

## A Note on the GMRES Method for Linear Discrete Ill-Posed Problems

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**Abstract.** In this paper, we are presenting a proposal for new modified algorithms for RRGMRRES and AGMRRES. It is known that RRGMRRES and AGMRRES are viable methods for solving linear discrete ill-posed problems. In this paper we have focused on the residual norm and have come-up with two improvements where successive updates and the stabilization of decreases for the residual norm improve performance respectively. Our numerical experiments confirm that our improved algorithms are effective for linear discrete ill-posed problems.

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**Key words:** Numerical computation, GMRES, iterative method, linear discrete ill-posed problem.

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### 1 Linear discrete ill-posed problems

Recently it is tried to use GMRES methods for *linear discrete ill-posed problems (LDIP)*. Conjugate gradient method and SVD is also applied to solve them, but we focus on the GMRES methods for LDIP in this paper. As an introduction, we will shortly describe the LDIP. The details of the GMRES methods for them are taken up in later sections.

Hansen [5], which is a good introduction to *discrete ill-posed problems (LDIP)*, says that the LDIP arise from the discretization of ill-posed problems such as the first kind of Fredholm integral equation. The first kind of Fredholm integral equation

$$\int_0^1 K(s, t)f(t)dt = g(s), \quad 0 \leq s \leq 1, \quad (1.1)$$

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where the right-hand side  $g(s)$  and the kernel  $K$  are known, but  $f$  is unknown, is one of inverse problems. We obtain "input" from "output" when we deal with inverse problems. After discretizing (1.1), a linear system like

$$Ax = \mathbf{b}, \tag{1.2}$$

where  $A \in \mathbb{R}^{n \times n}$ ,  $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$ , is derived. The coefficient matrix  $A$  appeared from the LDIP is generally ill-conditioned, because it has clustered tiny singular values or singular values decaying to zero. The right-hand side vector in (1.2) represents the "output", so it often includes measurement errors. Then the known right-hand side vector is

$$\bar{\mathbf{b}} = \mathbf{b} + \mathbf{b}_{error}. \tag{1.3}$$

Since usually we don't know  $\mathbf{b}, \mathbf{b}_{error}$ , the approximate solution is written as

$$\bar{\mathbf{x}}_* = \arg \min_{\bar{\mathbf{x}}_j, j \geq 0} \|\bar{\mathbf{x}}_j - \mathbf{x}\|, \tag{1.4}$$

in which  $\bar{\mathbf{x}}_j, j \geq 0$  is generated in  $j$  steps of the GMRES methods. When the size of LDIP is small, the analog of SVD are used for them. However, some iterative methods such as the CG method [5,6,8] and the GMRES method [1-3] are applied to the large scale LDIP for regularization.

## 2 GMRES methods for LDIP

The GMRES method by Saad and Shultz [10] is one of the popular iterative methods for the linear system like (1.2) In particular the method works well when the coefficient matrix  $A$  is non-symmetric. The GMRES generates an approximate solution whose residual norm is minimum by using a Krylov subspace as follow.

$$\|\mathbf{b} - A\mathbf{x}_j\|_2 = \min_{\mathbf{x}_0 + \mathcal{K}_j(A, \mathbf{r}_0)} \|\mathbf{b} - A\mathbf{x}\|_2, \tag{2.1}$$

$$\mathcal{K}_j(A, \mathbf{r}_0) = \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, \dots, A^{j-1}\mathbf{r}_0\}, \tag{2.2}$$

where  $j$  is the iteration number,  $\mathbf{x}_0$  is the initial guess and  $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$  is the initial residual.

One of the GMRES methods for solving LDIP is the Range Restricted GMRES (RRGMRES) method by Calvetti et al. [2]. This method restricts the Krylov subspace to generating an approximate solution within the range of coefficient matrix  $A$ . The least squares problem is solved as follows:

$$\|\mathbf{b} - A\mathbf{x}_j\|_2 = \min_{\mathbf{x}_0 + \mathcal{R}(A, A\mathbf{r}_0)} \|\mathbf{b} - A\mathbf{x}\|_2, \tag{2.3}$$

$$\mathcal{R}_j(A, \mathbf{r}_0) = \text{span}\{A\mathbf{r}_0, A^2\mathbf{r}_0, \dots, A^j\mathbf{r}_0\}. \tag{2.4}$$

Calvetti et al. [3] have confirmed that RRGMRRES performs well when solving LDIP. Another option for this is the augmented GMRES (AGMRRES) method developed by Baglama and Reichel [1]. The augmented GMRES method generates an approximate solution by using not only the Krylov subspace but also a user-supplied space  $\mathcal{W}$  as follows:

$$\|\mathbf{b} - A\mathbf{x}_j\|_2 = \min_{\mathbf{x}_0 + \mathcal{K}_j(A, \mathbf{r}_0) + \mathcal{W}} \|\mathbf{b} - A\mathbf{x}\|_2, \quad (2.5)$$

It works well when the space  $\mathcal{W}$  compensate features of exact solution. The augmentation is available for the RRGMRRES.

In a previous study, we made a proposal for an adaptive augmented GMRES and RRGMRRES (AAGMRRES and AARRGMRRES) method in Kuroiwa and Nodera [7] where we concentrated on the selection of the best user-supplied space  $\mathcal{W}$  for the augmentation. In this paper, we are making a proposal for a new modification, which focuses on successive updates and decreases of residual norms.

### 3 Improvements for RRGMRRES and AGMRRES

In this section, we have explored two ideas that improve the performances of RRGMRRES and AGMRRES, and have detailed our modified algorithms here. These ideas are relevant to successive updates and transition of residual norms.

