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Novel Iterative Algorithms Based on Regularization Total Least Squares for Solving the Numerical Solution of Discrete Fredholm Integral Equation

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Abstract: Discretization of inverse problems often leads to systems of linear equations with a highly ill-conditioned coefficient matrix. To find meaningful solutions of such systems, one kind of prevailing and representative approaches is the so-called regularized total least squares (TLS) method when both the system matrix and the observation term are contaminated by some noises. We will survey two such regularization methods in the TLS setting. One is the iterative truncated TLS (TTLS) method which can solve a convergent sequence of projected linear systems generated by Lanczos bidiagonalization. The other one is to convert the Tikhonov regularization TLS problem to an unconstrained optimization problem with the properties of a convex function. The optimization problem will be solved with the state-of-the-art conjugate gradient (CG) method, and moreover, the adaptive strategy for selecting regularization parameter is also established. Finally, both the new methods are applied to tackle several Fredholm integral equations of the first kind which are known to be typical ill-posed problems. The results of numerical examples demonstrate that the robustness and effectiveness of the two novel algorithms make a significant improvement in the solution of ill-posed linear problems, i.e., yield more accurate regularized solution than other typical methods.

Keywords: Ill-posed, Total least squares, regularization parameter, Fredholm integral equation, Conjugate gradient.

1 Introduction

Inverse problems often arise in engineering praxis. They originate from various fields like acoustics, optics, model updating, computerized tomography, statistics,

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load identification and signal processing, etc. When we deal with the term inverse problem, we will ask "inverse to what" immediately. Roughly speaking, inverse problem is a general framework that is used to convert observed measurements into information about a physical object or system in which we are interested. Thus, one might say the inverse problems are concerned with determining causes for a desired or an observed effect [Heinz, Martin and Andreas (1996)].

As we will see, most inverse problems are often ill-posed problems Therefore, the necessary conditions for stability of solutions in a well-posed problem are often violated. That is to say, the total measured data does not allow the existence of a solution; the solution is also not unique, even further, not stable due to disturbances in the data [Heinz, Martin and Andreas (1996)]. One central example of a linear inverse problem is Fredholm integral equations of the first kind which have been introduced by [Aster and Borchers (2004); Liu and Atluri (2009a)], such as for one-dimension:

$$\int_{\Omega} K(X,Y)f(Y) = T(X)\Omega = [a,b] \tag{1}$$

for two-dimensions:

$$\int\int_{\Omega} K(X,Y)f(Y) = T(X)\Omega = [a,b]\times[c,d] \tag{2}$$

where $K(X,Y)$ and $T(X)$ are known functions and $f(Y)$ is an unknown function. We also suppose that $K(X,Y)$ and $T(X)$ are perturbed by random noise. As we know, many physical problems, such as industrial control, geophysical exploration, image processing and signal processing [Aster and Borchers (2004); Liu and Atluri (2009a); Micheli and Viano (2011); Ioannou, Fyrillas and Doumanidis (2012)], could usually be reduced to the problem of solving one or two-dimensions Fredholm integral equations of the first kind. Such integral equation may often be discretized into linear equation $\boldsymbol{Ax} \approx \boldsymbol{b}, (\boldsymbol{A} \in \mathrm{R}^{m\times n}, \boldsymbol{b} \in \mathrm{R}^{m\times 1})$ in order to acquire numerical solution. A common feature of the discrete integral equation is ill-posed (the matrix $\boldsymbol{A}$ is typically ill-conditioned) or unstable i.e., small changes like measurement errors or roundoff errors in the measured effect may result in large fluctuations in the estimated cause. This significant feature makes the ill-posed equations impossible to be solved directly. Thence, some indirect numerical methods for solving above ill-posed problems have been discussed in [Liu (2008); Liu and Atluri (2009b); Liu, Yeih and Chang (2009); Liu and Kuo (2011)]. These processes could be summarized as regularization approach based on Least Squares (LS) which is one of the most significant methods for settling the linear ill-posed problems. In the ordinary LS-based approaches the measurement matrix $\boldsymbol{A}$ are assumed to be free of error and hence, all errors are confined to the right hand side $\boldsymbol{b}$. However, in engineering applications this assumption is often unrealistic: sampling errors, human errors, modeling errors and instrument errors may imply inaccuracies in the matrix $\boldsymbol{A}$ as well. For those cases, the regularization total least squares (RTLS) approach has been devised and amounted to solving the ill-posed linear equations reasonably [Goulb, Hanse and O'Leary (1999)].

The RTLS problem has been investigated in its algebraic setting for decades. There are two kinds of RTLS methods which are analogous to the truncated SVD and the Tikhonov regularization based on LS. The former one is called truncated total least squares (TTLS), which has already been studied by Fierro, Golub, Hansen and O'Leary (1997). Unfortunately, when the dimensions of $\boldsymbol{A}$ are too large, computing the complete SVD of $(\boldsymbol{A},\boldsymbol{b})$ will result in higher complexity. And in some cases, there is no clear gap in the singular value of the matrix $(\boldsymbol{A},\boldsymbol{b})$. This makes it difficult to decide the best truncation index. Moreover, it usually encounters that the singular vectors corresponding to smaller and smaller singular values have raising complexity (meaning that they include more and more sign change, oscillations) [Sima and Huffel (2007)]. Another typical RTLS method for solving ill-posed problem is the Tikhonov regularization approach. The main emphasis of this work was on quadratically constrained TLS problems [Sima, Huffel and Goubl (2004)]. The regularization approach with a quadratic constraint is highly suitable when some knowledge about the characteristics of the exact solution is known at priority. However, it is difficult to obtain prior knowledge about the true solution and the magnitude of the noise. Recently, Schaffrin and Wieser (2008) have derived the RTLS solution using a non-linear Lagrange function approach which could be implemented by a suitable and efficient iteration algorithm. Unfortunately their convergence rate is always slower, and the convergence properties of these methods for Tikhonov RTLS problems aren't also guaranteed.

Currently, the regularized TLS algorithms possess few deficiencies in practical applications, but many scholars [Renaut and Gou (2005); Markovsky and HUffel (2007); Lampe and Voss (2012)] have demonstrated that the regularized TLS method is a feasible approach for solving linear ill-posed problems if both the system matrix $\boldsymbol{A}$ and the right-hand side $\boldsymbol{b}$ are contaminated by some noises. Therefore, it is necessary to overcome above deficiencies, and then, improve the efficiency and robustness of the RTLS method for solving ill-posed problem.

