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A New Stopping Rule: GMRES for Linear Discrete Ill-posed Problems

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Abstract

The GMRES is a commonly used iterative method for the numerical solution of a system of linear equations derived from the Fredholm integral equation of the first kind. Such a system of linear equation is categorized as a linear discrete ill-posed problem. It has been analyzed by many researchers to illustrate various phenomena. However, its property as an ill-posed problem has resulted in many unresolved issues. Our proposed stopping rule is based on the Tikhonov regularization, which is one of the traditional regularization methods for an ill-posed problem. The conventional way to stop the iteration of the GMRES is to employ the relative residual norm. This, however, does not work for any ill-posed problems. In this study, we are proposing a new stopping rule for the GMRES, utilizing a simplified Tikhonov value to stop the iteration appropriately. Numerical experiments have been used to illustrate the effectiveness of this proposed algorithm.

1 Introduction

The GMRES is one of the popular iterative methods for the numerical solution of a system of linear equations:

$$A\boldsymbol{x} = \boldsymbol{b}, \quad A \in \mathbb{R}^{n\times n},\ \boldsymbol{b},\ \boldsymbol{x} \in \mathbb{R}^n, \tag{1}$$

where the coefficient matrix A is non-symmetric. This paper specifically studies the type of linear systems derived from the discretization of Fredholm integral equations of the first kind, which are classified as a linear discrete ill-posed problem. These problems commonly occur during the restoration of blurred satellite images, computed tomography images, oil exploration and gravity surveys.

Ill-posed problems are unable to secure at least one of following: uniqueness, existence and/or stability of a solution. To resolve this issue, regularization methods are often applied

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to them to enable arrival at a meaningful solution. With small problems, regularization methods related to singular value decomposition is a viable alternative. However, problems of computational effort and accuracy arise when dealing with solutions to large-scale problems. Currently, Krylov subspace methods are the most frequently used regularization method for large-scale problems. Björck [2], Hanke [6, Ch.4] and Hansen [8] illustrated the effectiveness of the conjugate gradient (CG), one of the Krylov subspace methods, as a plausible regularization method for linear discrete ill-posed problems. However, when coefficient matrix A is non-symmetric, methods utilizing the CG are rendered ill-conditioned for use during the step of introducing a normal equation of (1). The GMRES, another Krylov subspace method works better than the CG in such a situation, because the GMRES can solve non-symmetric linear systems. Calvetti et al. [3] suggested using the GMRES for linear discrete ill-posed problems and proposed the RRGMRES. The RRGMRES is a modified GMRES restricting the Krylov subspace within the range of A to make solutions more stable [4]. The augmented GMRES/RRGMRES proposed by Baglama et al. [1] supplements a user-supplied subspace to the Krylov subspace generated by the GMRES/RRGMRES to improve the accuracy of approximate solutions and to reduce the number of iterations necessary. Kuroiwa et al. [9, 10] proposed the adaptive augmented GMRES/RRGMRES to automate the selection of subspaces to augment, when applying the augmented GMRES/RRGMRES. While these GMRES algorithms work well as a regularization method, they do not have an adequate stopping rule like the residual norm in well-posed problems. The residual norm can be obtained naturally in the steps of the GMRES, but it does not work as a stopping rule for linear discrete ill-posed problems. The reasons for this will be discussed in the following section. Our findings indicate that the GMRES for linear discrete ill-posed problems is inadequate for determining an appropriate solution. From this perspective, we have attempted to modify the GMRES and have incorporated a new stopping rule for linear discrete ill-posed problems.

Linear discrete ill-posed problems are discussed in Section 2, followed by a proposal of the simplified Tikhonov value along with a modification of the GMRES as a new index for terminating the iterations of the GMRES in Section 3. In Section 4, numerical experiments are used to illustrate the effectiveness of this method. Lastly in Section 5 which constitutes the conclusion of this paper, there is a short discussion on the future issues that need to be resolved.

2 Linear Discrete Ill-posed Problems

When we discretize a linear Fredholm integral equation of the first kind such as:

$$\int_a^b K(s,t) f(t)\, dt = g(s), \quad c \le s \le d, \tag{2}$$

where $K(s,t)$ and $g(s)$ are known smooth functions and $f(t)$ is a desired unknown function, a linear system of equation (1) is obtained. The functions $g(s)$ and $K(s,t)$ correspond to a measurement value and a phenomenon making $f(t)$ change, respectively. The Fredholm integral equation of the first kind is one of the models of an inverse problem. Inverse problems are often ill-posed and when this is the case, the derived linear systems become ill-conditioned. The coefficient matrix A in equation (1) derived from equation (2) is characterized by a property wherein the larger the problem scale n becomes, the more the singular values are likely to cluster around zero. This property means that the larger n becomes, the larger the condition number of A is likely to be. Thus, the derived linear system (1) is rendered sensitive to the perturbation of each element. In particular, the right hand side vector $\boldsymbol{b}$ is often contaminated by measurement error $\boldsymbol{b}_{\mathrm{error}}$ as a perturbation in the following manner:

$$\tilde{\boldsymbol{b}} = \boldsymbol{b} + \boldsymbol{b}_{\mathrm{error}}. \tag{3}$$

If only the contaminated vector $\tilde{\boldsymbol{b}}$ is known, the following system is rendered inconsistent:

$$A\boldsymbol{x} \neq \boldsymbol{b}. \tag{4}$$

Applying the GMRES to a known set of $A, \tilde{\boldsymbol{b}}$ solves the following system of equation and obtains the approximate solution to $\tilde{\boldsymbol{x}}$.

