Different Tikhonov Regularization Operators for Elementary Residual Method

J. Hasani Eskandari* & H. Zareamoghaddam**

*Kashmar Branch, Islamic Azad University, Kashmar, IRAN. E-Mail: hasanieskandari{at}gmail{dot}com
**Young Researchers and Elite Club, Kashmar Branch, Islamic Azad University, Kashmar, IRAN.
E-Mail: zareamoghaddam{at}yahoo{dot}com

***Abstract*—**ELeMentary RESidual (ELMRES) method is a recently proposed krylov subspace method, which its implementation is similar to GMRES; however this does not use any Arnoldi orthogonalization technique. The implementation of ELMRES is based on Hessenberg decomposition. The main aim of this work is to solve (nearly) singular linear system of equations by ELMRES using Tkhonov regularization. But, the more important issue is that we collect several different appropriate sets of Tikhonov regularization parameters for ELMRES and compare the performances of these operators by some popular numerical tests to find some more practical class of Tikhonov operators for this iterative method. Therefore, some numerical experiments, which compare the performances of these operators, as well as conclusion, are drawn at the end of this work.

***Keywords*—**Elementary Residual; Hessenberg Decomposition; Ill-Posed Linear Systems; Regularization Techniques; Tikhonov Regularization.

***Abbreviations*—**Conjugate Gradient (CG); ELeMentary RESidual (ELMRES); Generalized Minimal Residual (GMRES); Partial Differential Equation (PDE); Quasi Minimal Residual (QMR); Truncated Singular Value Decomposition (TSVD).

I. INTRODUCTION

THERE are varieties of applications for the solution of a linear system of equations.

$$Ax = b, \tag{1}$$

where the coefficient matrix $A \in R^{n\times n}$ is a large and sparse matrix, $b \in R^n$ is a given right hand side column, and $x \in R^n$ is an unknown vector. Different areas such as Physics, Statistics, Engineering as well as Social Science need the solution of such linear systems. Due to importance of such solutions, many authors have had different researches about this sort of problem; see [Saad & Schultz, 1986; Kelley, 1998; Howell & Stephens, 2000; Saad, 2003; Salahi & Zareamoghaddam, 2009; Matinfar et al., 2012; Delkhosh & Zareamoghaddam, 2013]. In many cases, the coefficient matrix A is singular or ill-conditioned. This sort of problem is called as ill-posed linear system of equations. These systems may be extracted from discretization of some Partial Differential Equations (PDEs) and Fredholm integral equations of the first kind with a smooth kernel, as well as linearization of some nonlinear equations.

Usually, the entries of right hand side vector b are obtained through observations and they are contaminated by some noise or measurement errors. Suppose the sum of these errors is denoted by $e \in R^n$ and $\hat{b} \in R^n$ is the error-free right hand side vector. Then, $b = \hat{b} + e$ and the original linear system is,

$$A\hat{x} = \hat{b}, \tag{2}$$

while we normally access to the error-contaminated system of equations (1).

In practical problems, the solution of linear system of equations is computed by some efficient iterative methods such as CG variants, QMR, GMRES, etc. Normally, the mentioned iterative methods are not able to compute some meaningful solution for ill-posed problems directly; however, some regularization techniques are required to compute a meaningful approximation for such a problem. The main aim of these techniques is to reduce the ill-posedness of these problems. Several authors have investigated on various regularization techniques to develop them or to demonstrate the positive and negative points of such techniques, see [Plato, 1990; Engl et al., 1996; Hansen, 1997; Calvetti et al., 1998; Calvetti & Reichel, 2003; Scherzer, 2003; Viloche Bazán & Borges, 2010; Kindermann, 2011; Elden & Simoncini, 2012; Hamarik et al., 2012]. Generally, there are two more popular regularization techniques of Truncated Singular Value Decomposition (TSVD) variants [Hansen, 1989; Hansen, 1990; Morigi et al., 2006] as well as Tikhonov regularization. In this work, we focus on Tikhonov regularization [Engl et al., 1995; Calvetti & Reichel, 2003; Lewis & Reichel, 2009; O'Leary, 2011; Martin & Reichel, 2013] and this technique is discussed in section 2, because it is more popular. However, the interested readers can refer to [Hansen, 1989; Hansen, 1990; Engl et al., 1996; Hansen, 1997; Morigi et al., 2006] to know more about TSVD variants.

