of the residual norm is $|\gamma_{m+1}|$. The residual vector $\mathbf{r}_m$ at this time,

$$
\begin{aligned}
\mathbf{r}_m &= \mathbf{b} - \mathbf{A}\mathbf{x} && (27)\\
&= \mathbf{V}_m Q_m^T (\bar{\mathbf{g}}_m - \bar{R}_m \mathbf{y}_m) && (28)\\
&= \mathbf{V}_m Q_m^T (\gamma_{m+1} \mathbf{e}_{m+1}) && (29)
\end{aligned}
$$

become that way. Incidentally,

$$
\mathbf{y}_m = R_m^{-1} \mathbf{g}_m \tag{30}
$$

Calculation of R_m is an upper triangular matrix can be easily obtained using back substitution. Using these, GMRes algorithm is as follows.

2.3.1 Algorithm of GMRes method (upper triangle, back substitution)

1. *make* $\mathbf{V}_m$ $\bar{\mathbf{H}}_m$ *with Arnoldi method*
2. *make* $\bar{\mathbf{g}}_m$ $\bar{R}_m$ $from$ $\mathbf{H}_m$
3. *Compute* $\mathbf{y}_m = R_m^{-1} \mathbf{g}_m$
4. $\mathbf{x}_m = \mathbf{x}_0 + \mathbf{V}_m \mathbf{y}_m$

2.4 How to find the magnitude of residuals successively

In the past method, we have found a solution $\mathbf{x}_m$ that minimizes the square norm of the residual after making m base $\mathbf{V}_m$, but in practice the residual magnitude $||\mathbf{r}_k||_2$ is found for each iteration, It is possible to obtain a solution without wasteful repetition by getting iterated by the stage when it becomes smaller than the required smallness. Here we consider the method of updating the orthonormal basis, the upper triangular matrix, and the magnitude of the residual for each iteration.

2.4.1 Basis update

The basis vector $\mathbf{v}_{k+1}$ of the Krylov subspace generated in the k-th iteration from the algorithm of Arnordi method is normalized after orthogonalizing the vector $\omega = \mathbf{A}\mathbf{v}_k$ with the vector sequence $\mathbf{v}_1, \ldots, \mathbf{v}_k$ using Gram-Shumit's orthogonalization method or Hausholder transformation It was.

2.4.2 update upper triangular matrix

The $h_{k,1}, \ldots, h_{k,k} = (\mathbf{A}\mathbf{v}_k, \mathbf{v}_1), \ldots, (\mathbf{A}\mathbf{v}_k, \mathbf{v}_k)$ coefficient during orthogonalization when making $\mathbf{v}_{k+1}$, and the $h_{k,k+1}$ coefficient when normalizing after orthogonalization. Here put the vector $\mathbf{h}_k$ as follows.

$$\mathbf{h}_k = \{h_{k,1}, \ldots, h_{k,k+1}\} \tag{31}$$

Using this $\mathbf{h}_k$, the Hessenberg matrix $\bar{\mathbf{H}}_k$ in the k iteration is expressed as follows.

$$\bar{\mathbf{H}}_k = [\bar{\mathbf{H}}'_{k-1}, \mathbf{h}_k] \tag{32}$$

However, $\bar{\mathbf{H}}'_{k-1}$ is a matrix obtained by adding a row whose components are all zeros under the Hessenberg matrix $\bar{\mathbf{H}}_{k-1}$ in the $k-1$th iteration. Consider a method of finding the upper triangular matrix $\mathbf{R}_k$ in the k iteration from the upper triangular matrix $\mathbf{R}_{k-1}$ in $k-1$ iteration The matrix with $\mathbf{R}_k$'s bottom row with all rows of 0 elements was $\bar{\mathbf{R}}_k$. This matrix could be obtained from the Hessenberg matrix $\bar{\mathbf{H}}_k$ using the rotation matrix as follows.

$$\bar{\mathbf{R}}_k = \mathbf{Q}_k \bar{\mathbf{H}}_k = \Omega_k \Omega_{k-1} \ldots \Omega_1 \bar{\mathbf{H}}_k \tag{33}$$

Here, substitute the previous relationship in $\bar{\mathbf{H}}_k$

$$\begin{aligned}
\bar{\mathbf{R}}_k &= \Omega_k \Omega_{k-1} \ldots \Omega_1 \bar{\mathbf{H}}_k & (34)\\
&= \Omega_k \Omega_{k-1} \ldots \Omega_1 [\bar{\mathbf{H}}'_{k-1}, \mathbf{h}_k] & (35)\\
&= \Omega_k [\Omega_{k-1} \ldots \Omega_1 \bar{\mathbf{H}}'_{k-1},\ \Omega_{k-1} \ldots \Omega_1 \mathbf{h}_k] & (36)\\
&= \Omega_k [\bar{\mathbf{R}}'_{k-1},\ \tilde{\mathbf{h}}_k] & (37)
\end{aligned}$$