In this paper, our purpose is to tackle the linear discrete ill-posed problems by two novel regularization methods in the TLS setting described in Section 2. One is to extend the Lanczos TTLS algorithm to the iterative TTLS method which can solve a convergent sequence of projected linear systems in Section 2.1. The other one in section 2.2 is the iterative RTLS method based on conjugate gradient algorithm, which includes three creative schemes: establishing an modified unconstrained optimization problem with the properties of a convex function; giving the adaptive strategy for selecting regularization parameters; using a state-of-the-art CG method to solve the modified unconstrained optimization problem. In Section 3, several numerical examples related to Fredholm integral equations of the first kind are presented, and the efficiency and robustness of the two novel algorithms, compared with other typical regularization methods, are also demonstrated. Concluding remarks can be found in Section 4.

2 Regularized TLS

The TLS method is a generalized version of the original least squares method. Let the Errors-in-Variables model be defined by the functional relationship

$$\boldsymbol{b}-\boldsymbol{r}=(\boldsymbol{A}-\boldsymbol{E})\boldsymbol{x} \tag{3}$$

where $\boldsymbol{A}$ is the $m\times n$ system matrix affected by the random error matrix $\boldsymbol{E}$, the observation vector $\boldsymbol{b}\in \mathrm{R}^{m\times 1}$ is contaminated by random error vector $\boldsymbol{r}$, $\boldsymbol{x}$ is the (unknown) parameter vector. In the TLS method one allows a residual matrix as well as a residual vector, and then the computational problem becomes

$$\begin{aligned}&\min_{A_0,b_0}\|(\boldsymbol{A},\boldsymbol{b})-(\boldsymbol{A}_0,\boldsymbol{b}_0)\|_F\\ \text{or }&\min_{A_0,b_0}\|(\boldsymbol{E},\boldsymbol{r})\|_F,\ \text{ subject to }\ \boldsymbol{b}_0=\boldsymbol{A}_0\boldsymbol{x}\end{aligned} \tag{4}$$

If the matrix $\boldsymbol{A}$ is well conditioned a solution can be found using Eq. (4). While solving discrete ill-conditioned systems, regularization methods in the TLS setting should be used to introduce mild assumptions on the solution and prevent overfitting. In this section we survey two regularization methods in the TLS setting. One is similar in spirit to truncated SVD, which suitable for the singular values of $(\boldsymbol{A},\boldsymbol{b})$ have one or more small (nonzero) singular values away from the large ones, namely, with an obvious gap in the singular values spectrum. Other one is analogous to the Tikhonov regularized method, which adapt to the singular values of $(\boldsymbol{A},\boldsymbol{b})$ decay gradually to zero, i.e., with no particular gap in the singular values spectrum.

2.1 Iterative TTLS approach based on a Lanczos Bidiagonalization Algorithm

The first TLS-based regularization approach is inspired by the TSVD method. The major difference between the two methods lies in the way that this is done: in TSVD method the small singular values of $\boldsymbol{A}$ are discarded, while in TTLS method the key idea is to neglect the small singular values of $(\boldsymbol{A},\boldsymbol{b})$ by treating small singular values below a given threshold as zeros. See, for example, in [Fierro, Golub, Hansen and O'Leary (1997)]. The details of the TTLS algorithm can be summarized as follow

Algorithm. 1

1) execute the SVD of the augmented matrix $(\boldsymbol{A},\boldsymbol{b})$

$$(\boldsymbol{A},\boldsymbol{b}) = \mathrm{U}\sum \boldsymbol{V}^{\mathrm{T}} = \sum_{\mathrm{i}=1}^{\mathrm{n}+1} \mathrm{u_i}\sigma_{\mathrm{i}}\mathrm{v_i^T}$$

where $\boldsymbol{U} \in \mathrm{R}^{m\times(n+1)}$, $\boldsymbol{V} \in \mathrm{R}^{(n+1)\times(n+1)}$ is orthonormal matrices. The diagonal matrix $\sum = diag(\sigma_1,\cdots,\sigma_{n+1})$ holds that $\sigma_1 \geq \cdots \geq \sigma_{n+1}$.

2) select a truncation parameter $k \leq \min(n, rank(\boldsymbol{A},\boldsymbol{b}))$

3) block-partition $\boldsymbol{V} \in \mathrm{R}^{(n+1)\times(n+1)}$ as

$$\boldsymbol{V} = \begin{pmatrix} \boldsymbol{V}_{11} & \boldsymbol{V}_{12} \\ \boldsymbol{V}_{21} & \boldsymbol{V}_{22} \end{pmatrix}, \boldsymbol{V}_{11}^{\in}\mathrm{R}^{n\times k},\ \boldsymbol{V}_{22}^{\in}\mathrm{R}^{1\times(n+1-k)}$$

4) compute the TTLS solution $x_{TTLS,k}$ as

$$\boldsymbol{x}_{TTLS,k} = -\boldsymbol{V}_{12}\boldsymbol{V}_{22}^{+} = -\frac{\boldsymbol{V}_{12}\boldsymbol{V}_{22}^{T}}{\|\boldsymbol{V}_{22}\|_2^2}$$

where $\boldsymbol{V}_{22}^{+} = \boldsymbol{V}_{22}^{T}\|\boldsymbol{V}_{22}\|_2^{-2}$ is the pseudoinverse of $\boldsymbol{V}_{22}$, and $\boldsymbol{V}_{22} \neq 0$.

The TTLS method which simultaneously considers error and noise on both sides can be applied to handle ill-posed problems, especially when there are obvious gap in the singular values spectrum. And its performance is usually better than conventional Tikhonov method. However, when the dimensions of $\boldsymbol{A}$ become large, the efficiency and robustness of this approach become increasingly poor because the SVD algorithm is of high complexity. We shall therefore describe that a Lanczos technique which can project large-scale TLS problems onto the smaller subspaces may improve the efficiency of the TTLS algorithm.

The typical algorithm is the Lanczos bidiagonalization method which can generate a sequence of bidiagonal matrices. Here, the extremal singular values of bidiagonal matrices are progressively better estimates of the extremal singular values of the given matrices [Goulb, Hanse and O'Leary (1999)]. The main advantages of the Lanczos method are that the original matrix is not overwritten and little storage is required since only matrix-vector products are computed. Therefore, the computation cost of SVD of a matrix may be more attractive, which makes the Lanczos method interesting for large matrices especially if they are sparse and there exists fast routines for computing matrix-vector products.