Recently, ELMRES as a new iterative method proposed by Howell and Stephens (2000), which it is explained here, shortly. This is a Krylov subspace method, which uses Hessenberg decomposition technique to generate a basis for the corresponding Krylov subspace and by this way, the coefficient matrix A is transferred into an upper hessenberg matrix $\overline{H}_k$ with less dimensions. To become more familiar with this method, at first, its algorithm is described below.

Algorithm 1: ELMRES

1. Choose x_0, set $r_0 = b - Ax_0$, $\beta = r_0(1)$, $v_1 = r_0/\beta$.
   $w = Av_1$, $h(1{:}2,1) = w(1{:}2)$,
   $v_2(2 \dots n) = w(2 \dots n)/h(2,1)$, $v_2(1) = 0$.
2. For $j = 1, \dots, k$, until satisfied do
   $w = Av_j$,
   For $i = 1, \dots, j+1$ do
   $h(i, j+1) = w(i)$, $w = w - h(i, j+1)v_i$.
   End
   $h(j+2, j+1) = w(j+2)$, $v_{j+2} = w/h(j+2, j+1)$,
   $v_{j+2}(1, \dots, j+1) = 0$.
   End
3. Compute $\bar{y}$ as the solution of $\min_{y \in R^k} \|\beta e_1 - \overline{H}_k y\|$,
   where $\overline{H}_k = h(i,j) \in R^{(k+1)\times k}$ is an upper Hessenberg matrix.
   Set $x_k = x_0 + V_k \bar{y}$, where $V_k = [v_1, \dots, v_k]$. If x_k does not satisfied go to 1.

From the above algorithm, it is seen that $V_k = [v_1, \dots, v_k]$ is a basis for the krylov subspace,

$$K_k(A, r_0) = span\{r_0, Ar_0, \dots, A^{k-1}r_0\}.$$

The two main similarities of ELMRES and GMRES are that, at first, both of these methods try to reduce the coefficient matrix A using different projection techniques (hessenberg decomposition technique is applied for ELMRES and Arnoldi orthogonalization process is for GMRES) and secondly, the approximate iterations of both methods are updated by the solution of similar upper Hessenberg least square problems (i.e. step 3 of Algorithm 1).

By this algorithm, the vectors v_is are extracted such that we have,

$$v_{k+1} \perp \{e_1, e_2, \dots, e_k\}, k = 1,2, \dots \tag{3}$$

By setting $\hat{L}_i = I_n + v_i e_i^T$ and $\tilde{L}_k = \hat{L}_1 \hat{L}_2 \dots \hat{L}_k$, we have $\hat{L}_i^{-1} = I_n - v_i e_i^T$ and $\tilde{L}_k^{-1} = \hat{L}_k^{-1} \hat{L}_{k-1}^{-1} \dots \hat{L}_1^{-1}$ are the inverses of $\hat{L}_i$ and $\tilde{L}_k$, respectively. If V_k be the first k columns of $\tilde{L}_k$ then,

$$AV_k = V_{k+1} \overline{H}_k, \tag{4}$$

which is the basic reduction technique of ELMRES. Finally, the last computed approximation is modified as,

$$x_k = x_0 + V_k \bar{y}, \text{ where } \bar{y} = \arg min_{y \in R^k} \|\beta e_1 - \overline{H}_k y\|. \tag{5}$$

Here and throughout this paper, $\|\cdot\|$ is used for Euclidean norm of a vector and the associated induced norm for square matrices.

Theorem 1: [Howell & Stephens, 2000; Delkhosh & Zareamoghaddam, 2013] The kth iteration x_k of ELMRES is the solution of $\min_{x \in K_k(A, r_0)} \left\|\tilde{L}_k^{-1}(b - Ax)\right\|$.

For more information about this iterative method refer to [Howell & Stephens, 2000; Delkhosh & Zareamoghaddam, 2013].