$$A\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{b}}. \tag{5}$$

The GMRES will generate an approximate solution which has a minimum residual norm in the Krylov subspace $\mathcal{K}_j$:

$$\mathcal{K}_j(A, \tilde{\boldsymbol{r}}_0) = \mathrm{span}\{\tilde{\boldsymbol{r}}_0, A\tilde{\boldsymbol{r}}_0, \ldots, A^{j-1}\tilde{\boldsymbol{r}}_0\}, \tag{6}$$

where the index j is an iteration number, $\tilde{\boldsymbol{r}}_0$ is the initial residual $\tilde{\boldsymbol{r}}_0 = \tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}_0$ in equation (5), and $\tilde{\boldsymbol{x}}_0$ is the initial guess. When we apply GMRES to a discrete ill-posed problem, an appropriate approximate solution $\tilde{\boldsymbol{x}}_j$ is determined by a constraint which helps the approximate solution $\tilde{\boldsymbol{x}}_j$ becomes closer to the exact solution $\boldsymbol{x}$. Therefore, we solve the least squares problem with constraint Ψ as follows:

$$\min_{\tilde{\boldsymbol{x}} \in \tilde{\boldsymbol{x}}_0 + \mathcal{K}_j(A, \tilde{\boldsymbol{r}}_0)} \|\tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}\|_2 \quad \text{subject to} \quad \tilde{\boldsymbol{x}}_j \text{ satisfies } \Psi, \tag{7}$$

where the most ideal constraint is:

$$\Psi: \ \min \| \tilde{\boldsymbol{x}}_j - \boldsymbol{x} \|_2. \tag{8}$$

It is unrealistic to use the exact solution $\boldsymbol{x}$ in this scenario, and it has made it necessary to investigate other constraints to determine an appropriate approximate solution without the use of $\boldsymbol{x}$.

In a classical GMRES, the constraint Ψ for GMRES to equation (1), requires that the relative residual norm $\|\boldsymbol{r}_j\|/\|\boldsymbol{r}_0\|$ becomes small enough. However, when solving discrete ill-posed problems, not only does $\tilde{\boldsymbol{b}}$ including perturbation cause equation (5) to become unstable. It also fails to guarantee that the resulting approximate solution $\tilde{\boldsymbol{x}}_j$ will get closer to $\boldsymbol{x}$ when the iteration number j becomes larger. The instability of this system can increase the margin of error of the approximate solution as the iterations of the GMRES proceeds.

Due to this, the norm of residual $\tilde{\boldsymbol{r}}_j = \tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}_j$ from equation (5) fails to play the role of the index to halt the iterations of the GMRES for linear discrete ill-posed problems.

Calvetti et al. [5] proposed condition L-curves for determinating an adequate approximate solution. Condition L-curves use a condition number of a matrix appearing in each iteration step of the GMRES. Unfortunately, there are two issues with this method. Expensive and complicated computation is required to calculate the condition number of the matrices. Additionally, there is the unresolved issue of when the iteration of the GMRES should be stopped. With this background in mind, we have explored the possibility of using a new constraint. This not only enables us to determine a suitable approximate solution, but also to stop the iteration of the GMRES without additional computations. Details of the new constraint follows.

3 Modified GMRES Utilizing a New Stopping Rule

This section discusses a new modified GMRES that addresses some of the issues posed by discrete ill-posed problems. The new method introduces a new constraint, which uses a certain value based on Tikhonov regularization to generate adequate approximate solutions.

3.1 Tikhonov Regularization

The Tikhonov regularization [13] is one of the popular classical regularization methods. When solving equation (5) with this method, the desired approximate solution is generated by the least squares problem as follows:

$$\min_{\tilde{\boldsymbol{x}}} \{\|\tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}\|_2^2 + \lambda\|L\tilde{\boldsymbol{x}}\|_2^2\}, \tag{9}$$

where $\lambda \in \mathbb{R}$ is the Tikhonov regularization parameter and $L \in \mathbb{R}^{n\times n}$ is the Tikhonov regularization matrix. In this example, the identity matrix I, the diagonal matrix, or the matrix yielding the first or second derivative are often used as L. The identity matrix I affects nothing, but the other matrices are applied to reduce the effects of perturbation. The Tikhonov regularization matrix L is determined a priori because the appropriate L will be different for each problem. For simplicity's sake, $L = I$. In addition, it should be noted that there is no confirmed way to determine the exact λ. In most cases, the most likely parameter is found through running a few numerical experiments and identifying which one appears to produce a smooth approximate solution. In relation to the Krylov subspace methods as regularization methods, Lewis [11] proposed the RRAT method, which includes a scheme to calculate λ, to solve linear discrete ill-posed problems.

We considered utilizing the philosophy of the Tikhonov regularization method as constraint Ψ for the GMRES in formula (9). As shown in (9), the Tikhonov regularization determines the approximate solution which minimizes the sum of the residual norm and solution norm with λ and L. The Tikhonov regularization parameter λ and matrix L seem to play a role in balancing the effect of the norms. The parameter is key to determining the approximate solution. This means that it is integral to balance the effect of the norms. Hence, the new formula:

$$\log_j \|\tilde{\boldsymbol{r}}_j\|_2^2 + \log_j \|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2^2. \tag{10}$$

When applying the GMRES, the residual norm decreases as the number of iterations increases. Simultaneously, small unknown errors in $\tilde{\boldsymbol{b}}$ are enhanced by singular values close to zero. The resulting approximate solution $\tilde{\boldsymbol{x}}_j$ would have a large norm due to the enhanced errors as the iterations proceed. This suggests that the difference between them would grow, in correspondence to the iteration number. Logarithms in formula (10) help to scale their magnitudes. It should be noted that the change of the residual norm and the solution norm will affect the iteration number j. In view of this property, j was set to be the base of each logarithm.