#### 3.1 Successive Updates on GMRES

GMRES can apply a value for checking residual norm  $\|\mathbf{r}_j\|_2$  at every iteration step without any extra calculations [9]. As a result, it is possible to determine approximate solution  $\mathbf{x}_j$  with optimal iterations. However, if it were possible to obtain an alternative to calculating residual norm  $\|\mathbf{r}_j\|_2$  in RRGMRRES and AGMRRES, these methods would be further optimized.

We first reviewed the successive updates and how it applies to GMRES, when the Arnoldi decomposition is represented as

$$AV_j = V_{j+1}H, \quad (3.1)$$

where  $V_j = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_j] \in \mathbb{R}^{n \times j}$  and  $H \in \mathbb{R}^{(j+1) \times j}$  are orthonormal and upper Hessenberg matrices, respectively,  $\forall \mathbf{x} \in \mathcal{K}_j(A, \mathbf{r}_0)$  is  $\mathbf{x}_0 + V_j\mathbf{y}$ , and  $\mathbf{y} \in \mathbb{R}^j$  is an arbitrary vector. The first column of  $V_j$  is  $\mathbf{r}_0 / \|\mathbf{r}_0\|_2$ . Therefore, the residual form is able to be transformed to

$$\begin{aligned} & \mathbf{b} - A\mathbf{x} \\ &= \mathbf{b} - A(\mathbf{x}_0 + V_j\mathbf{y}) = \mathbf{r}_0 - V_{j+1}H\mathbf{y} \\ &= V_{j+1}(\|\mathbf{r}_0\|_2\mathbf{e}_1 - H\mathbf{y}) = V_{j+1}G^T(\mathbf{g} - U\mathbf{y}), \end{aligned}$$

where  $G = \Omega_j \Omega_{j-1} \cdots \Omega_1$ ,  $\mathbf{g} = G \|\mathbf{r}_0\|_2 \mathbf{e}_1$ , and  $U = GH$  is an upper triangular matrix and  $\mathbf{e}_1$  is an identity vector whose first element is 1. Here,  $\Omega_i$  is a rotation matrix defined by

$$\Omega_i = \begin{pmatrix} I_{i-1} & & & \\ & c_i & s_i & \\ & -s_i & c_i & \\ & & & I_{n-i-2} \end{pmatrix}, \tag{3.2}$$

where  $I_i$  is an  $i \times i$  identity matrix and

$$s_i = \frac{h_{i+1,i}}{\sqrt{(h_{i-2}^{ii})^2 + h_{i+1,i}^2}}, \quad c_i = \frac{h_{i,i}^{(i-1)}}{\sqrt{(h_{i-2}^{ii})^2 + h_{i+1,i}^2}}, \quad s_i^2 + c_i^2 = 1, \tag{3.3}$$

with  $H \equiv [h_{i,j}]$ . Since  $V_{j+1}$  and  $G$  are orthogonal and unitary matrices, respectively,

$$\|\mathbf{b} - A\mathbf{x}\|_2 = \|\mathbf{g} - U\mathbf{y}\|_2 = |\gamma| + \|\hat{\mathbf{g}} - \hat{U}\mathbf{y}\|_2,$$

where

$$\mathbf{g} = \begin{pmatrix} \hat{\mathbf{g}} \\ \gamma \end{pmatrix}, \quad U = \begin{pmatrix} \hat{U} & & \\ 0 & \cdots & 0 \end{pmatrix}.$$

The  $j$  th approximate solution is

$$\mathbf{x}_j = \mathbf{x}_0 + V_j \mathbf{y}_j, \quad \text{with } \mathbf{y}_j = \arg \min_{\mathbf{y}} \|\hat{\mathbf{g}} - \hat{U}\mathbf{y}\|_2. \tag{3.4}$$

When  $\gamma$  represents the  $j$  th residual norm  $\|\mathbf{r}_j\|_2$ , it is no need to compute the approximate solution  $\mathbf{x}_j$  for the residual norm at every step.

The second consideration was the successive updates and how it is applied to the RRGMRRES method. The first columns of  $V_j$  is  $A\mathbf{r}_0 / \|A\mathbf{r}_0\|_2$  in the RRGMRRES. Applying  $V_{j+1}^T$  to the residual vector  $\mathbf{b} - A\mathbf{x}_j$ , we obtain

$$V_{j+1}^T(\mathbf{b} - A\mathbf{x}_j) = V_{j+1}^T \mathbf{r}_0 - H\mathbf{y} = G^T(GV_{j+1}^T \mathbf{r}_0 - GH\mathbf{y}) = G^T(\mathbf{g}_R - U_R\mathbf{y}).$$

Then the residual norm is

$$\|\mathbf{b} - A\mathbf{x}_j\|_2 = \|\mathbf{g}_R - U_R\mathbf{y}\|_2 = |\gamma_R| + \|\hat{\mathbf{g}}_R - \hat{U}_R\mathbf{y}\|_2,$$

in which  $\gamma_R$  is the last element of  $\mathbf{g}_R$ . The  $j$  th approximate solution in the RRGMRRES is

$$\mathbf{x}_j = \mathbf{x}_0 + V_j \mathbf{y}_j, \quad \text{with } \mathbf{y}_j = \arg \min_{\mathbf{y}} \|\hat{\mathbf{g}}_R - \hat{U}_R\mathbf{y}\|_2, \tag{3.5}$$

and

$$|\gamma_R| = \|\mathbf{b} - A\mathbf{x}_j\|_2. \quad (3.6)$$

Eq. (3.6) enables RRGMRES to use alternative  $\gamma_R$  instead of residual norm  $r_j$  without computing approximate solution  $\mathbf{x}_j$ . This type of RRGMRES will be referred to as RRGMRES with Successive Updates (SRRGMRES) from here on.