II. Tikhonov Regularization

Tikhonov regularization is the most popular iterative technique for computing the solution of ill-posed linear system of equations (1) by minimizing the following least square problem,

$$\min_{x \in R^n} \{\|Ax - b\|^2 + \beta \|Lx\|^2\}, \tag{6}$$

where the matrix L is referred to as the regularization operator and the scalar $0 < \beta$ as the regularization parameter [Engl et al., 1996; Calvetti & Reichel, 2003; Lewis & Reichel, 2009; O'Leary, 2011; Martin & Reichel, 2013].

It has been proved that the minimization problem (6) can be replaced by its equivalent linear system of equations,

$$\left(A^T A + \beta L^T L\right) x = A^T b. \tag{7}$$

Therefore, the solution of this regularization technique is theoretically obtained by,

$$x = \left(A^T A + \beta\, L^T L\right)^{-1} A^T b.$$

There are many investigations on Tikhonov regularization. Some authors have explored various regularization operators and parameters for (6), and several authors have studied on the implementations of such a regularization technique, as well as its benefits for computing the solution of ill-posed linear system of equations. This paper aims to study some classes of Tikhonov regularization operators suitable for ELMRES algorithm. For this purpose, several set of applicable regularization operators are discussed for finding the best class of such operators. To see the performance of such operators, they are tested by some popular numerical examples in section 4.

III. Different Classes of Tikhonov Operators

To use Tikhonov regularization, we need a regularization operator L and a scalar parameter β. There may be some appropriate options for such required operators. Here, we introduce some more important classes of Tikhonov operators.

3.1. Identity matrix

The most common and the simplest operator for implementation of Tikhonov regularization is the identity matrix with the same dimension of the coefficient matrix A.

In this case, the regularized problem (6) is replaced by minimization problem,

$$\min_{x \in R^n} \{\|Ax - b\|^2 + \beta \|x\|^2\},$$

and simultaneously, this problem is transferred into the following regularized linear system,

$$\left(A^T A + \beta I_n\right) x = A^T b . \quad (8)$$

Due to the above regularization operator, just the elements of the diagonals of the symmetric coefficient matrix $A^T A$ of the normal equation $A^T A x = A^T b$ are regularized by adding the positive value β. Using this approach usually improves the condition number of final linear system and it causes that a solution with more accuracy precision could be computed for the problem (1).

3.2. Operators based on Scaled Discretizations of One-Dimensional Finite Differences

It is an old approach to estimate partial differential equations by some Finite Differences Method (FDM) such as the following one-dimensional finite differences.

$$\left.\frac{df}{dx}\right|_{x=x_k} \approx \frac{f_k - f_{k-1}}{h}, \quad \left.\frac{df}{dx}\right|_{x=x_k} \approx \frac{f_{k+1} - f_k}{h} \text{ and}$$

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x_k} \approx \frac{f_{k+1} - 2 f_k + f_{k-1}}{h^2} .$$

There are several different FDM approaches with various orders of accuracy for estimating of one-dimensional differential equations. Based on the coefficients of each FDM, a Toeplitz-like upper triangular rectangular matrix can be extracted. Usually, from such FDM techniques, the scaled discretizations of one-dimensional finite difference approaches are used as the fixed elements of diagonals and above of matrices which are used as regularization operators. The corresponding operators related to the above illustrated finite differences are,

$$L_1 = \begin{pmatrix} 1 & -1 & & & 0 \\ & 1 & -1 & & \\ & & \ddots & \ddots & \\ 0 & & & 1 & -1 \end{pmatrix} \in R^{(n-1)\times n} \text{ and}$$

$$L_2 = \begin{pmatrix} 1 & -2 & 1 & & & 0 \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ 0 & & & 1 & -2 & 1 \end{pmatrix} \in R^{(n-2)\times n} .$$

3.3. The Coefficients of Newton Expansion

Newton expansion is a well-known polynomial expansion that the coefficients of such formula are used in many practical problems. Generally, the kth order of this expansion is,

$$(a-b)^k = \sum_{i=0}^{k} (-1)^i a^{k-i} b^i . \quad (9)$$

To obtain such scalars regularly, the following well-known triangular shape of the coefficients is helpful.