Here, $\bar{\mathbf{R}}'_{k-1}$ is a matrix with $\bar{\mathbf{R}}_{k-1}$'s bottom row with a row with all zero components. Ω_k was a rotation matrix whose diagonal is a unit matrix except for the diagonal element whose bottom size is 2.

$$\Omega_k = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & & c_k & s_k \\ & & & -s_k & c_k \end{pmatrix} \tag{38}$$

$\bar{\mathbf{R}}'_{k-1}$ is $\Omega_k \bar{\mathbf{R}}_{k-1} = \bar{\mathbf{R}}_{k-1}$ because the bottom two rows are 0. The rotation matrix Ω_k is chosen so that the $k+1$-th component of the vector $\Omega_k \tilde{\mathbf{h}}_k$ is zero. That is, it satisfies

$-s_k(\tilde{\mathbf{h}}_k)_k + c_k(\tilde{\mathbf{h}}_k)_{k+1} = 0$. Also Ω_k is a unitary matrix so it is $s_k^2 + c_k^2 = 1$. That is, it is $s_k = \frac{(\tilde{\mathbf{h}}_k)_{k+1}}{\sqrt{(\tilde{\mathbf{h}}_k)_k^2+(\tilde{\mathbf{h}}_k)_{k+1}^2}}$ $c_k = \frac{(\tilde{\mathbf{h}}_k)_k}{\sqrt{(\tilde{\mathbf{h}}_k)_k^2+(\tilde{\mathbf{h}}_k)_{k+1}^2}}$. With these

$$\bar{\mathbf{R}}_k = \Omega_k[\bar{\mathbf{R}}'_{k-1},\ \tilde{\mathbf{h}}_k] = [\bar{\mathbf{R}}'_{k-1},\ \Omega_k\Omega_{k-1}\ldots\Omega_1\mathbf{h}_k] \tag{39}$$

In this way, the upper triangular matrix $\mathbf{R}_k$ in the k iteration from the upper triangular matrix $\mathbf{R}_{k-1}$ in the $k-1$ iteration can be obtained.

2.4.3 Update the magnitude of residuals

The magnitude of the residual in m times iteration is expressed as $|\gamma_{m+1}|$. However, the vector γ is $\bar{\mathbf{g}}_m$ and γ_{m+1} was the $m+1$th component of the vector $\bar{\mathbf{g}}_m$. That is, the absolute value of the last component of the vector $\mathbf{g}$ is the norm of the residual. Here, we examine how the vector $\mathbf{g}$ is updated. It is expressed as $\bar{\mathbf{g}}_k = \mathbf{Q}_k(\beta\mathbf{e}_1) = \Omega_k\mathbf{Q}_{k-1}(\beta\mathbf{e}_1) = \Omega_k\bar{\mathbf{g}}'_{k-1}$. Where $\bar{\mathbf{g}}'_{k-1}$ is a vector whose size is $k+1$ by adding 0 to the last component of the k vector. Ω_k is a matrix in which diagonal elements 1 to $k-1$ are unit matrices, k components and $k+1$ components are rotation matrices $\bar{\mathbf{g}}_k$ can be obtained as follows based on the value $\bar{\mathbf{g}}_{k-1}$ of the vector one step before.

$$\bar{\mathbf{g}}_k = \Omega_k\bar{\mathbf{g}}'_{k-1} = \Omega_k\begin{pmatrix} g_{k-1,1} \\ g_{k-1,2} \\ \vdots \\ g_{k-1,k} \\ 0 \end{pmatrix} = \begin{pmatrix} g_{k-1,1} \\ g_{k-1,2} \\ \vdots \\ c_k g_{k-1,k} \\ -s_k g_{k-1,k} \end{pmatrix} = \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_k \\ -s_k g_{k-1,k} \end{pmatrix} \tag{40}$$

Therefore, the norm λ_k of the residuals at k times iteration is as follows

$$\lambda_k = |-s_k g_{k-1,k}| = |s_k||g_{k-1,k}| = |s_k|\lambda_{k-1} \tag{41}$$

Since it is $|s_k| \leq 1$, it can be confirmed that the residual will not increase. To summarize the above, at the k th iteration, first create a normal orthogonal basis $\mathbf{v}_{k+1}$ of the new Krylov subspace, multiply the coefficient vector $\mathbf{h}_k$ at the time of creating the orthonormal basis by the previous rotation matrix $\Omega_{k-1}\Omega_{k-2}\cdots\Omega_1$, Create a new rotation matrix Ω_k that reduces the size of the vector by 1, and creates an upper triangular matrix. Update the $\mathbf{g}$ vector by multiplying the new rotation matrix by the $\mathbf{g}$ vector and find the norm of the current residual from the last component of the $\mathbf{g}$ vector.