The Lanczos TTLS algorithm is proposed by considering Lanczos bidiagonalization of the matrix $\boldsymbol{A}$ rather than $(\boldsymbol{A},\boldsymbol{b})$. Firstly, we compute the bidiagonal matrix

$\boldsymbol{B}_k \in \mathrm{R}^{(k+1)\times k}$ of $\boldsymbol{A}$ with $\tilde{\boldsymbol{U}}_{k+1} \in \mathrm{R}^{m\times(k+1)}$, $\tilde{\boldsymbol{V}}_k \in \mathrm{R}^{n\times k}$ such that

$$\boldsymbol{A}\tilde{\boldsymbol{V}}_k = \tilde{\boldsymbol{U}}_{k+1}\boldsymbol{B}_k$$

where $\tilde{\boldsymbol{V}}_k = [\tilde{\boldsymbol{v}}_1, \tilde{\boldsymbol{v}}_2, \cdots, \tilde{\boldsymbol{v}}_k], \tilde{\boldsymbol{v}}_1, \tilde{\boldsymbol{v}}_2, \cdots, \tilde{\boldsymbol{v}}_k \in \mathrm{R}^n$, $\tilde{\boldsymbol{U}}_{k+1} = [\tilde{\boldsymbol{u}}_1, \tilde{\boldsymbol{u}}_2, \cdots, \tilde{\boldsymbol{u}}_{k+1}]\tilde{\boldsymbol{u}}_1, \tilde{\boldsymbol{u}}_2, \cdots, \tilde{\boldsymbol{u}}_{k+1} \in \mathrm{R}^m$.

$$\boldsymbol{B}_k = \begin{bmatrix} \alpha_1 & & & & \\ \beta_2 & \alpha_2 & & & \\ & & \cdots & & \\ & & & \beta_k & \alpha_k \\ & & & & \beta_{k+1} \end{bmatrix} \in {}^{(k+1)\times k}$$

with starting vector $\tilde{\boldsymbol{u}}_1 = \boldsymbol{b}/\beta_1$, $\beta_1 = \|\boldsymbol{b}\|_2$, the bidiagonal iterative process is as follows

$$\alpha_1 \tilde{\boldsymbol{v}}_1 = \boldsymbol{A}^T \tilde{\boldsymbol{u}}_1$$

$$\left.\begin{array}{l} \beta_{i+1}\tilde{\boldsymbol{u}}_{i+1} = \boldsymbol{A}\tilde{\boldsymbol{v}}_i - \alpha_i \tilde{\boldsymbol{u}}_i \\ \alpha_{i+1}\tilde{\boldsymbol{v}}_{i+1} = \boldsymbol{A}^T\tilde{\boldsymbol{u}}_{i+1} - \beta_{i+1}\tilde{\boldsymbol{v}}_i \end{array}\right\rangle, i = 1, 2, \cdots$$

$$\tilde{\boldsymbol{U}}_{k+1}(\beta_1 \boldsymbol{e}_1) = \boldsymbol{b}$$

$$\boldsymbol{A}\tilde{\boldsymbol{V}}_k = \tilde{\boldsymbol{U}}_{k+1}\boldsymbol{B}_k$$

$$\boldsymbol{A}^T\tilde{\boldsymbol{U}}_{k+1} = \tilde{\boldsymbol{V}}_k\boldsymbol{B}_k^T + \alpha_{k+1}\tilde{\boldsymbol{v}}_{k+1}\boldsymbol{e}_{k+1}^T$$

Thus after k Lanczos iterations, the projected TLS problem mentioned in Eq. (4) is given by

$$\min \left\| \tilde{\boldsymbol{U}}_{k+1}^T \left((\boldsymbol{A}, \boldsymbol{b}) - (\boldsymbol{A}_0, \boldsymbol{b}_0) \right) \begin{pmatrix} \tilde{\boldsymbol{V}}_k & 0 \\ 0 & 1 \end{pmatrix} \right\|_F \tag{5}$$

or

$$\min \|(\boldsymbol{B}_k, \beta_1 \boldsymbol{e}_1) - (\boldsymbol{B}_{0,k}, \boldsymbol{e}_{0,k})\|_F, \quad \boldsymbol{B}_{0,k} y = \boldsymbol{e}_{0,k} \tag{6}$$

where $\boldsymbol{e}_1 = (1, 0, \cdots, 0)^T$. In each Lanczos step we can now compute a TLS solution $\tilde{\boldsymbol{x}}_{TTLS,k} = \tilde{\boldsymbol{V}}_k \boldsymbol{y}_k$ by applying the TTLS algorithm to the small-size problem (2). To obtain an optimal TLS solution of the Eq. (4), we must determine a suitable iteration parameter k which has a similar meaning as a truncated index. An effective criterion is the discrete L-curve criterion which plotted in log-log scale via solutions norm $\|\tilde{\boldsymbol{x}}_{TTLS,k}\|_2$ versus the residual norm $\|(\boldsymbol{A}, \boldsymbol{b}) - (\boldsymbol{A}_{0,k}, \boldsymbol{b}_{0,k})\|_F$ [Fierro, Golub, Hansen and O'Leary (1997)]. Nevertheless, the solutions of the Lanczos T-TLS algorithm would be repeated for $k_{\max}$ times, which cost amount of time. And the maximal truncate index $k_{\max}$, as a critical precondition, isn't easy to get. If the maximal truncate index $k_{\max}$ is larger, the advantage of the lanczos method may disappear, while smaller $k_{\max}$ may make the L-curve method invalidation for determining optimal truncation index k. At present, we can only determinate the maximal truncate index $k_{\max}$ by means of experiential knowledge.

To overcome these deficiencies, we note that it is easy to extend the above algorithm to an iterative TTLS method without any prior knowledge. This method can solve a convergent sequence of projected linear systems generated by the Lanczos bidiagonalization method, which is a potentially inexpensive task. The structure of this algorithm is as follows

Algorithm. 2 (iteration Lanczos TTLS called I-LTTLS)

1) set starting vector $\tilde{\boldsymbol{x}}_{TTLS}^{(0)}$, $k = 0$

2) for $k = 1, 2, \cdots$ until convergence do

3) obtain the projected TLS problem of (4) based on Lanczos bidiagonalization.

$$\min \|(\boldsymbol{B}_k, \beta_1 \boldsymbol{e}_1) - (\boldsymbol{B}_{0,k}, \boldsymbol{e}_{0,k})\|, \boldsymbol{B}_{0,k} y = \boldsymbol{e}_{0,k}$$

4) compute the TTLS solution $\boldsymbol{y}_{k,l}$ via **algorithm.1**, l denotes truncate parameter.