This is why the solution norm is used as an index to measure how much difference the perturbation is causing, as the number of iterations proceeds. The norm $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$ is used to omit the effects of the initial guess $\tilde{\boldsymbol{x}}_0$.

Formula (10) can be rewritten as follows:

$$\begin{aligned}\log_j \|\tilde{\boldsymbol{r}}_j\|_2^2 + \log_j \|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2^2 &= 2\log_j \|\tilde{\boldsymbol{r}}_j\|_2 + 2\log_j \|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2 \\ &= 2(\log_j \|\tilde{\boldsymbol{r}}_j\|_2 \|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2),\end{aligned}$$

where we define τ_j as the Tikhonov value:

$$\tau_j = \log_j \|\tilde{\boldsymbol{r}}_j\|_2 \|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2. \tag{11}$$

Using τ_j, a new constraint Ψ_j can be defined based on the Tikhonov regularization:

$$\Psi_j \colon \tau_j < \tau_{j-1}. \tag{12}$$

3.2 Derivation of the Simplified Tikhonov Value

The constraint Ψ_j is applied to the GMRES here. τ_j in Ψ_j consists of the residual norm $\|\tilde{\boldsymbol{r}}_j\|_2$ and $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$. In consideration of the constraint Ψ_j being applied to the GMRES, the Tikhonov value τ_j in Ψ_j consists of the residual norm and the norm $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$ with an approximate solution. The calculation of the Tikhonov value τ_j can be simplified, by using the approximate values obtained from the GMRES iterations.

3.2.1 Approximation of the Residual Norm

It is a given that the residual norm is approximated by certain values in the steps of a GMRES. When applying a classical GMRES to a system of linear equations (5), the Arnoldi decomposition of A after j iterations is expressed as follows:

$$AV_j = V_{j+1}H_j, \tag{13}$$

where the columns of $V_j \in \mathbb{R}^{n\times j}$ are the orthonormal basis of the Krylov subspace $\mathcal{K}(A, \tilde{\boldsymbol{r}}_0)$ and $H_j \in \mathbb{R}^{(j+1)\times j}$ is an upper-Hessenberg matrix. The approximate solution $\tilde{\boldsymbol{x}}_j$ in the Krylov subspace $\mathcal{K}(A, \tilde{\boldsymbol{r}}_0)$ is written as follows:

$$\tilde{\boldsymbol{x}}_j = \tilde{\boldsymbol{x}}_0 + V_j\boldsymbol{y}_j. \tag{14}$$

Using relations (13) and (14), the jth residual is rewritten as follows (see Saad [12]):

$$\begin{aligned}\tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}_j &= \tilde{\boldsymbol{b}} - A(\tilde{\boldsymbol{x}}_0 + V_j\boldsymbol{y}) \\ &= \tilde{\boldsymbol{r}}_0 - V_{j+1}H_j\boldsymbol{y} \\ &= V_{j+1}(\|\tilde{\boldsymbol{r}}_0\|_2\boldsymbol{e}_1 - H_j\boldsymbol{y}) \\ &= V_{j+1}G_j^T G_j(\|\tilde{\boldsymbol{r}}_0\|_2\boldsymbol{e}_1 - H\boldsymbol{y}) \\ &= V_{j+1}G_j^T(\tilde{\boldsymbol{g}}_j - R_j\boldsymbol{y}),\end{aligned}$$

where $\boldsymbol{y} \in \mathbb{R}^j$, $G_j = \Pi_1^{i=j}\Omega_i$ and Ω_i is a Givens rotation matrix. Let γ_j be a last element of $\tilde{\boldsymbol{g}}_j$, and $\tilde{\boldsymbol{g}}'_j$ and R'_j be a vector and matrix which will remove the last element of $\tilde{\boldsymbol{g}}_j$ and the last row of R_j. As G_j and V_j are both orthogonal matrices, the norm of the residual is written as follows:

$$\|\tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}_j\|_2 = \|\tilde{\boldsymbol{g}}'_j - R'_j\tilde{\boldsymbol{y}}_j\|_2 + |\gamma_j| \tag{15}$$

$$\boldsymbol{y}_j = \underset{\boldsymbol{y}}{\operatorname{argmin}} \|\tilde{\boldsymbol{g}}'_j - R'_j\boldsymbol{y}\|_2, \tag{16}$$

where $\boldsymbol{y}_j$ minimizes the norm $\|\tilde{\boldsymbol{g}}'_j - R'_j\boldsymbol{y}\|_2$, i.e. the approximate solution of the linear system of equations $R'\boldsymbol{y} = \boldsymbol{g}'_j$. Since the resulting norm $\|\boldsymbol{g}'_j - R'_j\boldsymbol{y}_j\|_2$ must be small enough, the residual norm can be approximated as follows:

$$\|\tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}_j\|_2 \approx |\gamma_j|. \tag{17}$$

3.2.2 Approximation of the Solution Norm

Consider the norm $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$ with the approximate solution. Using relations (13) and (14), the norm can be rewritten as follows:

$$\begin{aligned}\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2 &= \|\tilde{\boldsymbol{x}}_0 + V_j\boldsymbol{y}_j - \tilde{\boldsymbol{x}}_0\|_2 \\ &\leq \|V_j\boldsymbol{y}_j\|_2.\end{aligned}$$

Moreover, since V_j has orthonormal columns, the norm is approximated as follows:

$$\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2 \leq \|\boldsymbol{y}_j\|_2. \tag{18}$$