In AGMRES, the user-supplied space is

$$\mathcal{W} = \text{range}W, \quad (3.7)$$

Apply the QR factorization

$$AW = QR, \quad (3.8)$$

where  $W \in \mathbb{R}^{n \times p}$ ,  $Q \in \mathbb{R}^{n \times p}$  and  $R \in \mathbb{R}^{p \times p}$ . After applying Arnoldi process, we get

$$A[W, V_j] = [Q, V_{j+1}] \begin{bmatrix} R & H_1 \\ 0 & H_2 \end{bmatrix}, \quad (3.9)$$

where  $H_2$  is upper Hessenberg and the first column of  $V_j$  is

$$\frac{(I - QQ^T)\mathbf{r}_0}{\|(I - QQ^T)\mathbf{r}_0\|_2}.$$

Since any vector  $\mathbf{x}$  in  $\mathbf{x}_0 + \mathcal{K}_j(\mathbf{r}_0, A\mathbf{r}_0) + \mathcal{W}$  can be written as  $\mathbf{x} = \mathbf{x}_0 + [W, V_j]\mathbf{y}$ ,

$$\mathbf{b} - A\mathbf{x} = \mathbf{b} - A(\mathbf{x}_0 + [W, V_j]\mathbf{y}) = \mathbf{r}_0 - [Q, V_{j+1}] \begin{bmatrix} R & H_1 \\ 0 & H_2 \end{bmatrix} \mathbf{y}, \quad (3.10)$$

Applying  $[Q, V_{j+1}]^T$  to the above equation (3.10), we immediately obtain

$$\begin{aligned} [Q, V_{j+1}]^T(\mathbf{b} - A\mathbf{x}) &= [Q, V_{j+1}]^T\mathbf{r}_0 - \begin{bmatrix} R & H_1 \\ 0 & H_2 \end{bmatrix} \mathbf{y} \\ &= G_A^T \left( G_A [Q, V_{j+1}]^T \mathbf{r}_0 - G_A \begin{bmatrix} R & H_1 \\ 0 & H_2 \end{bmatrix} \mathbf{y} \right) \\ &= G_A^T (\mathbf{g}_A - U_A \mathbf{y}), \end{aligned}$$

where  $G_A = \Omega_{p+j} \Omega_{p+j-1} \cdots \Omega_{p+1}$ . Then the residual norm can be written as

$$\|\mathbf{b} - A\mathbf{x}_j\|_2 = \|\mathbf{g}_A - U_A \mathbf{y}\|_2 = |\gamma_A| + \|\hat{\mathbf{g}}_A - \hat{U}_A \mathbf{y}\|_2,$$

where  $\gamma_A$  is the last element of  $\mathbf{g}_A$ . The  $j$  th approximate solution in the AGMRES is represented as

$$\mathbf{x}_j = \mathbf{x}_0 + [W, V_j]\mathbf{y}_j, \quad \text{with} \quad \mathbf{y}_j = \arg \min_{\mathbf{y}} \|\hat{\mathbf{g}}_A - \hat{U}_A \mathbf{y}\|_2. \quad (3.11)$$

and  $|\gamma_A| = \|\mathbf{b} - A\mathbf{x}_j\|_2$ . It is possible to update the residual norm successively in AGMRES without calculating approximate solution  $\mathbf{x}_j$ . This method will be referred to as AGMRES with Successive Updates (SAGMRES) from here on. Similarly, SARRGMRES is determined if successive updates are applied to RRGMRES.

Both RRGMRES and AGMRES are able to use a temporary value which represents the residual norm at each step of their internal iteration without computing approximate solution  $\mathbf{x}_j$ .

### 3.2 Transition of residual norms

One good feature of GMRES is that its residual norm is non-increasing. The residual norm will converge when coefficient matrix  $A$  is positive definite, and it will stagnate but not increase when  $A$  is not positive definite. It has been confirmed that since residual norm  $\|\mathbf{r}_j\|_2$  is equal to the last element of  $\mathbf{g} = G\|\mathbf{r}_0\|_2\mathbf{e}_1$  and  $0 \leq |s_i| \leq 1$ , it can be denoted as

$$\|\mathbf{r}_j\|_2 = |(-1)^j s_j s_{j-1} \cdots s_1| \|\mathbf{r}_0\|_2 = |-s_j| \|\mathbf{r}_{j-1}\|. \tag{3.12}$$