5) compute solutions $\tilde{\boldsymbol{x}}_{TTLS,l}^{(k)} = \tilde{\boldsymbol{V}}_k \boldsymbol{y}_{k,l}$ of the Eq. (4)

6) end for

7) output the approximate truncated TLS solution $\tilde{\boldsymbol{x}}_{TTLS}^{(k)}$

We now discuss details how to efficiently execute algorithm. 2.

· Typically the starting vector $\tilde{\boldsymbol{x}}_{TTLS}^{(0)} = \boldsymbol{0}^{n\times 1}$is reasonable.

· We apply an modified generalized cross validation (GCV) combined with the TTLS method to obtain truncate parameter l in step 4, which has been proposed in [Sima and Huffel (2007)] , see Eq.(4)

$$\min_l \frac{\|\boldsymbol{H}\boldsymbol{x}_{TTLS,l} - \boldsymbol{b}\|_2^2}{(m - p_l^{eff})^2} \tag{7}$$

where p_k^{eff} is computed as the sum of the TTLS filter factors.

· The convergence criteria is determined by considering the relative change of two restoration solution vector $\tilde{\boldsymbol{x}}_{TTLS}^{(k)}$ and $\tilde{\boldsymbol{x}}_{TTLS}^{(k-1)}$ is smaller terminate tolerance ε, i.e., $\eta = \|\boldsymbol{x}_{TTLS}^{k} - \boldsymbol{x}_{TTLS}^{k-1}\| / \|\boldsymbol{x}_{TTLS}^{k-1}\| < \varepsilon$.

2.2 Iterative Tikhonov RTLS approach based on conjugate gradient method

For some discrete ill-posed problems the TTLS method is efficient, but cutting off filtering strategy is not the best choice when facing that the singular value of $(\boldsymbol{A},\boldsymbol{b})$ decay gradually to zero. In this case, the TTLS algorithm faces several deficiencies that the truncation index is hard to determine and the truncated singular values may be the useful system information. To solve such problems, the second TLS-base regularization method based on the Tikhonov formulation is proposed in this section. We adopt the Tikhonov regularization concept to stabilize the TLS problem described as Eq. (4), i.e., consider the problem

$$\min_{x,E,r}\left\{\|\boldsymbol{E}\|^2+\|\boldsymbol{r}\|^2+\lambda\,\|\boldsymbol{Lx}\|^2:(\boldsymbol{A}+\boldsymbol{E})\boldsymbol{x}=\boldsymbol{b}+\boldsymbol{r}\right\} \tag{8}$$

where $\boldsymbol{L}\in \mathrm{R}^{(n-1)\times n}$ is a full row rank matrix (regularization matrix) and $\lambda>0$ is a penalty parameter (regularization parameter).

The Lagrangian of the problem (8) is given by

$$\Phi(\boldsymbol{E},\boldsymbol{r},\tilde{\boldsymbol{\lambda}})=\|\boldsymbol{E}\|^2+\|\boldsymbol{r}\|^2+\lambda\,\|\boldsymbol{Lx}\|^2+2\tilde{\boldsymbol{\lambda}}^T\left((\boldsymbol{A}+\boldsymbol{E})\boldsymbol{x}-\boldsymbol{b}-\boldsymbol{r}\right) \tag{9}$$

where $\tilde{\boldsymbol{\lambda}}\in \mathrm{R}^{m\times 1}$denotes Lagrange coefficient.

Let us first consider the minimization problem with respect to the variables $\boldsymbol{E}$ and $\boldsymbol{r}$. Obviously the Eq. (9) is a convex optimization problem, and the KKT conditions [Maziar and Hossein (2009)] are necessary and sufficient for optimality that follows:

$$2\boldsymbol{E}+2\tilde{\boldsymbol{\lambda}}\boldsymbol{x}^T=0\quad(\nabla_E\Phi=0) \tag{10}$$

$$2\boldsymbol{r}-2\tilde{\boldsymbol{\lambda}}=0\quad(\nabla_r\Phi=0) \tag{11}$$

$$(\boldsymbol{A}+\boldsymbol{E})\boldsymbol{x}=\boldsymbol{b}+\boldsymbol{r} \tag{12}$$

Substituting (11) into (10) we have

$$\boldsymbol{E}=-2\boldsymbol{r}\boldsymbol{x}^T \tag{13}$$

Combining (12) with (13) we can conclude

$\boldsymbol{r}=\frac{\boldsymbol{Ax}-\boldsymbol{b}}{\|\boldsymbol{x}\|^2+1},\quad \boldsymbol{E}=-\frac{(\boldsymbol{Ax}-\boldsymbol{b})\boldsymbol{x}^T}{\|\boldsymbol{x}\|^2+1}$

Finally, by substituting $\boldsymbol{r}$ and $\boldsymbol{E}$ into the objective function of the problem (8), then regularized problem becomes

$$\min_{\boldsymbol{x}\in \mathrm{R}^{n\times 1}} f(\boldsymbol{x}):=\frac{\|\boldsymbol{Ax}-\boldsymbol{b}\|^2}{1+\|\boldsymbol{x}\|^2}+\lambda\,\|\boldsymbol{Lx}\|^2 \tag{14}$$

It can be observed that the Eq. (14) is an unconstrained optimization problem, which is not known to be convex or concave in general. Beck and Ebn-Tal (2006) computed a value and a derivative of the problem (14) consists of solving a sequence of trust region subproblems. The suggested TRTLSG algorithm converges to the global minimum when the function $f(x)$ is unimodal. If, for some reason, the function $f(x)$ is not unimodal, the TRTLSG algorithm doesn't necessarily converge to global minimum and more sophisticated one dimensional global solver should be employed.

The classical Newton iterative method has been used to tackle the unconstrained optimization problem (14) in [Maziar and Hossein (2009)], which is an extremely powerful technique—in general the convergence is quadratic. The Newton iterative method requires that the gradient and hessian of the objective function can be calculated directly. However, an analytical expression for the derivative may not be easily obtainable and may be expensive to evaluate. For situations where the method fails to converge, it is because the assumption such as the second derivative of the positive definite made in the proof is not met. Lampe and Voss (2013) proposed an iterative projection method which was an efficient method for solving large-scale TLS problem. This algorithm requires a suitable starting basis called orthogonal basis of the Krylov space, which has a great influence on the computational efficiency and is hard to be determined. The main computational cost is again building up the search space, in general, which is not a Krylov subspace. In particular, the new space basis vector cannot be computed with a short recurrence relation.