2.4.4 GMRes algorithm (sequential update type)

1. Compute $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ $\mathbf{v}_1 = \mathbf{r}_0/||\mathbf{r}_0||$
2. For $k = 1, 2, \ldots, m$ Do:

(a) $\mathbf{w} = \mathbf{A}\mathbf{v}_k$

(b) For $i = 1, 2, \ldots, k$ Do:

- $h_{k,i} = (\mathbf{w}, \mathbf{v}_i)$
- $\mathbf{w} = \mathbf{w} - h_{k,i}\mathbf{v}_i$

(c) End Do

(d) $h_{k,k+1} = \|\mathbf{w}\|_2$

(e) $\mathbf{v}_{k+1} = \mathbf{w}/\|\mathbf{w}\|_2$

(f) $Compute\ \tilde{\mathbf{h}}_k = \Omega_{k-1} \cdots \Omega_1 \mathbf{h}_k\ and\ make\ \Omega_k\ from\ \tilde{\mathbf{h}}_k$

(g) $Compute\ \bar{R}_k = [\bar{R}'_{k-1}, \Omega_k \tilde{\mathbf{h}}_k]\ and\ \bar{\mathbf{g}}_k = \Omega_k \bar{\mathbf{g}}'_{k-1}$

(h) $if\ |\bar{\mathbf{g}}_{k,k+1}| < tolerance$ Break Loop

3. End Do:

4. $Compute\ \mathbf{y}_k = R_k^{-1}\mathbf{g}_k$

5. $\mathbf{x}_k = \mathbf{x}_0 + \mathbf{V}_k \mathbf{y}_k$

2.5 Full-GMRes method, GMRes (m) method

The Full-GMRes method is a method of repeating the iteration until the norm of the residual becomes small without determining an appropriate iteration number m. The Full-GMRes method repeats iteratively indefinitely until the residual becomes small, and the orthonormal basis continues to infinitely increase until convergence. Since resources are limited on the computer, it is not realistic. The GMRes (m) method is also called restarted GMRes method. When the number of iterations reaches m, the basis of the Krylov subspace up to that point and the upper triangular matrix etc are all discarded and the iterative solution at that point is initialized (Re-start) the algorithm. It is difficult to find the optimum value of the iteration number m up to this restart. If m is smaller than a certain problem dependent value, it is known that convergence is difficult even if the restart is repeated. This method is often used.

It is a program to solve the matrix arising from

3 Preconditioned GMRes method

3.1 right front processing

We transform the equation $\mathbf{Ax} = \mathbf{b}$ to be solved as follows using the preprocessing matrix M.

$$\mathbf{AM}^{-1}\mathbf{u} = \mathbf{b}, \quad \mathbf{x} = \mathbf{M}^{-1}\mathbf{u} \tag{42}$$

This is called right front process because $\mathbf{M}^{-1}$ is hanging from the right of $\mathbf{A}$. The coefficient matrix has changed from $\mathbf{A}$ to $\mathbf{AM}^{-1}$. If the property of $\mathbf{AM}^{-1}$ is close to the unit matrix, convergence is expected to be faster than the original equation. Basically, using this preprocessing method to solve the problem with GMRes method is basically changing the $\mathbf{A}$ part to $\mathbf{AM}^{-1}$ with $\mathbf{AM}^{-1}$, finding $\mathbf{u}$, finally solving once to solve $\mathbf{u}$ without any special change. For the residuals

$$\mathbf{r} = \mathbf{b} - \mathbf{Ax} = \mathbf{b} - \mathbf{AM}^{-1}\mathbf{u} \tag{43}$$

So the residuals for $\mathbf{u}$ are also the residuals for $\mathbf{x}$ as they are. Therefore, the magnitude of the residual obtained when $\mathbf{u}$ is obtained while sequentially updating the magnitude of the residual is also the magnitude of the residual for $\mathbf{x}$. Therefore, since the magnitude of the residual can be obtained even in the middle of the iteration, the right front process is often used for sequential updating.