On the other hand, the residual norm of the range restricted or augmented methods, e.g., RRGMRES and SRRGMRES or AGMRES and SAGMRES, respectively, do not perform in the same manner as that of GMRES. In SRRGMRES, since  $\gamma_R$ , which represents the residual norm and the last element of  $\mathbf{g}_R$ , is written as

$$|\gamma_R| = \|\mathbf{r}_j\|_2 = |-s_j| \|\mathbf{r}_{j-1}\|_2 + c_j(\mathbf{v}_{j+1}, \mathbf{r}_0), \tag{3.13}$$

the difference between  $\|\mathbf{r}_j\|_2$  and  $\|\mathbf{r}_{j-1}\|_2$  is

$$\begin{aligned} \|\mathbf{r}_j\|_2 - \|\mathbf{r}_{j-1}\|_2 &= |s_j| \|\mathbf{r}_{j-1}\|_2 - c_j(\mathbf{v}_{j+1}, \mathbf{r}_0) - \|\mathbf{r}_{j-1}\|_2 \\ &= \begin{cases} c_j(\mathbf{v}_{j+1}, \mathbf{r}_0) - (1 + s_j) \|\mathbf{r}_{j-1}\|_2, & \text{if } \gamma_R \geq 0, \\ (s_j - 1) \|\mathbf{r}_{j-1}\|_2 - c_j(\mathbf{v}_{j+1}, \mathbf{r}_0), & \text{if } \gamma_R < 0, \end{cases} \end{aligned} \tag{3.14}$$

where  $(\cdot, \cdot)$  represents an inner product. This means that the residual norm of the range restricted methods will not necessarily decrease monotonously. In SAGMRES, temporary value  $\gamma_A$  is

$$|\gamma_A| = \|\mathbf{r}_j\|_2 = |-s_j| \|\mathbf{r}_{j-1}\|_2 + c_j(\mathbf{v}_{j+1}, \mathbf{r}_0). \tag{3.15}$$

Then the difference between  $\|\mathbf{r}_j\|_2$  and  $\|\mathbf{r}_{j-1}\|_2$  is represented as (3.14). The residual norm  $\|\mathbf{r}_j\|_2$  in the SAGMRES does not always decrease as well as the SRRGMRES.

Consequently, the range restricted methods and the augmented methods may not reduce their residual norm at each step of their inner iterations. This feature is an impediment to generating approximate solutions because these residuals have the possibility of not diverging. In such a case, it is necessary to locate and define a condition in this manner:

$$\text{Stop iteration if } |s_j| \|\mathbf{r}_{j-1}\|_2 - c_j(\mathbf{v}_{j+1}, \mathbf{r}_0) - \|\mathbf{r}_{j-1}\|_2 \geq 0, \tag{3.16}$$

This condition applies to both the range restricted and augmented methods and makes it possible to determine whether residual norm  $\|r_j\|_2$  is increasing or stagnating. The  $j - 1$  th computed solution is assumed to be the approximate solution. Condition (3.16) helps generate better approximate solutions than either SRRGMRES or SAGMRES.

### 3.3 Modified algorithms for RRGMRES and AGMRES

We have found two remedies for the algorithms of RRGMRES and AGMRES in sections 3.1 and 3.2 respectively. One of the remedies involves the successive updates of residual norm  $\|r_j\|_2$ , and the other involves the transition of this.

Our modified algorithm for SRRGMRES will be referred to as the Decreasing-Residual RRGMRES with Successive Updates (SDRRGMRES). Its algorithm is shown in Algorithm 3.1. The remedy for transition of residual norms is applied to SDRRGMRES. Thus we added condition 3.16 to SRRGMRES. Steps for the successive updates are detailed in lines 2, 11-13 and 18-22.  $g_R$  and  $U_R$  are updated at every iteration to determine whether to stop the iteration process or not. Lines 14-17 define the criterion for when residual norm  $\|r_j\|_2$  should not increase.

**Algorithm 3.1:** Decreasing-residual RRGMRES with successive update

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1: Compute  $r_0 = b - Ax_0$  and  $v_1 := Ar_0 / \|Ar_0\|_2$ 
2: Define  $g = (n + 1)$ -vector  $[g_1, g_2, \dots, g_{n+1}]$ ,  $g_1 = (v_1, r_0)$ 
3: for  $j = 1, \dots, n$  do
4:   Compute  $w := Av_j$ 
5:   for  $i = 1, \dots, j$  do
6:      $h_{ij} := (w, v_i)$ 
7:      $w := w - h_{ij}v_i$ 
8:   end for
9:    $h_{j+1,j} = \|w\|_2$ 
10:   $v_{j+1} = w / h_{j+1,j}$ 
11:   $g_{j+1} := (v_{j+1}, r_0)$ 
12:  Multiply  $\Omega_i, i = j - 1, \dots, 1$  by the  $j$  th column of  $H$ 
13:  Compute  $s_j, c_j$  in (3.3)
14:  if  $|-s_j\|r_{j-1}\|_2 + c_j g_{j+1}| - \|r_{j-1}\|_2 \geq 0$  then
15:     $j := j - 1$ 
16:    break loop
17:  end if
18:  Multiply  $\Omega_j$  by the  $j$  th column of  $H$  and  $g$ 
19:   $\|r_j\|_2 := g_{j+1}$ 
20:  if  $\|r_j\|_2$  is small enough then
21:    break loop
22:  end if
23: end for
24: Compute  $y_j$  the minimizer of (3.5) and  $x_j = x_0 + V_j y_j$ 

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Our improved algorithm for SAGMRES will be referred to from here on as the

Decreasing-Residual AGMRES with Successive Updates (SDAGMRES). Its algorithm is shown in Algorithm 3.2. The remedy for transition of residual norms is applied to SDAGMRES. Thus we added condition 3.16 to SAGMRES. Lines 4, 13-15 and 20-24 update  $g_A$  and  $U_A$  to obtain  $\gamma_A$  which is an alternative to residual norm  $\|r_j\|_2$ , and lines 16-19 help prevent residual norm  $\|r_j\|_2$  from increasing.