The nonlinear conjugate gradient (CG) methods[Liu, Hong and Atluri (2010)] are one of the most popular approaches for solving unconstrained minimum optimization problem (14) due to the simplicity of iteration formula and the lower memory requirements. A CG method can generate a sequence $\{\boldsymbol{x}_l\}$, starting from an initial point $\boldsymbol{x}_0 \in \mathrm{R}^{n\times 1}$, the iterative formula is given by

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \tilde{\alpha}_k \boldsymbol{d}_k \quad k = 0, 1, \cdots,$$

where $\boldsymbol{x}_k$ is the current iteration value, $\tilde{\alpha}_k > 0$ is a step length which is determined by kinds of line search methods, $\boldsymbol{d}_k$ is the search direction generated by the rule

$$\boldsymbol{d}_k = \begin{cases} -\boldsymbol{g}_k, & \text{if} \quad k = 0, \\ -\boldsymbol{g}_k + \beta_k \boldsymbol{d}_{k-1}, & \text{if} \quad k > 0. \end{cases}$$

here β_k is a scalar which determines the different conjugate gradient methods, and $\boldsymbol{g}_k = \nabla f(\boldsymbol{x}_k)$ is the gradient of $f(\boldsymbol{x})$.

The aim of this section is to propose a CG method to solve the Tikhonov RTLS problem (14). The main difficulty associated with problem (14) is its nonconvexity. This deficiency may result in a non-convergent sequence i.e., cannot get the global optimal solutions, and make the CG algorithm ineffective or difficult implementation. Nevertheless, we will propose in this section several creative schemes to solve the unconstrained optimization problem (14) efficiently and stably. The partial recovery solution $\boldsymbol{x}_{k-1}$ from every step of the iterative process, without losing premise of the generality, can be used as the prior knowledge of computing the next value $\boldsymbol{x}_k$ in the iterative formula. Therefore, substituting $\boldsymbol{x}_{k-1}$ into the denominator of the problem (14) in k^{th} iteration we can conclude

$$f(\boldsymbol{x}_k) := \frac{\|\boldsymbol{A}\boldsymbol{x}_k - \boldsymbol{b}\|^2}{1+\|\boldsymbol{x}_{k-1}\|^2} + \lambda \|\boldsymbol{L}_i\boldsymbol{x}_k\|^2 \tag{15}$$

It is obviously that the iteration Eq. (15) has adaptive characteristics which are able to fully reflect the continuity of recovery process. More importantly, the original Eq. (14) with a nonconvex function is transformed into a convex function, which can facilitate the optimization problem greatly and improve the computational efficiency significantly.

In above technique, it is important to choose an optimal regularization parameter. For the determination of regularization parameters in LS-based problems there are several well-known methods [Hansen (2007)]. At present, the main methods for determining regularization parameter of TLS problem are original from the LS-based methods. However, it is hard to obtain effective regularization parameter since the complexity of Tikhonov RTLS problem. In [Lampe J (2010)] the L-curve method has been applied to the Tikhonov RTLS problem to determine a suitable regularization parameter λ. The L-curve method derives from the characteristic shape of this curve, for RTLS case, which is plot—for all valid regularization parameters—of the regularization solution $\|\boldsymbol{L}_i\boldsymbol{x}_\lambda\|^2$versus the size of the corresponding residual $\|\boldsymbol{A}\boldsymbol{x}_\lambda - \boldsymbol{b}\|^2 \Big/ 1+\|\boldsymbol{x}_\lambda\|^2$. We choose the optimal parameter which is the closest to the L-shape left bottom corner as a regularization parameter λ. The parameter λ controls the trade-off between a good fit of regularization solution and a smoothness requirement. The L-curve criterion has its limitations is that the repeated solutions of the corresponding RTLS problem are required for many values of the regularization parameter λ, a potentially very costly task. However, the L-curve method has been proved to be better than other methods for tackling RTLS problem in many real-world applications if no previous knowledge about its error is available.

Oraintara, Karl, Castanon, and Nguyen (2000) have proposed an algebraic condition for choosing the optimal regularization parameter of regularized LS. The main idea is to identify the corner of the L-curve as the point of tangency between a straight line of arbitrary slope and the L-curve. The main restrictions are that the object function should be differentiable, non-negative and convex scalar function of their vector arguments. Owing to these restrictions, the algebraic method cannot be used to acquire regularization parameter for RTLS optimization problem (14). Fortunately, for the modified optimization problem (15) with the properties of a convex function, the algebraic method can be extended to obtain the regularization parameter of Tikhonov RTLS. That is also an important way to make the conjugate gradient method converge to a global minimum point.

For convenience in what follows, the function of the parameter$\lambda$is

$$\xi(\lambda) = \frac{\beta \varphi(b, x_\lambda)}{\phi(x_\lambda)} \tag{16}$$

with $\varphi(\boldsymbol{b}, \boldsymbol{x}_{k,\lambda}) = \frac{\|\boldsymbol{A}\boldsymbol{x}_k - \boldsymbol{b}\|^2}{1+\|\boldsymbol{x}_{k-1}\|^2}$, $\varphi(\boldsymbol{x}_{k,\lambda}) = \|\boldsymbol{L}\boldsymbol{x}_k\|^2$, β is a scalar.

As a consequence, we demonstrate that extreme points of $\xi(\lambda)$ are fixed points of a related function, and a fixed point iterative algorithm for computing the optimal parameter λ is as follows

$$\lambda_{k+1} = \zeta(\lambda_k) = \frac{\beta \varphi(\boldsymbol{b}, \boldsymbol{x}_{k,\lambda})}{\phi(\boldsymbol{x}_{k,\lambda})} \tag{17}$$

In particular, if λ_k converges, it is guaranteed to converge to the L-corner. The formula is able to choose the regularization parameter adaptively and get higher efficiency attributed to the convex properties of the problem (15).

To solve the minimum optimization problem (15) efficiently, we apply a state-of-the-art nonlinear CG methods established by Zhang, Zhou and Li (2006), which is a CG algorithm of the modified PRP. The attractive properties of this modified CG method are that the search direction is always a descent direction for the minimum optimization problem (15) i.e. $\boldsymbol{d}_k^T \boldsymbol{g}_k = -\|\boldsymbol{g}_k\|^2 < 0$, and this new technique is globally convergent for convex optimization problem if the search satisfies Armijo-type condition.