$$\begin{array}{lccccccccc} k=0: & & & & & 1 & & & & \\ k=1: & & & & 1 & & 1 & & & \\ k=2: & & & 1 & & 2 & & 1 & & \\ k=3: & & 1 & & 3 & & 3 & & 1 & \\ k=4: & 1 & & 4 & & 6 & & 4 & & 1 \\ \vdots & & & & & \vdots & & & & \end{array} \quad (10)$$

For each positive integer k, the absolute values of corresponding coefficients of kth order of (9) are obtained as the scalars located in the kth row of (10) and the exact values are so that the first scalar in each row (i.e. 1) is positive and the sign of other scalars are changed one by one regularly. Similar to previous subsection, using the scalars of each row, a Toeplitz-like rectangular matrix can be generated. To emphasis this class of operators, kth operator of this class is illustrated by $L_k^{'} \in R^{(n-k)\times n}$. It is obviously seen that for $k = 0$, the corresponding operator $L_0^{'}$ is I_n. As an example, for $k = 4$, we have,

$$L_4' = \begin{pmatrix} 1 & -4 & 6 & -4 & 1 & & & & \\ & 1 & -4 & 6 & -4 & 1 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & & 1 & -4 & 6 & -4 & 1 \end{pmatrix} \in R^{(n-4)\times n} .$$

3.4. Orthogonal Projection Operators

There are some matrices with orthogonal columns that are used as regularization operators. To identify different regularization operators, this class of orthogonal projection operators are shown by $L^{''}$. Due to Gram-Schmidt orthogonalization algorithm [Saad & Schultz, 1986; Saad, 2003], it is possible to generate a set of orthogonal basis vectors for an arbitrary set of independent vectors. Calvatti et al., (2003) suggested the following structure to find an orthogonal regularization operator. Suppose $W_k \in R^{n\times k}$ is a matrix with orthogonal columns, the corresponding orthogonal operator for Tikhonov regularization method is obtained by,

$$L_k'' = I_n - W_k W_k^T, \ \left(L_k'' \in R^{n\times n}\right). \quad (11)$$

It has been proved that the Vandermonde matrix,

$$V = \begin{pmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \dots & x_2^{n-1} \\ 1 & x_3 & x_3^2 & \dots & x_3^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^{n-1} \end{pmatrix} \in R^{n\times n} , \quad (12)$$

is nonsingular (if $\forall i \neq j: x_i \neq x_j$) because its determinant is

$$Det(V) = \prod_{1\le i<j\le n} \left(x_j - x_i\right).$$

Consequently, all of its column vectors are independent. To generate an orthogonal matrix $W_k \in R^{n\times k}$, the first k columns of kth in (12) are orthogonalized by Gram-Schmidt algorithm. Using (11), the kth required orthogonal operator for Tikhonov regularization is obtained.

IV. NUMERICAL TESTS

In previous section, several different classes of Tikhonov regularization operators have been introduced. Now, the influences of such operators on some numerical examples are illustrated. Here, the following operators for regularizing the ill-posed linear system of equations are considered. I_n is the identity matrix of order n, L_1 and L_2 are two operators based on scaled discretization of finite difference methods described in subsection 2.2, $L_4^{'}$ is an operator based on Newton's expansion of order 4, as well as two orthogonal operators $L_2^{''}$ and $L_4^{''}$ of the form (11). All the Tikhonov regularized problems are solved just by the ELMRES algorithm. For this algorithm, the initial guess $x_0 = (0,\ldots,0)^T$, the tolerance $eps = 10^{-10}$, the maximum iteration number $k\,max = 100$, the restarted number k (i.e. ELMRES(k)) and the convergence condition $\|b - Ax_n\| < eps$ are considered. The following numerical examples have been selected from the well-known package "Regularization Tools" collected by Hansen (2007).