**Algorithm 3.2:** Decreasing-residual AGMRES with successive update

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1: Apply QR factorization for  $AW = QR$ 
2: Compute  $r_0 = b - Ax_0$ 
3: Compute  $v_1 = (I - QQ^T)r_0 / \|(I - QQ^T)r_0\|_2$ 
4: Define  $g = (p + n + 1)$ -vector  $[g_1, g_2, \dots, g_{p+n+1}]$ ,  $V := [Q, v_1]$ ,  $H := R$ ,  $g := V^T r_0$ 
5: for  $j = p + 1, \dots, p + n$  do
6:   Compute  $w := Av_j$ 
7:   for  $i = 1, \dots, j$  do
8:      $h_{ij} := (w, v_i)$ 
9:      $w := w - h_{ij}v_i$ 
10:  end for
11:   $h_{j+1,j} = \|w\|_2$ 
12:   $v_{j+1} = w / h_{j+1,j}$ ,  $V := [V, v_{j+1}]$ 
13:   $g_{j+1} := (v_{j+1}, r_0)$ 
14:  Multiply  $\Omega_i$ ,  $i = j - 1, \dots, p + 1$  by the  $j$  th column of  $H$ 
15:  Compute  $s_j, c_j$  in (3.3)
16:  if  $| -s_j \|r_{j-1-p}\|_2 + c_j g_{j+1} | - \|r_{j-1-p}\|_2 \geq 0$  then
17:     $j := j - 1$ 
18:    break loop
19:  end if
20:  Multiply  $\Omega_j$  by the  $j$  th column of  $H$  and  $g$ 
21:   $\|r_{j-p}\|_2 := g_{j+1}$ 
22:  if  $\|r_{j-p}\|_2$  is small enough then
23:    break loop
24:  end if
25: end for
26: Compute  $y_j$  the minimizer of (3.11) and  $x_j = x_0 + [W, V_{p+1:p+j}]y_j$ 

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SDRRGMRES and SDAGMRES can be restarted in the same manner as the standard GMRES. From here on, these methods will be referred to as SDRRGMRES( $m$ ) and SDAGMRES( $m$ ) respectively. When we restart these algorithms, the upper limit of the inner iteration is set to  $m$ . After approximate solution  $x_j$  is generated, let  $x_0 := x_j$ , and then go to line 1 in Algorithm 3.1 or line 2 in Algorithm 3.2.

## 4 Numerical experiments

Three numerical experiments of LDIP, are shown in this section. We solved them with SGMRES( $m$ ), SRRGMRES( $m$ ), SAGMRES( $m$ ), SARRGMRES( $m$ ), SDRRGMRES( $m$ ), SDA-GMRES( $m$ ) and SDRRGMRES( $m$ ), which have been discussed in previous sections,



and compared their results. SGMRES( $m$ ) represents classical GMRES with successive update. The LDIP is usually too ill-conditioned for obtaining well-approximated solutions even if restart cycle  $m$  or the iteration number is large. Hence in every example restart cycle  $m$  was set to be from 1 to 50. Each method had 50 variations, and the maximum iteration number was set to 1500. Matrices  $W$  for user-supplied spaces  $\mathcal{W}$  were

$$W_1 = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \quad W_2 = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ \vdots & \vdots \\ 1 & n \end{pmatrix}, \quad W_3 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ \vdots & \vdots & \vdots \\ 1 & n & n^2 \end{pmatrix}, \quad (4.1)$$

$$\mathcal{W}_i = \text{range } W_k, \quad 1 \leq i \leq 3, \quad (4.2)$$

based on Baglama [1]. We used spaces  $\mathcal{W}_1$ ,  $\mathcal{W}_2$  or  $\mathcal{W}_3$  when augmenting the Krylov subspace. Thus there are 4 types of augmentation, for we are able to use  $\mathcal{W}_i$ ,  $1 \leq i \leq 3$  or we don't augment any spaces. Then each method has 4 augmentations and 50 restart cycles, i.e., there are 200 patterns of computation in each method.

All programs were written in C. An SGI Altix 450, configured with a Dual-Core Intel Itanium 2 1.4 GHz processor was used. Error vector  $\mathbf{b}_{error}$  had a 0 mean and  $1/3n^2$  variant normal random numbers for its elements. The elements of error vectors  $\mathbf{b}_{error}$  for each example were the same. The condition for finishing the iteration was

$$\frac{\|\mathbf{r}_j\|_2}{\|\mathbf{r}_0\|_2} = 1.0 \times 10^{-12}.$$

**Example 4.1.** Our first example is a type of the Fredholm integral equation of the first kind:

$$\int_0^\pi \exp(s \cos t) x(t) dt = 2 \frac{\sin s}{s}, \quad t \in \left[0, \frac{\pi}{2}\right],$$

which is a test problem baart from the Regularization Tools developed by Hansen [4]. Exact function  $x(t)$  is equal to  $\sin t$ . Each function is discretized with size  $n = 1000$ . The condition number of coefficient matrix  $A$  is  $\|A\| \|A^{-1}\| = 6.604 \times 10^{18}$ .

We solved this problem with SRRGMRES( $m$ ), SARRGMRES( $m$ ), SDRRGMRES( $m$ ) and SDARRGMRES( $m$ ). The results of the analogues of SGMRES( $m$ ) are not shown because they did not perform as well as those of SRRGMRES( $m$ ). Table 1 shows that, the decreasing-residual methods are more stable than methods only with successive updates.