Therefore, we propose three creative schemes in this section in order to solve Tikhonov RTLS problem. Firstly, the modified minimum optimization problem (15) characterized by the properties of a convex function is established. Secondly, the adaptive strategy for selecting regularization parameter is given, which gets better quality of the result in view of the former one. Finally, a state-of-the-art CG method is used to solve the unconstrained optimization problem (15). More precisely, this iterative RTLS method based on conjugate gradient (called CGRTLS method) can be described as follows

Algorithm 3 (The CGRTLS algorithm)

1) set the outer iteration terminate tolerance ε, $0 < \varepsilon \ll 1$, and the largest admissible number of outer iteration $k_{\max}$

2) set the inner iteration terminate tolerance ξ, $0<\xi\ll 1$, and the largest admissible number of inner iteration $l_{\max}$

3) set the iteration vector $\boldsymbol{x}_{k-1}=\boldsymbol{x}_k\in \mathrm{R}^{n\times 1}$ and the regularization parameter λ_0, $k=1$

4) begin outer iteration

4.1) given function $f(\boldsymbol{x}_k)$ and the gradient $\nabla f(\boldsymbol{x}_k)$ of the function $f(\boldsymbol{x}_k)$

4.2) inner iteration processes

(a) set $\boldsymbol{x}_k^{(0)}=\boldsymbol{x}_{k-1}$, compute $g_0=\nabla f(\boldsymbol{x}_k^{(0)})$ when $l=0$

(b) if $\|\boldsymbol{g}_l\|\le\xi$ or $l>l_{\max}$, then stop inner iteration processes, and output $\boldsymbol{x}_k^*\approx\boldsymbol{x}_k^{(l)}$

(c) else go step (d)

(d) compute search orientation $\boldsymbol{d}_l$:

$$\boldsymbol{d}_l=\begin{cases}-\boldsymbol{g}_l, & l=0\\ -\boldsymbol{g}_l+\tilde{\beta}_{l-1}^{PRP}\boldsymbol{d}_{l-1}-\theta_l y_{l-1}, & l\ge 1\end{cases}$$

$$\tilde{\beta}_l^{PRP}=\frac{\boldsymbol{g}_l^H\boldsymbol{y}_{l-1}}{\boldsymbol{g}_{l-1}^T\boldsymbol{g}_{l-1}},\quad \theta_l=\frac{\boldsymbol{g}_l^T\boldsymbol{d}_{l-1}}{\left\|\boldsymbol{g}_{l-1}\right\|^2},\quad \boldsymbol{y}_{l-1}=(\boldsymbol{g}_k-\boldsymbol{g}_{k-1})$$

(e) determine a step $\tilde{\alpha}_l=\rho^j(j=0,1,2,\cdots)$ satisfying Armijo-type condition

$$f(\boldsymbol{x}_k^{(l)}+\tilde{\alpha}_l\boldsymbol{d}_l)<f(\boldsymbol{x}_k^{(l)})-\mu\tilde{\alpha}_2^2\|\boldsymbol{d}_l\|^2$$

with the scalar ρ, $\mu\in(0,1)$

(f) set $\boldsymbol{x}_k^{(l+1)}:=\boldsymbol{x}_k^{(l)}+\tilde{\alpha}_l\boldsymbol{d}_l$, and compute $\boldsymbol{g}_{l+1}=\nabla f(\boldsymbol{x}_k^{(l+1)})$

(g) set $l:=l+1$, go to (b)

4.3) update $\lambda_k=\frac{\beta\varphi(\boldsymbol{b},\boldsymbol{x}_k)}{\phi(\boldsymbol{x}_k)}$ by Eq. (17)

4.4) $\eta=\|\boldsymbol{x}_k-\boldsymbol{x}_{k-1}\|^2\big/\|\boldsymbol{x}_{k-1}\|^2$

4.5) $k:=k+1$

4.6) until the convergence condition $\eta<\varepsilon$ or $k>k_{\max}$, execute step 5

5) end outer iteration

To improve convergence performance of the CG algorithm, $\boldsymbol{x}_{k-1}$ is chosen as the initial vector for inner CG iteration at k^{th} outer iteration. Here, we set the parameter $\rho=0.5$, $\mu=0.6$.

3 Numerical examples

To evaluate the effectiveness of the Algorithm 2 and 3, we consider the one and two-dimensional Fredholm integral equations of the first kind, which are known to be severely ill-posed problems. We compare the solutions computed by two novel algorithms with the solutions obtained from several typical methods, i.e., Tikhonov regularization LS (RLS) [Hansen (2007)], Lanczos TTLS (L-TTLS) established in[Sima and Huffel (2007)] and RTLSQEP introduced in [Lampe and Voss (2012)]. All algorithms are carried out by MATLAB software. Firstly, we discuss how to efficiently execute these algorithms for solving the ill-posed inverse problems.

· Tikhonov regularization LS (RLS): we determinate regularization parameter using L-curve method withλin the range$(10^{-10}, 10^{2})$, and then, chose regularization matrix$L$which equals to the approximate first derivative operator i.e.,

$$\boldsymbol{L} = \begin{bmatrix} -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & & \cdots & & \\ & & & -1 & 1 & \\ & & & & -1 & 1 \end{bmatrix} \in {}^{(n-1)\times n}$$

·Lanczos TTLS (L-TTLS): the maximal truncate index$k_{\max} = 15$, the truncate index is acquired by L-curve method.

· RTLSQEP algorithm: the quadratic constraint δ is obtained by L-curve method, to create a suitable L-curve scenario, $r = 60$ RTLS problems with $0 \leq \delta_1 < \cdots < \delta_r \leq \|\boldsymbol{Lx}_{TLS}\|$, i.e., regularization parameter rang $\delta \in [0, \|\boldsymbol{Lx}_{TLS}\|]$.

· I-LTTLS's truncate parameter is determined by an modified generalized cross validation (GCV) in Eq.(7), terminate tolerance $\varepsilon = 10^{-6}$.

· CGRTLS: the tolerance parameters $\varepsilon = 10^{-6}$ and $\xi = 10^{-6}$, we also select iteration starting vector $\boldsymbol{x}_0 = 0^{n\times 1}$, the regularization parameter $\lambda_0 = 10^{-2}$, and the maximal iteration number $k_{\max} = 500$, $l_{\max} = 5000$.