3.2.3 The Simplified Tikhonov value

It has been confirmed that the residual norm $\|\tilde{\boldsymbol{r}}_j\|_2$ and the norm $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$ are approximated to equations (17) and (18), respectively. The Tikhonov value τ_j introduces the following relation:

$$\begin{aligned}\tau_j &= \log_j(\|\tilde{\boldsymbol{r}}_j\|_2 \, \|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2) \\ &\lessapprox \log_j(|\gamma_j| \, \|\boldsymbol{y}_j\|_2),\end{aligned}$$

where we define τ_j^S as the simplified Tikhonov value:

$$\tau_j^S = \log_j(|\gamma_j| \, \|\boldsymbol{y}_j\|_2). \tag{19}$$

As elements constructing the simplified Tikhonov value do not need extra computations, the calculation of τ_j^S allows us to omit the following computations from τ_j:

1. Solve system $R'\boldsymbol{y} = \boldsymbol{g}'$ ($O(j^2)$)
2. Compute $\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0 = V\boldsymbol{y}_j$ ($O(jn)$)
3. Compute $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$ ($O(n)$)

3.3 The Modified Algorithm of the GMRES

The other alternative for a new constraint Ψ_j^S, using the simplified Tikhonov value τ_j^S, is defined as follows:

$$\Psi_j^S : \tau_j^S < \tau_{j-1}^S. \tag{20}$$

The following problem is redefined with Ψ_j^S:

$$\min_{\tilde{\boldsymbol{x}} \in \tilde{\boldsymbol{x}}_0 + \mathcal{K}_j(A, \tilde{\boldsymbol{r}}_0)} \|\tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}\|_2 \quad \text{subject to} \quad \tilde{\boldsymbol{x}}_j \text{ satisfies } \Psi_j^S. \tag{21}$$

This means that the iterations to generate the approximate solution will proceed until the simplified Tikhonov value τ_j^S increases. When value τ_j^S increases, the iterations of the GMRES will stop and it will determine the approximate solution $\tilde{\boldsymbol{x}}_j = \tilde{\boldsymbol{x}}_{j-1}$. In this manner, the simplified Tikhonov value can be used as an index of a stopping criteria for the GMRES. In addition, it can determine the appropriate approximate solution automatically.

Figure 1 is the aforementioned modified algorithm of the GMRES, using the simplified Tikhonov value. Steps 4–14 generate the orthonormal basis of the Krylov subspace, and the simplified Tikhonov value τ_j^S is computed at step 11. If the dimension of the Krylov subspace is larger than 2 and τ_j^S is less than τ_{j-1}^S, the iteration continues. If τ_j^S increases or the iteration number is maximized, the final approximate solution is determined in step 15.

4 Numerical Experiments

In this section, numerical experiments were used to illustrate the effectiveness of the modified GMRES with the simplified Tikhonov value shown in Figure 1. All computations were run on the following equipment:

- Computer : ThinkPad X201s
- CPU : Intel(R) Core(TM) i7 2.13GHz
- OS : Ubuntu 10.10

Input $A \in \mathbb{R}^{n\times n}, \tilde{\boldsymbol{x}}_0, \tilde{\boldsymbol{b}} \in \mathbb{R}^n, m$
Output $\tilde{\boldsymbol{x}}_j$
$\tilde{\boldsymbol{r}}_0 := \tilde{\boldsymbol{b}} - A\tilde{\boldsymbol{x}}_0, \boldsymbol{v}_1 := \tilde{\boldsymbol{r}}_0$
For $j = 1, \ldots, m$ do
  $\boldsymbol{w}_j := A\boldsymbol{v}_j$
  For $i = 1, \ldots, j$ do
    $h_{ij} := (\boldsymbol{w}_j, \boldsymbol{v}_i)$
    $\boldsymbol{w}_j := \boldsymbol{w}_j - h_{ij}\boldsymbol{v}_i$
  End for
  $h_{j+1,j} := \|\boldsymbol{w}_j\|_2$
  $\boldsymbol{v}_{j+1} := \boldsymbol{w}_j / h_{j+1,j}$
  Compute $\boldsymbol{y}_j$ of (16)
  Compute τ_j^S of (19)
  If $j > 2$ and $\tau_j^S > \tau_{j-1}^S$ then
    Set $j = j - 1$ and break
End for
$\tilde{\boldsymbol{x}}_j := \tilde{\boldsymbol{x}}_0 + V_j \boldsymbol{y}_j$

Figure 1: The Modified GMRES Using the Simplified Tikhonov Value

Table 1: Properties of the Numerical Experiments

	function	A	$\|A^{-1}\|_2\|A\|_2$
Ex.1	`foxgood`	Symmetric	1.85×10^{19}
Ex.2	`baart`	Non-symmetric	2.55×10^{19}
Ex.3	`gravity`	Non-symmetric	1.80×10^{22}

- Software : Octave 3.2.4

These methods were applied under the conditions detailed below:

- Initial guess : $\tilde{\boldsymbol{x}}_0 = \boldsymbol{0}$
- Elements of $\boldsymbol{b}_{\text{error}}$: normal random numbers with 0 mean and 1.0×10^{-5} variance

The Fredholm integral equations of the first kind which are used as test problems in the "Regularization Tools" by Hansen [7] were implemented. "Regularization Tools" is a MATLAB package including functions to analyze linear discrete ill-posed problems. The properties of each experiment are shown in Table 1. One symmetric problem and two non-symmetric problems were solved. The second non-symmetric problem was derived from a real world problem. In every experiment, the problem (21) with A, $\boldsymbol{b}$, $\boldsymbol{x}$ discretized by the functions of the "Regularization Tools" were considered.