Table 1: Example 4.1 Distribution of the minimal error norms  $\|\bar{\mathbf{x}}_* - \mathbf{x}\|_2$  by each method in each interval.

method	$\leq 0.5$	$< \ \bar{\mathbf{x}}_0 - \mathbf{x}\ _2$	$= \ \bar{\mathbf{x}}_0 - \mathbf{x}\ _2$
SRRGMRES, SARRGMRES	16	3	181
SDRRGMRES, SDARRGMRES	193	6	1

Table 2: Example 4.1 Methods whose error norm is minimal in each of SRRGMRES( $m$ ), SARRGMRES( $m$ ), SDRRGMRES( $m$ ) and SDARRGMRES( $m$ ).

method	augmentation	iteration	$\ r_j\ _2$	$\ \bar{x}_* - x\ _2$
SRRGMRES(5)	-	30	$1.564 \times 10^{-3}$	$2.416 \times 10^{-3}$
SARRGMRES(3)	$\mathscr{W}_2$	294	$1.193 \times 10^{-5}$	$1.090 \times 10^{-3}$
SDRRGMRES(40)	-	29	$1.042 \times 10^{-5}$	$1.288 \times 10^{-3}$
SDARRGMRES(27)	$\mathscr{W}_3$	13	$1.023 \times 10^{-5}$	$1.085 \times 10^{-3}$

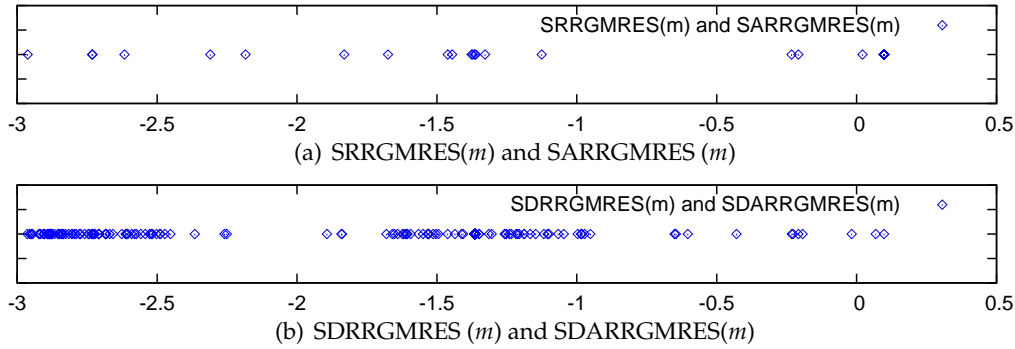


Figure 1: Experiment 4.2 Distribution of  $\log_{10} \|\bar{x}_* - x\|_2$ . Let restart cycle  $m$  be  $1 \leq m \leq 50$  and the space for augmentation be  $\mathscr{W}_i$  where  $1 \leq i \leq 3$ . Each figure has 200 points.

Table 1 shows the distribution of minimum error norm  $\|\bar{x}_* - x\|_2$ . 90.5% of all results from SRRGMRES( $m$ ) and SARRGMRES( $m$ ) were equal to initial error norm  $\|\bar{x}_0 - x\|_2$ . In other words, their error norm was not reduced through iterations, whereas 96.5 % of all the results obtained through methods with decreasing-residual conditions were under 0.5.

The distribution of  $\log_{10} \|\bar{x}_* - x\|_2$  can be seen in Fig. 1. Fig. 1(a) has 200 points obtained through SRRGMRES( $m$ ) and SARRGMRES( $m$ ), and Fig. 1(b) has 200 points obtained through SDRRGMRES( $m$ ) and SDARRGMRES( $m$ ), where  $1 \leq m \leq 50$ . Space  $\mathscr{W}_i$ , where  $1 \leq i \leq 3$  was used for the augmentations.

According to Table 1 and Fig. 1, the conditions under which an increasing residual norm is avoided, help make better approximate solutions.

The results with the smallest error norm in each method are shown in Table 2. We can see that SDARRGMRES(27) with  $\mathscr{W}_3$  performs best both in terms of error norm  $\|\bar{x}_* - x\|_2$  and the iteration number. The smallest error norm  $\|\bar{x}_* - x\|_2$  of SDARRGMRES(27) with  $\mathscr{W}_3$  was a little smaller than that of SARRGMRES(3) with  $\mathscr{W}_2$ , which exhibited the best performance among these methods without the decreasing-residual condition. The iteration number of SDARRGMRES(27) with  $\mathscr{W}_3$  was about 1/20 that of SARRGMRES(3) with  $\mathscr{W}_2$ .

**Example 4.2.** Our second example is a test problem called foxgood from the Regularization Tools developed by Hansen [4]:

$$\int_0^1 (s^2 + t^2)^{\frac{1}{2}} x(t) dt = \frac{1}{3} \left( (1 + s^2)^{\frac{3}{2}} - s^3 \right), \quad t \in [0, 1].$$

Table 3: Example 4.2 Distribution of the minimal error norms  $\|\bar{x}_* - x\|_2$  by each method in each interval.

method	$\leq 0.5$	$< \ \bar{x}_0 - x\ _2$	$= \ \bar{x}_0 - x\ _2$
SRRGMRES, SARRGMRES	29	15	106
SDRRGMRES, SDARRGMRES	200	0	0

Table 4: Example 4.2 Methods whose error norm is minimal in each of SRRGMRES( $m$ ), SARRGMRES( $m$ ), SDRRGMRES( $m$ ) and SDARRGMRES( $m$ ).

method	augmentation	iteration	$\ r_j\ _2 (10^{-5})$	$\ \bar{x}_* - x\ _2$
SRRGMRES(4)	-	816	3.029	$7.193 \times 10^{-3}$
SARRGMRES(1)	$\mathscr{W}_2$	1	2.971	$1.429 \times 10^{-4}$
SDRRGMRES(20)	-	802	3.039	$5.040 \times 10^{-3}$
SDARRGMRES(17)	$\mathscr{W}_2$	1	2.840	$4.917 \times 10^{-6}$

Exact function  $x(t)$  equals  $t$ . We discretized each function with size  $n = 500$ . The condition number of coefficient matrix  $A$  was  $\|A\| \|A^{-1}\| = 6.317 \times 10^{19}$ .