We want to compare the optimal solutions that can be attained by any of the above methods. To do this, for each algorithm we define relative error γ between the optimal regularized solution $\boldsymbol{x}_{TLS}$ and the exact solution. For example, for CGRTLS

$$\gamma = \frac{\|\boldsymbol{x}_{true} - \boldsymbol{x}_{CRGTLS}\|}{\|\boldsymbol{x}_{true}\|} \tag{18}$$

Then we add perturbations $\boldsymbol{E}$ and $\boldsymbol{r}$ in Eq. (3), and the perturbations satisfy a Gaussian distribution with zero mean and unit variance, which is put in relation to the norm of true system matrix $\boldsymbol{A}_{ture}$ and true right-hand side $\boldsymbol{b}_{ture}$ respectively. We refer to the quotient

$$\rho = \frac{\|\boldsymbol{r}\|_2}{\|\boldsymbol{b}_{true}\|_2} = \frac{\|\boldsymbol{E}\|_F}{\|\boldsymbol{A}_{true}\|_F}$$

as the noise level. In the tests we select the noise levels $\rho_1 = 1 \times 10^{-3}$ and $\rho_2 = 1 \times 10^{-2}$.

3.1 One-dimensional Fredholm integral equation of the first kind

Firstly, we consider one-dimensional Fredholm integral equation of the first kind, which is a classical ill-posed problem. The Fredholm integral equation with a square integrate kernel is of the form

$$\int_a^b K(s,t)f(t)dt = T(s) \quad s \in [c,d] \tag{19}$$

in which the kernel K represents a known model for the physical phenomenon, the right-hand side T is a given date function, and$f$is a function to be determined.

To solve (19) numerically, it is necessary to make the variables discrete and replace the integral equation by a set of finite linear equations. Firstly, let us discretize the intervals of $[a,b]$ and $[c,d]$ into m_1 and m_2 equally. The integral equation can then be replaced by a set of numerical equations

$$T(s_i) = \int_a^b K(s_i,t)f(t)dt \approx \sum_{j=1}^{m1} w_j K(s_i,t_j)f(t_j) \tag{20}$$

where $i = 1,2,\cdots,m_2$, and w_j are the weighting coefficients for the quadrature formula. Through a trapezoidal rule, Eq . (20) can be rewritten as

$$K(s_i,t_1)f(t_1)w_1 + K(s_i,t_2)f(t_2)w_2 + \cdots + K(s_i,t_{m_1})f(t_{m_1})w_{m_1} = T(s_i) i = 1,2,\cdots,m_2$$

The above equations may be abbreviated as

$$\boldsymbol{Ax} = \boldsymbol{b} \tag{21}$$

where $\boldsymbol{A}(i,j) = w_j K(s_i,t_j)$ is a rectangular matrix with dimensions $m_2 \times m_1$, vectors $\boldsymbol{x} = f(t_j)$, $\boldsymbol{b} = T(s_i)$ is $m_1 \times 1$ and $m_2 \times 1$ column vector respectively. Then the regularized TLS algorithms can be used to solve the TLS algebraic equation (21) when not only the right-hand side $\boldsymbol{b}$ but the system matrix $\boldsymbol{A}$ is also contaminated by some noises.

We examine our TLS approaches by considering the numerical solution of the following one-dimensional Fredholm integral equations of the first kind.

Example. 1: the one problem is the discretization of the inverse Laplace transformation by means of Gauss-Laguerre quadrature. The kernel K is given by

$$K(s,t) = e^{-st}$$

and both integration interval $[a,b]$ and $[c,d]$ are $[0,\infty)$.

The right-hand side $T(s) = \frac{1}{s+1/2}$, and the exact solution $f(t) = e^{-t/2}$ is a function to be determined.

Example.2: other one is the famous one-dimensional Fredholm integral equation of the first kind devised by Phillips [Hansen, P. C. (2007)], which is described as follows:

$$K(s,t) = \phi(s-t)$$

$$f(t) = \phi(t)$$

$$T(s) = (6-|s|)(1+\frac{1}{2}\cos(\frac{\pi s}{3})) + \frac{9}{2\pi}\sin(\frac{\pi |s|}{3})$$

Both the integration intervals are $[-6,6]$. Where the function ϕ is

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

Here, solving the function f (the same as $\boldsymbol{x}$ mentioned in Eq. (21)), arising from an inverse problem, is usually prone to errors. These arise due to a combination of errors in the measurement and the ill-conditioning of the system matrix to be inverted. The most famous approach for measuring the ill-conditioning matrix is condition number, which is defined as the ratio of the largest singular value versus the smallest singular value. If the errors are significant and the condition numbers of the system matrix are small then the errors simply propagate to the solution $\boldsymbol{x}$ without much amplification. On the other hand, high condition numbers of the system matrix $\boldsymbol{A}$ can result in small errors of $\boldsymbol{b}$ and $\boldsymbol{A}$ being magnified into large $\boldsymbol{x}$ errors. The condition numbers of the matrix $\boldsymbol{A}$ of above examples are computed in different matrix dimensions, which can be seen in Table 1.

Table 1: The condition numbers of different matrix dimensions in two examples.

$m_1 = m_2$	20	40	100	200	300	600
Eg1-cond(A)	1.026×10^{30}	1.880×10^{32}	1.499×10^{32}	1.233×10^{33}	7.203×10^{32}	Inf
Eg2-cond(A)	3.958×10^{3}	6.604×10^{4}	2.638×10^{6}	4.228×10^{7}	2.412×10^{8}	2.423×10^{9}

It is known that the condition numbers of two types of system matrices are high, which indicate that the system matrices are much stronger ill-condition, especially in the first example. And the condition numbers of the system matrices grow as the m_1 and m_2 increase. Therefore, a small perturbation of the given date will be amplified greatly, such that the solution $\boldsymbol{x}$ in Eq. (21) may be contaminated seriously by some measurement errors.

Test 1. This test was carried out with matrix dimensions $m_1 = m_2 = 20$ and $m_1 = m_2 = 100$ in Example.1, the noise level $\rho_1 = 1\times10^{-3}$. For one thing, we consider the distribution of singular values of the augmented matrix $(\boldsymbol{A},\boldsymbol{b})$ with degressive ratio of neighboring eigenvalues. In Fig.1 we have plotted the declining ratio of neighboring eigenvalues i.e., plot $\left(i,\sigma_i/\sigma_{i+1}\right)$, i is the number of singular value of the matrix $(\boldsymbol{A},\boldsymbol{b})$. For case of $m_1=m_2=20$, the computed results obtained from the plots on the left of the Fig.1 show that there is a great declining ratio of eigenvalues when the number of singular value $i=12$, hence, existing larger gap in the eigenvalues spectrum. On the contrary, the plot on the right-hand side of this figure shows that the ratio of eigenvalues changes slowly i.e., the singular values of $(\boldsymbol{A},\boldsymbol{b})$ decay gradually to zero.