In each of the numerical experiments, the behavior of the simplified Tikhonov value τ_j^s versus the Tikhonov value τ_j were compared. Further to this, the performance of the

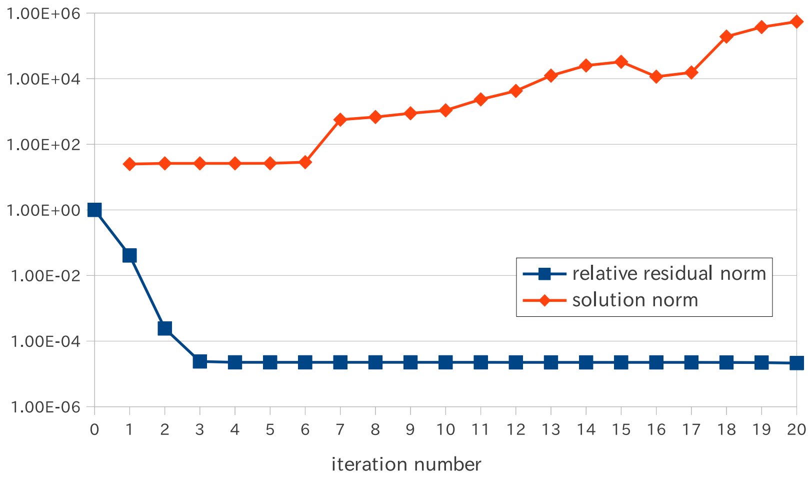

Figure 2: Numerical Experiment 1: The Relative Residual Norm $\|\tilde{\boldsymbol{r}}_j\|_2/\|\tilde{\boldsymbol{r}}_0\|_2$ and the Solution Norm $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$ by GMRES

modified GMRES with the simplified Tikhonov value versus the classical GMRES were also compared and evaluated

4.1 Numerical Experiment 1

The first experiment dealt with the Fredholm integral equation of the first kind:

$$\int_0^1 (s^2 + t^2)^{\frac{1}{2}} f(t)\, dt = \frac{1}{3}\left((1 + s^2)^{\frac{3}{2}} - s^3\right), \quad 0 \le s \le 1, \tag{22}$$

where the exact solution $f(t) = t$. In this particular case, $A, \boldsymbol{b}, \boldsymbol{x}$ were generated on Octave by using the `foxgood(2048)` command.

The results of the classical GMRES are shown in Figure 2, 3 and 4. Figure 2 shows the history of the relative residual norm $\|\tilde{\boldsymbol{r}}_j\|_2/\|\tilde{\boldsymbol{r}}_0\|_2$ and $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$ corresponding to the iteration numbers. The former decreases, then stagnates, while the latter increases. Thus, the difference between them grows as the iterations proceed. Figure 3, illustrates the changes in the absolute values $|\tau_j - \tau_j^S|$ of the Tikhonov value τ_j and the simplified Tikhonov value τ_j^S. Even though it may appear to be increasing, it should be noted that the value at the 20th iteration is less than 1.0×10^{-9}. This indicates that the simplified Tikhonov value τ_j^S has enough accuracy for τ_j. In Figure 4, the relative error norm $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}_j\|_2/\|\boldsymbol{x}\|_2$ and the simplified Tikhonov value τ_j^S were compared. The features of their history appear to be similar. In particular, it should be noted that they become minimal at the same iteration.

The results from the exercises with the GMRES with constraints Ψ in (8), Ψ_j in (12) and Ψ_j^S in (20) have been tabulated in Table 2. Each resulted in the same relative error norm. In Figure 4, it is shown that the simplified Tikhonov value increases at the 4th iteration for

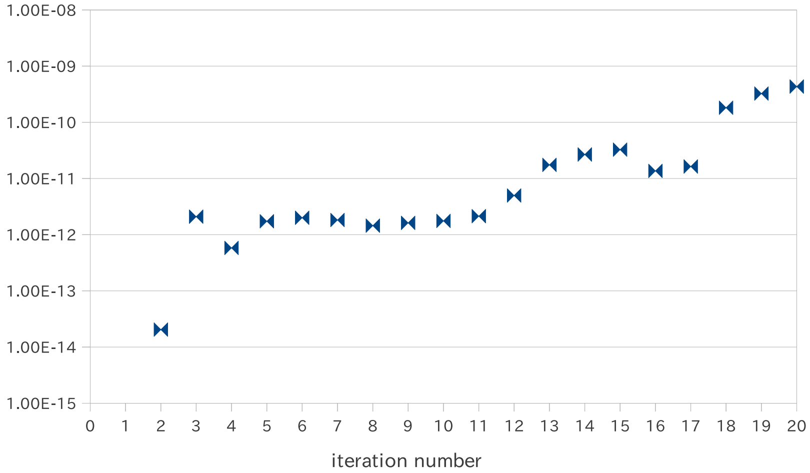

Figure 3: Numerical Experiment 1: The Distance between Tikhonov Value τ_j and the Simplified Tikhonov Value τ_j^S by GMRES

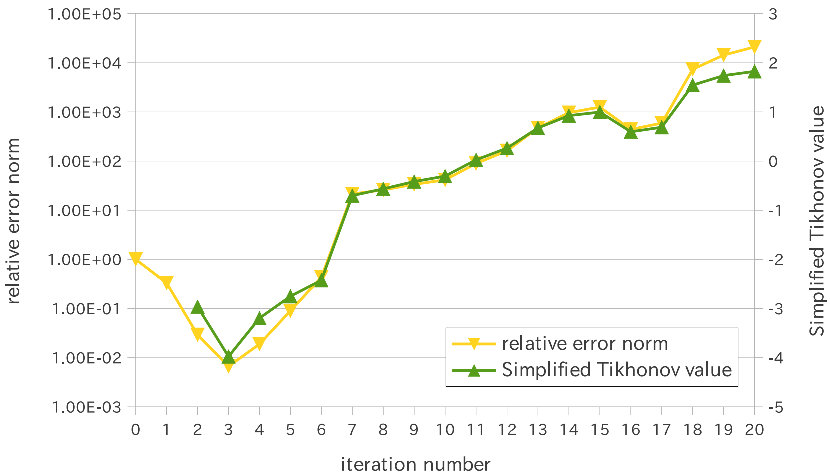

Figure 4: Numerical Experiment 1: The Relative Error Norm $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}_j\|_2 / \|\boldsymbol{x}\|_2$ and the Simplified Tikhonov Value τ_j^S by GMRES