Example 1: In this example, the following Fredholm integral equation of the first kind

$$\int_{-\pi/2}^{\pi/2} h(s,t)ds = b(t), \qquad -\pi/2 \le t \le \pi/2., \tag{13}$$

with $h(s,t) = \left(cos(s) + cos(t)\right)\left(\frac{sin(u)}{u}\right)^2$ with $u = \pi\left(sin(s) + sin(t)\right)$ where $b(t) = 2exp(-6(t-0.8)^2) + exp(-2(t+0.5)^2)$ discussed by Shaw (1972) is considered. By using the discretized MATLAB code shaw [Hansen, 2007] with $n = 200$, a linear system (1) with nonsymmetric matrix $A \in R^{200\times200}$ and right hand side vector $\hat{b} \in R^{200}$ are obtained.

By adding the noise vector $e = 10^{-4} * randn(200,1)$ to vector $\hat{b}$ as $b = \hat{b} + e$, the linear system of equations $Ax = b$ is solved by GMRES(20) using different discussed regularization operators. The following table shows some numerical results of this example using different regularization operators.

Table 1: Numerical Results of Example 1

Regularization Operators ➔	I_n	L_1	L_2	$L_4^{'}$	$L_2^{''}$	$L_4^{''}$
Error ($\|b - Ax_n\|$)	3.352e-12	1.497e-07	1.2147e-07	1.6334e-09	1.8269e-13	5.2524e-14
Iterations	2	100	100	100	3	4
Time	0.1092	0.3744	0.1872	0.1716	0.0156	0.0312

To compare the results of table 1, it is concluded that the regularization operators I_n, $L_2^{''}$ as well as $L_4^{''}$ have so better performances while the system will be solved for other operators within more than 100 iterations.

Example 2: The following Fredholm integral equation of the first kind, which discussed by Phillips (1962), is considered.

$$\int_{-6}^{6} k(s,t)x(t)dt, \qquad -6 \le t \le 6, \tag{14}$$

The function,

$$x(t) = \begin{cases} 1+\cos(\pi t/3), & |t| < 3, \\ 0, & Otherwise, \end{cases}$$

is the solution of (14) where $k(s,t) = x(s-t)$ and

$$b(s) = (6-|s|)\left(1+(\cos(\pi s/3))/2\right) + (9/2s)\sin(\pi|s|/3).$$

Using the discretized MATLAB code *phillips* with $n = 500$ [Hansen, 2007], the symmetric linear system of (1) with $A \in R^{500\times500}$ is obtained.

Similar to the previous example, the linear system $Ax = \hat{b} + e = b$ is solved by GMRES(30) using the previous regularizations. The following table shows that the numerical results of orthogonal operators are here better too.

Table 2: Numerical Results of Phillips500

Regularization Operators ➔	I_n	L_1	L_2	$L_4^{'}$	$L_2^{''}$	$L_4^{''}$
Error	9.533e-11	3.4133e-11	2.5351e-11	1.1754e-08	7.0536e-11	3.0802e-11
Iterations	8	39	69	100	12	12
Time	0.0936	0.5304	0.9048	1.6380	0.1560	0.1248

The exact solution of this problem is illustrated below.

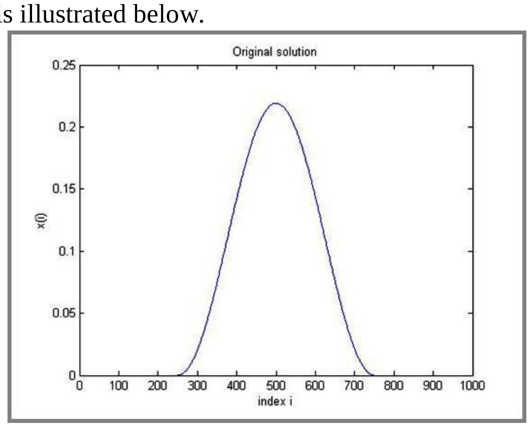

Figure 1: Exact Solution of Example 2

To compare the computed solutions of different methods, see the following graphs.