SRRGMRES( $m$ ), SARRGMRES( $m$ ), SDRRGMRES( $m$ ), SDARRGMRES( $m$ ) were applied to this example. In every case the analogue of SGMRES( $m$ ) did not perform as well as that of SRRGMRES( $m$ ). The data in Table 3 indicates that SDRRGMRES( $m$ ) and SDARRGMRES( $m$ ) are more stable than SRRGMRES( $m$ ) and SARRGMRES( $m$ ).

Table 3 and Fig. 2 show the distribution of minimal error norm  $\|\bar{x}_* - x\|_2$  of the applied methods with each restart cycle  $m$ , where  $1 \leq m \leq 50$  and space  $\mathscr{W}_i$ , where  $1 \leq i \leq 3$  for augmentations. All of the results from the methods with the decreasing-residual condition were under 0.5, while only about 3/10 of the results from the methods without this condition were under 0.5. The upper figures in Fig. 2(a) are from the methods with only successive updating of the residual norm, and the lower ones in Fig. 2(b) are from the methods which also had the decreasing-residual condition explained in Section 3.2. These figures indicate that the minimal error norms were significantly improved by this condition.

The best performances from the perspective of the error norm  $\|\bar{x}_* - x\|_2$  are seen in Table 4. According to Table 4, the iteration numbers of SDARRGMRES(17) with

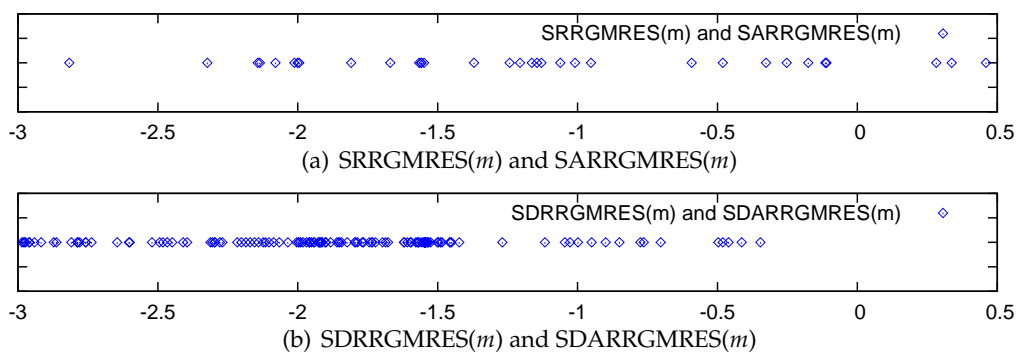


Figure 2: Experiment 4.2 Distribution of  $\log_{10} \|\bar{x}_* - x\|_2$ . Let restart cycle  $m$  be  $1 \leq m \leq 50$  and the space for augmentation be  $\mathscr{W}_i$  where  $1 \leq i \leq 3$ . Each figure has 200 points.

$\mathscr{W}_2$  and SARRGMRES(1) with  $\mathscr{W}_2$  are the same, but the error norm of the SDARRGMRES(17) with  $\mathscr{W}_2$  is the smallest and about 3/100 that of SARRGMRES(1) with  $\mathscr{W}_2$ .

**Example 4.3.** Our last example is phillips:

$$\int_{-6}^6 \phi(s-t)x(t)dt = (6 - |s|) \left( 1 + \frac{1}{2} \cos \left( \frac{\pi s}{3} \right) \right) + \frac{9}{2\pi} \sin \left( \frac{\pi |s|}{3} \right), \quad t \in [-6, 6],$$

$$\phi(u) = \begin{cases} 1 + \cos \left( \frac{\pi u}{3} \right), & |u| < 3 \\ 0, & |u| \geq 3 \end{cases}$$

which is also a test problem from the Regularization Tools developed by Hansen [4]. The exact function was set to  $x(t) = \phi(t)$ . We discretized each function with size  $n = 500$ . The condition number of the coefficient matrix  $A$  was  $\|A\| \|A^{-1}\| = 1.653 \times 10^9$ .

We compared the results of SGMRES( $m$ ), SRRGMRES( $m$ ), SAGMRES( $m$ ), SARRGMRES( $m$ ), SDRRGMRES( $m$ ), SDAGMRES( $m$ ) and SDRRGMRES( $m$ ) in this problem. Table 5 suggests that the decreasing-residual methods work better in particular in the RRGMRES methods.

The best results of each method have been tabulated in Table 6. Error norm  $\|\bar{x}_* - x\|$  of SAGMRES(5) with  $\mathscr{W}_2$  was the smallest among all the methods which did not have a guarantee that the residual norm would decrease. However, the method which had the smallest error norm of all was SDRRGMRES(20), which was about 1/3 that of SAGMRES(5) with  $\mathscr{W}_2$ .

Table 5 and Fig. 3 show the distribution of minimum error norm  $\|\bar{x}_* - x\|_2$  of each of the applied methods in each  $m$ , where  $1 \leq m \leq 50$  and space  $\mathscr{W}_i$ , where  $1 \leq i \leq 3$  for augmentation.