Table 2: Numerical Experiment 1: A Comparison of Each Constraint for the GMRES

Constraint	Iteration Count	Achieved Relative Error Norm	Time (Sec.)
Ψ	3	6.66×10^{-3}	–
Ψ_j	4	6.66×10^{-3}	0.05
Ψ_j^S	4	6.66×10^{-3}	0.03

Table 3: Numerical Experiment 2: A Comparison of Each Constraint for the GMRES

Constraint	Iteration Count	Achieved Relative Error Norm	Time (Sec.)
Ψ	3	3.61×10^{-2}	–
Ψ_j	4	3.61×10^{-2}	0.05
Ψ_j^S	4	3.61×10^{-2}	0.04

the first time. This indicates that the constraint Ψ_4^S determines the final approximate solution $\tilde{\boldsymbol{x}}_4 = \tilde{\boldsymbol{x}}_3$. Further to this, these exercises suggest that the GMRES converges faster when using Ψ_j^S rather than Ψ_j.

The results of these numerical experiments suggest that the simplified Tikhonov value is a feasible alternative for determining the best approximate solution.

4.2 Numerical Experiment 2

The following Fredholm integral equation is considered here:

$$\int_0^\pi \exp\left(s \cos t\right) f(t)\, dt = 2\frac{\sin s}{s}, \quad 0 \le s \le \frac{\pi}{2}, \tag{23}$$

where the exact solution is $f(t) = \sin t$. $A, \boldsymbol{b}, \boldsymbol{x}$ by using the baart(2048) command were generated on Octave.

The results of the numerical experiments performed with the classical GMRES are shown in Figure 5, 6 and 7. The history of the relative error norm $||\tilde{\boldsymbol{r}}_j||_2/||\tilde{\boldsymbol{r}}_0||_2$ and the solution norm $||\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0||_2$ have been tabulated in Figure 5. As in Experiment 1, their distance gradually increases. Figure 6 illustrates the changes in the absolute values $|\tau_j - \tau_j^S|$ of the Tikhonov value τ_j and the simplified Tikhonov value τ_j^S. The results indicate that the simplified Tikhonov value τ_j^S provides a good approximation of the nonsimplified version τ_j. The relative error norm $||\boldsymbol{x} - \tilde{\boldsymbol{x}}_j||_2/||\boldsymbol{x}||_2$ and the simplified Tikhonov value τ_j^S are compared in Figure 7.

The results of the numerical experiments implemented to find approximate solutions through the GMRES with three different constraints, Ψ, Ψ_j and Ψ_j^S, are shown in Table 3. All three constraints resulted in identical relative error norms. The GMRES using the constraint Ψ_j^S, resulted in the approximate solution $\tilde{\boldsymbol{x}}_4$, because τ_4^S became larger than τ_3^S. This constraint was also the most efficient in determining the final approximate solution. As in

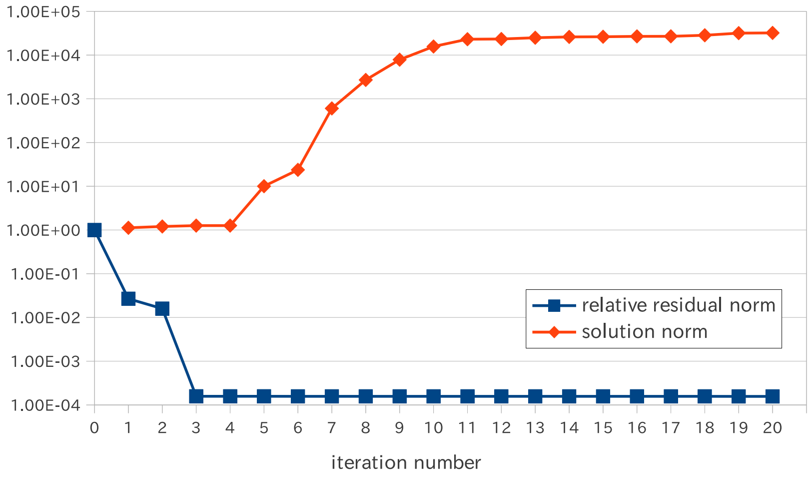

Figure 5: Numerical Experiment 2: The Relative Residual Norm $||\tilde{\boldsymbol{r}}_j||_2/||\tilde{\boldsymbol{r}}_0||_2$ and the Solution Norm $||\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0||_2$ by GMRES

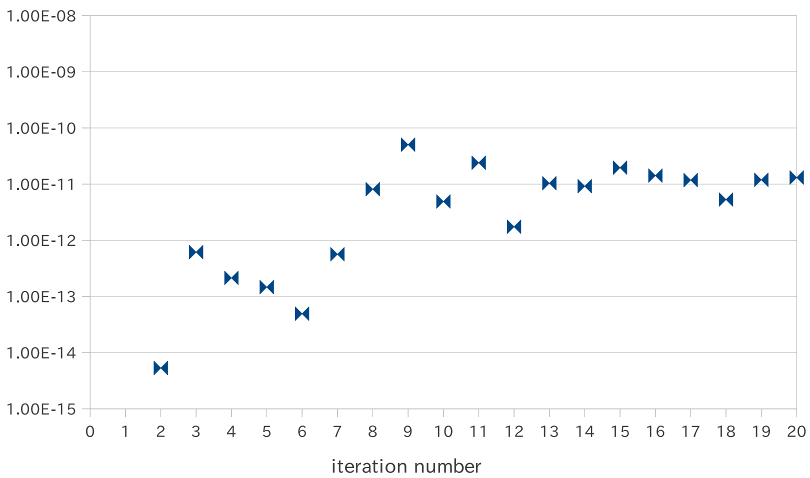

Figure 6: Numerical Experiment 2: The Distance Between Tikhonov value τ_j and the Simplified Tikhonov Value τ_j^S by GMRES