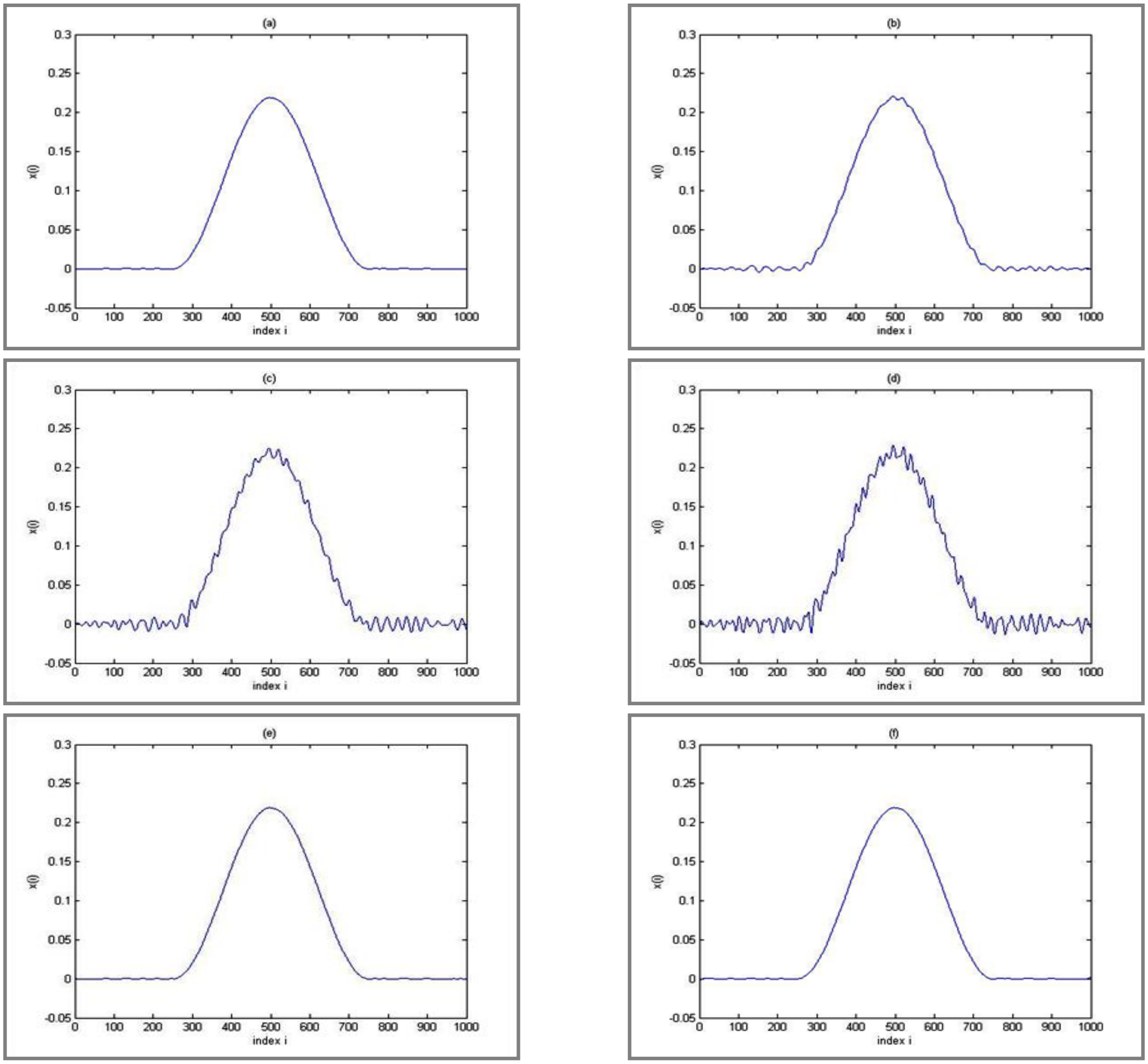

Figure 2: Numerical Results of Example 2

In figure 2, (a) is for the solution computed by ELMRES using identity regularization operator, (b) is for L_2, (c) is for L_2, ... and (f) is for the approximated solution applied L''_4 respectively. It is obviously seen that the graphs of (b), (c) and (d) are not as smooth as the others which used orthogonal operators.

V. Conclusion

In this work, several sorts of Tikhonov regularization operators have been studied and they have been compared with each other by the recently proposed iterative method ELMRES. Due to the numerical results of this work and other experiences of the authors, the orthogonal operators are the best set and the identity operator can be chosen as a simplest one which is an efficient and applicable operator for Tikhonov regularization for ELMRES algorithm.

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