Table 5: Example 4.3 Distribution of the minimal error norms  $\|\bar{x}_* - x\|_2$  by each method in each interval.

method	$\leq 0.5$	$< \ \bar{x}_0 - x\ _2$	$= \ \bar{x}_0 - x\ _2$
SGMRES, SAGMRES	196	2	2
SRRGMRES, SARRGMRES	150	22	28
SDGMRES, SDAGMRES	200	0	0
SDRRGMRES, SDARRGMRES	200	0	0

Table 6: Example 4.3 Methods whose error norm is minimal in each of SGMRES( $m$ ), SAGMRES( $m$ ), SDGMRES( $m$ ), SDAGMRES( $m$ ) SRRGMRES( $m$ ), SARRGMRES( $m$ ), SDRRGMRES( $m$ ) and SDARRGMRES( $m$ ).

method	augmentation	iteration	$\ r_j\ _2$	$\ \bar{x}_* - x\ _2$
SGMRES(4)	-	1496	$3.338 \times 10^{-4}$	$1.504 \times 10^{-2}$
SAGMRES(5)	$\mathscr{W}_2$	490	$2.369 \times 10^{-4}$	$7.830 \times 10^{-3}$
SDGMRES(4)	-	1496	$3.338 \times 10^{-4}$	$1.504 \times 10^{-2}$
SDAGMRES(5)	$\mathscr{W}_2$	490	$2.369 \times 10^{-4}$	$7.830 \times 10^{-3}$
SRRGMRES(7)	-	385	$1.023 \times 10^{-2}$	$1.769 \times 10^{-2}$
SARRGMRES(1)	$\mathscr{W}_2$	1500	$4.081 \times 10^{-4}$	$1.490 \times 10^{-2}$
SDRRGMRES(20)	-	514	$4.800 \times 10^{-5}$	$2.686 \times 10^{-3}$
SDARRGMRES(48)	$\mathscr{W}_2$	55	$3.100 \times 10^{-3}$	$1.246 \times 10^{-2}$

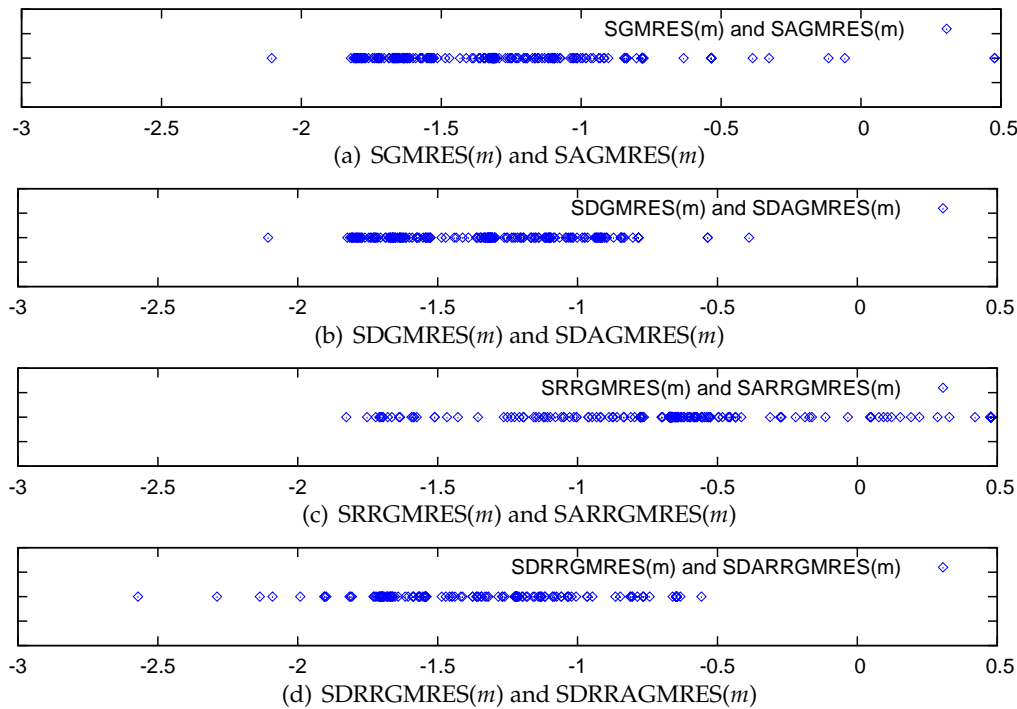


Figure 3: Experiment 2 Distribution of  $\log_{10} \|\bar{x}_* - x\|_2$ . Let restart cycle  $m$  be  $1 \leq m \leq 50$  and the space for augmentation be  $\mathcal{W}_i$  where  $1 \leq i \leq 3$ . Each figure has 200 points.

Table 5 shows that the decreasing-residual condition which helps prevent the residual norm from increasing also improves the figures for the minimum error norm. Figs. 4.3(a) and 4.3(b) show the results of the GMRES methods, and Figs. 4.3(c) and 4.3(d) show the results of the RRGMRES methods. The data indicates that the decreasing-residual conditions work well in both methods, but the RRGMRES methods are more influenced by this than the GMRES methods.

All examples show, that the modified algorithms with decreasing-residual conditions performed better than the algorithms with only successive updates of the residual norm.

## 5 Conclusions

We have made a proposal for modified versions of SDRRGMRES and SDAGMRES. One modification was the inclusion of successive updates which have already been applied to the standard GMRES. The other modification was the procedure of stabilizing the decreases of the residual norm in inner iterations. Numerical examples have illustrated that these generated more stable and better solutions than unmodified versions of SRRGMRES and SAGMRES.

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