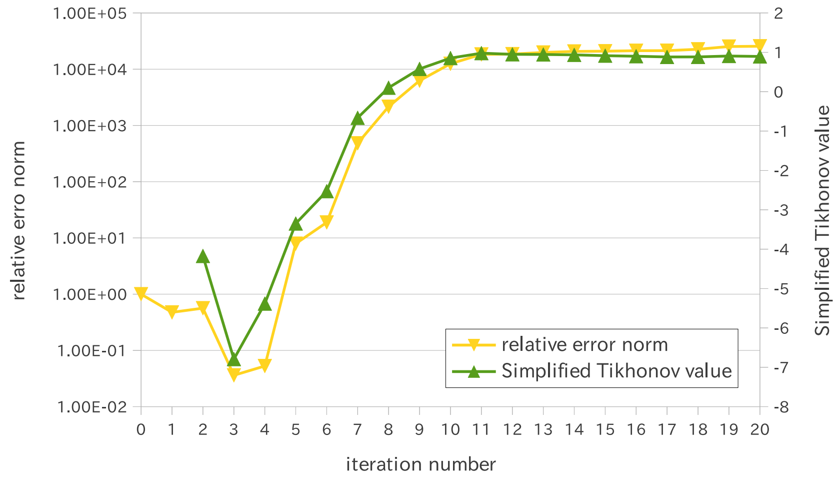

Figure 7: Numerical Experiment 2: The Relative Error Norm $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}_j\|_2/\|\boldsymbol{x}\|_2$ and the Simplified Tikhonov value τ_j^S by GMRES

Experiment 1, the simplified Tikhonov value was able to determine the best approximate solution in the shortest period of time.

4.3 Numerical Experiment 3

A 1D model from an actual gravity survey is solved here:

$$\int_0^1 (s^2 + t^2)^{\frac{1}{2}} f(t)\, dt = \frac{1}{3}\left((1 + s^2)^{\frac{3}{2}} - s^3\right), \quad 0 \le s \le 1. \tag{24}$$

The exact solution is $f(t)$ as $f(t) = \sin(\pi t) + 0.5 \sin(2\pi t)$. $A, \boldsymbol{b}, \boldsymbol{x}$ by gravity(2048,1.0,0.5) were generated on Octave.

The results from the numerical exercises using the classical GMRES are shown in Figure 8, 9 and 10. Figure 8 shows the history of the relative residual norms $\|\tilde{\boldsymbol{r}}_j\|_2/\|\tilde{\boldsymbol{r}}_0\|_2$ and $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$. As mentioned in the previous experiment, though the norms $\|\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0\|_2$ produce similar results during the early iterations, the difference between them grows after that. Figure 9 illustrates the changes in the absolute values $|\tau_j - \tau_j^S|$ of the Tikhonov value τ_j and the simplified Tikhonov value τ_j^S. Although this appears to be increasing, it should be noted that the value in the 20th iteration is less than 1.0×10^{-8} and still minimal. In Figure 10, the relative error norm $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}_j\|_2/\|\boldsymbol{x}\|_2$ and the simplified Tikhonov value τ_j^S are compared. Here, τ_j^S appears to roughly approximate the relative error norm.

The results of the GMRES numerical experiments using the constraints Ψ of (8), Ψ_j of (12) and Ψ_j^S of (20) are tabulated in Table 4. The achieved relative error norm by Ψ was 9.66×10^{-2} and smaller than those achieved by Ψ_j and Ψ_j^S. Figure 10 shows that the simplified Tikhonov value increases at the 8th iteration for the first time. The approximate

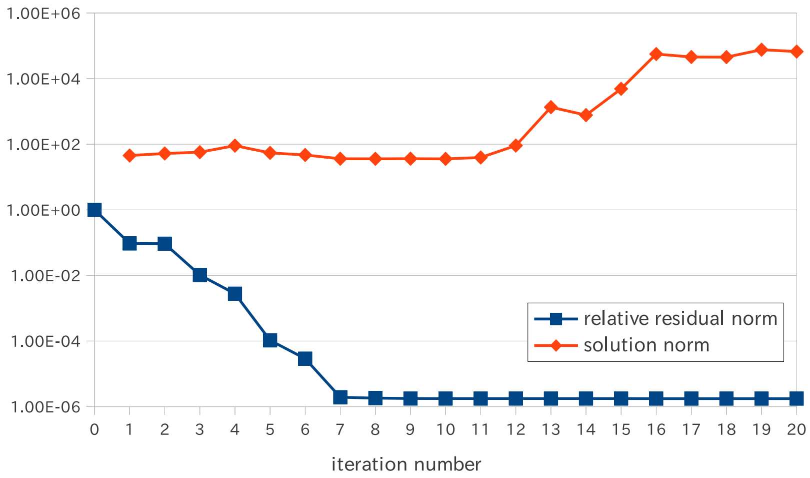

Figure 8: Numerical Experiment 3 : The Relative Residual Norm $||\tilde{\boldsymbol{r}}_j||_2/||\tilde{\boldsymbol{r}}_0||_2$ and Solution Norm $||\tilde{\boldsymbol{x}}_j - \tilde{\boldsymbol{x}}_0||_2$ by GMRES

Table 4: Numerical Experiment 3: The Comparison of Each Constraint for the GMRES

The Constraint	Iteration Count	Achieved Relative Error Norm	Time (sec.)
Ψ	10	1.84×10^{-2}	–
Ψ_j	8	1.15×10^{-1}	0.16
Ψ_j^S	8	1.15×10^{-1}	0.08

solution obtained by the modified GMRES was $\tilde{\boldsymbol{x}}_8 = \tilde{\boldsymbol{x}}_7$, while the best approximate solution by the GMRES with Ψ was generated at the 10th iteration. In this experiment, Ψ_j^S was not only unable to find the best approximate solution. The computed approximate solution contained too many errors.