3.1.1 Algorithm of Preconditioned GMRes Method (Sequential Update Type)

1. Compute $\mathbf{r}_0 = \mathbf{b} - \mathbf{Ax}_0$ $\mathbf{v}_1 = \mathbf{r}_0/||\mathbf{r}_0||$
2. For $k = 1, 2, \ldots, m$ Do:
   (a) $\mathbf{w} = \mathbf{AM}^{-1}\mathbf{v}_k$
   (b) For $i = 1, 2, \ldots, k$ Do:
      - $h_{k,i} = (\mathbf{w}, \mathbf{v}_i)$
      - $\mathbf{w} = \mathbf{w} - h_{k,i}\mathbf{v}_i$
   (c) End Do
   (d) $h_{k,k+1} = ||\mathbf{w}||_2$
   (e) $\mathbf{v}_{k+1} = \mathbf{w}/||\mathbf{w}||_2$
   (f) *Compute* $\tilde{\mathbf{h}}_k = \Omega_{k-1} \cdots \Omega_1 \mathbf{h}_k$ *and make* Ω_k *from* $\tilde{\mathbf{h}}_k$
   (g) *Compute* $\bar{R}_k = [\bar{R}'_{k-1}, \Omega_k \tilde{\mathbf{h}}_k]$ *and* $\bar{\mathbf{g}}_k = \Omega_k \bar{\mathbf{g}}'_{k-1}$
   (h) *if* $|\bar{\mathbf{g}}_{k,k+1}| < tolerance$ Break Loop
3. End Do:
4. *Compute* $\mathbf{y}_k = R_k^{-1}\mathbf{g}_k$
5. $\mathbf{u}_k = \mathbf{u}_0 + \mathbf{V}_k\mathbf{y}_k$
6. $\mathbf{x}_k = \mathbf{M}^{-1}\mathbf{u}_k$

This is a program to solve the matrix arising from

4 GMRes method for complex matrix

Basically, the GMRes method and the procedure for the real number matrix are the same, but in the case of the complex matrix, care is required only in the way of Givens rotation. Assuming that the rotation matrix is Ω, the rotation matrix does not change the value of the inner product so that for any complex vector $\mathbf{a}, \mathbf{b}$ the following holds.

$$(\Omega\mathbf{a}, \Omega\mathbf{b}) = (\mathbf{a}, \Omega^*\Omega\mathbf{b}) = (\mathbf{a}, \mathbf{b}) \tag{44}$$

That is, it turns out that it is a Hermetian matrix $\Omega^*\Omega = \mathbf{I}$. If we assume that the rotation Ω_i is a rotation in the $i, i+1$ plane, all but the $i, i+1$ component do not change. That is, Ω can be found to be an identity matrix except for $i, i+1$. So let Ω_i' be the small matrix for $i, i+1$. That is, Ω has the following matrix

$$\Omega_i = \begin{pmatrix} \mathbf{I} & & \\ & \Omega_i' & \\ & & \mathbf{I} \end{pmatrix} \leftarrow row\ i\ i+1 \tag{45}$$

In this case, in order for Ω_i to be a Hermitian matrix, the small matrix Ω_i' must also be a Hermitian matrix. Also, Ω_i is a vector The second component of $\Omega_k' \begin{pmatrix} (\tilde{\mathbf{h}}_k)_k \\ (\tilde{\mathbf{h}}_k)_{k+1} \end{pmatrix}$ was chosen to be zero. Ω_i' is not uniquely determined from the condition that these two conditions, that is, the condition that it is a Hermitian matrix, and the condition that the last component of the product with the vector $\tilde{\mathbf{h}}_k$ is 0. In other words, you can choose Ω_i' as long as these two conditions are satisfied. For example, here we consider Ω_i' as a matrix such that

$$\Omega_i' = \begin{pmatrix} c_k & \bar{s}_k \\ -s_k & c_k \end{pmatrix} \tag{46}$$

However, c_k is a real number. Then, the condition that Ω_i' is a Hermitian matrix can be written as follows.

$$c_k^2 + \bar{s}_k s_k = 1 \tag{47}$$

Also, the condition that the last component of the product with the vector $\tilde{\mathbf{h}}_k$ is 0 is as follows:

$$-s_k(\tilde{\mathbf{h}}_k)_k + c_k(\tilde{\mathbf{h}}_k)_{k+1} = 0 \tag{48}$$

When solving these, c_k, s_k becomes as follows.

$$c_k = \frac{||(\tilde{\mathbf{h}}_k)_k||}{\sqrt{(||\tilde{\mathbf{h}}_k)_k^2|| + ||(\tilde{\mathbf{h}}_k)_{k+1}^2||}} \quad s_k = c_k \frac{(\tilde{\mathbf{h}}_k)_{k+1}}{(\tilde{\mathbf{h}}_k)_k} \tag{49}$$

For example, using the rotation matrix Ω_i' with s_k, c_k like this, we can solve the complex matrix using the GMRes method. In the case of a complex number, it is $h_{k,i} = (\mathbf{w}, \mathbf{v}_i) \neq (\mathbf{v}_i, \mathbf{w})$. Attention is necessary because it is easy to make a mistake and it is easy to get into a bug.