4.4 Discussion

Numerical experiments 1 and 2 show that constraint Ψ_j^S with the simplified Tikhonov value τ_j^S helps stop the iterations of the modified GMRES, and it can determine the best approximate solution. In numerical experiment 3, the determined approximate solution was not the best one, but it had enough accuracy.

To evaluate effectiveness, the changes in the simplified Tikhonov value in each experiment were compared and analyzed. The first increments of τ_j^S in Figure 4 and Figure 7, equal to $\tau_4^S - \tau_3^S$ in each case, were large, compared to the increments in Figure 10, equal to $\tau_8^S - \tau_7^S$. The small changes in τ_j^S in Figure 10 continued to the 11th iteration.

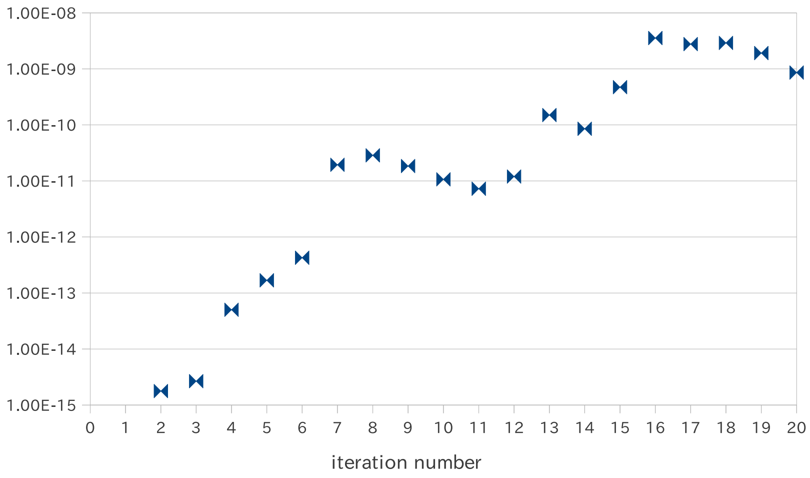

Figure 9: Numerical Experiment 3: The Distance Between Tikhonov value τ_j and the Simplified Tikhonov Value τ_j^S by GMRES

This suggests that the amount of the first increase of the simplified Tikhonov value influences the effectiveness of the value itself. If the amount of the increment is too small, the approximate solution determined by constraint Ψ_j^S has not yet reached the point where it delivers the highest possible accuracy. This problem can be resolved if we set the threshold for the increment of the simplified Tikhonov value τ_j^S in constraint Ψ_j^S.

5 Conclusion

This paper explored the possibilities of using the simplified Tikhonov value τ_j^S as a new index in constraint Ψ_j^S for stopping the iterations of the GMRES and determining an approximate solution. The proposed value, which is suspected to yield a property of the Tikhonov regularization, consists of some approximate values appearing in the iterations of the GMRES.

The numerical experiments have illustrated that the modified GMRES using this proposed value can automatically determine an approximate solution when the corresponding relative error norm becomes small enough.

Although this study has shown that the simplified Tikhonov value τ_j^S can work as a new index in constraint Ψ_j^S for stopping the iterations of the GMRES and determining an approximate solution, there are some outstanding issues that remain unresolved. Future work would include proposing constraints and preconditioners which can deliver a higher accuracy in terms of providing an appropriate approximate solution. The application of this proposed method to large-scale practical problems also needs further exploration.

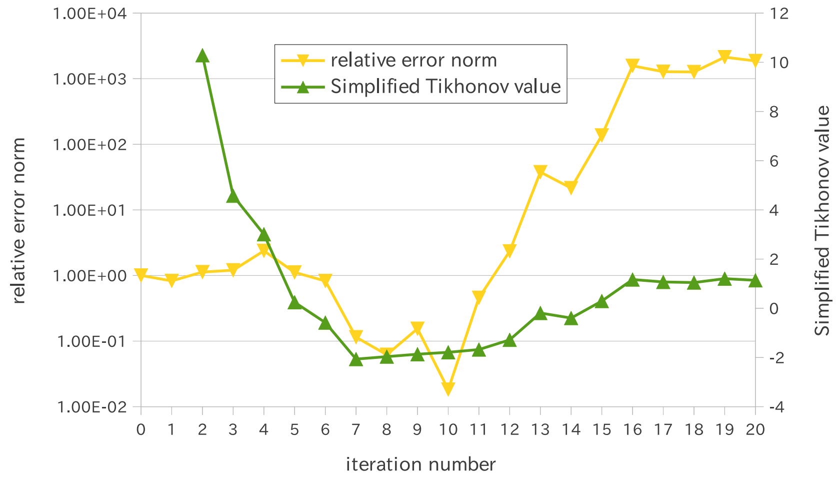

Figure 10: Numerical Experiment 3: The Relative Error Norm $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}_j\|_2/\|\boldsymbol{x}\|_2$ and the Simplified Tikhonov Value τ_j^S by GMRES

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