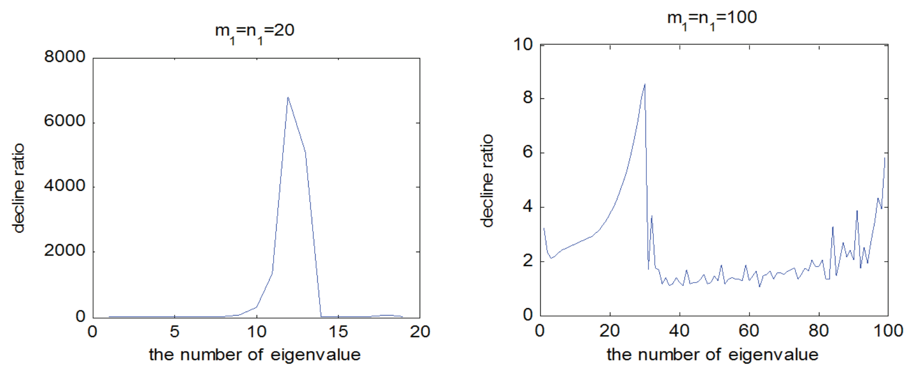

Figure 1: The declining ratio of neighboring eigenvalues

Fig.2 and Fig.3 show histograms of the relative errors γ for all five regularization methods in different matrix dimensions, respectively. And our results are obtained in the solution over 1000 independent simulations of the same example. It can be readily observed that the RLS method produces a worse solution than other RTLS algorithms. It is probably because the RLS cannot consider the errors of the system matrix efficiently. It is obvious that the I-LTTLS, CGRTLS and RTLSQEP methods are able to generate more accurate solutions than the classical regularization methods L-TTLS. Here, the effects of random noise on L-TTLS may reduce the accuracy of the solutions and increase dispersion of the solutions greatly, which is apt to obtain the unstable solutions. Furthermore, the I-LTTLS, CGRTLS and RTLSQEP methods possess lower noise sensitivity. Especially, the robustness of the I-LTTLS algorithm perfects best of these methods. The accuracy of the state-of-the-art RTLSQEP algorithm and CGRTLS algorithm is somewhere in between, where the latter one yields more accurate approximations. The RTLSQEP and L-TTLS algorithms are suitable when some knowledge about the characteristic of the exact solution or noise condition is known a priori, however, it is difficult to be obtained in some cases.

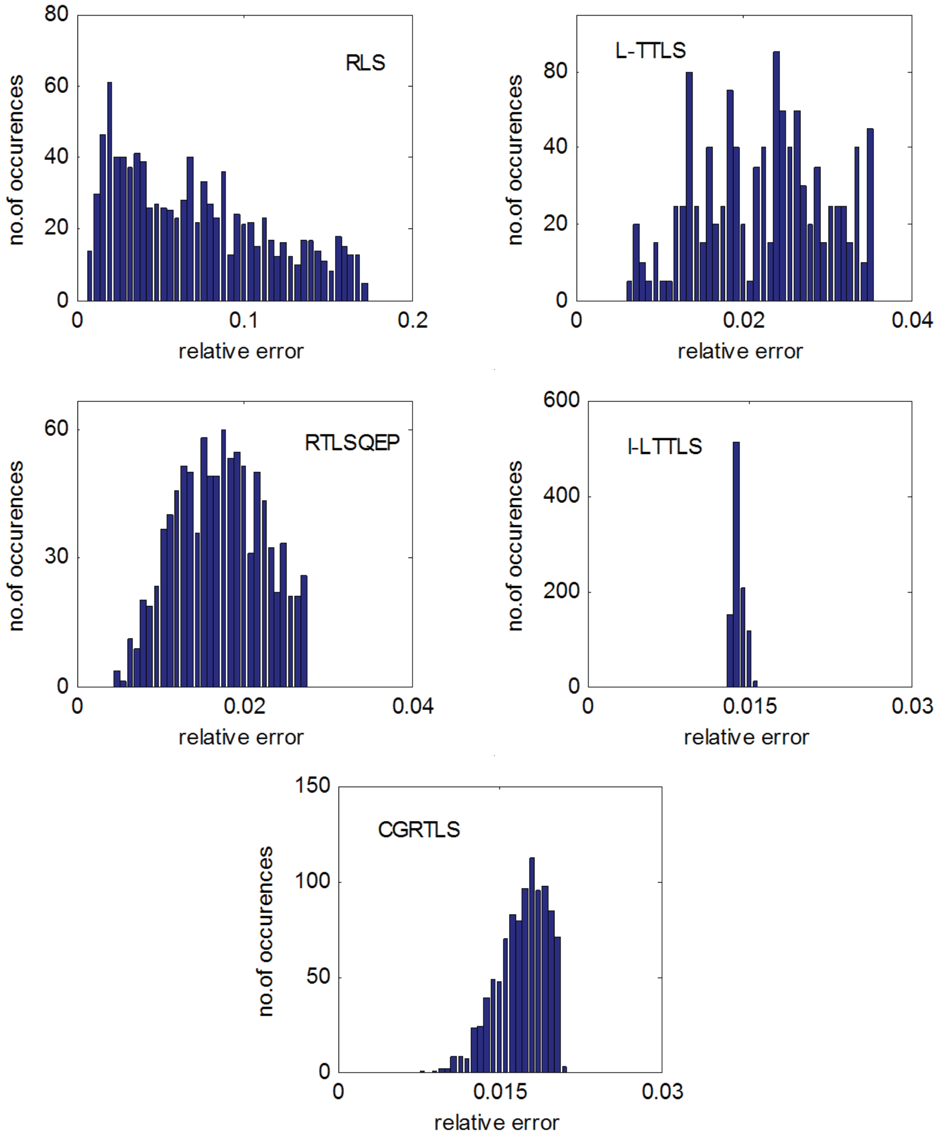

Figure 2: Histograms present the optimal relative errors of 1000 test problems solved by five different regularization methods for Example.1, with matrix dimensions $m_1 = m_2 = 20$, noise levels $\rho_1 = 1 \times 10^{-3}$

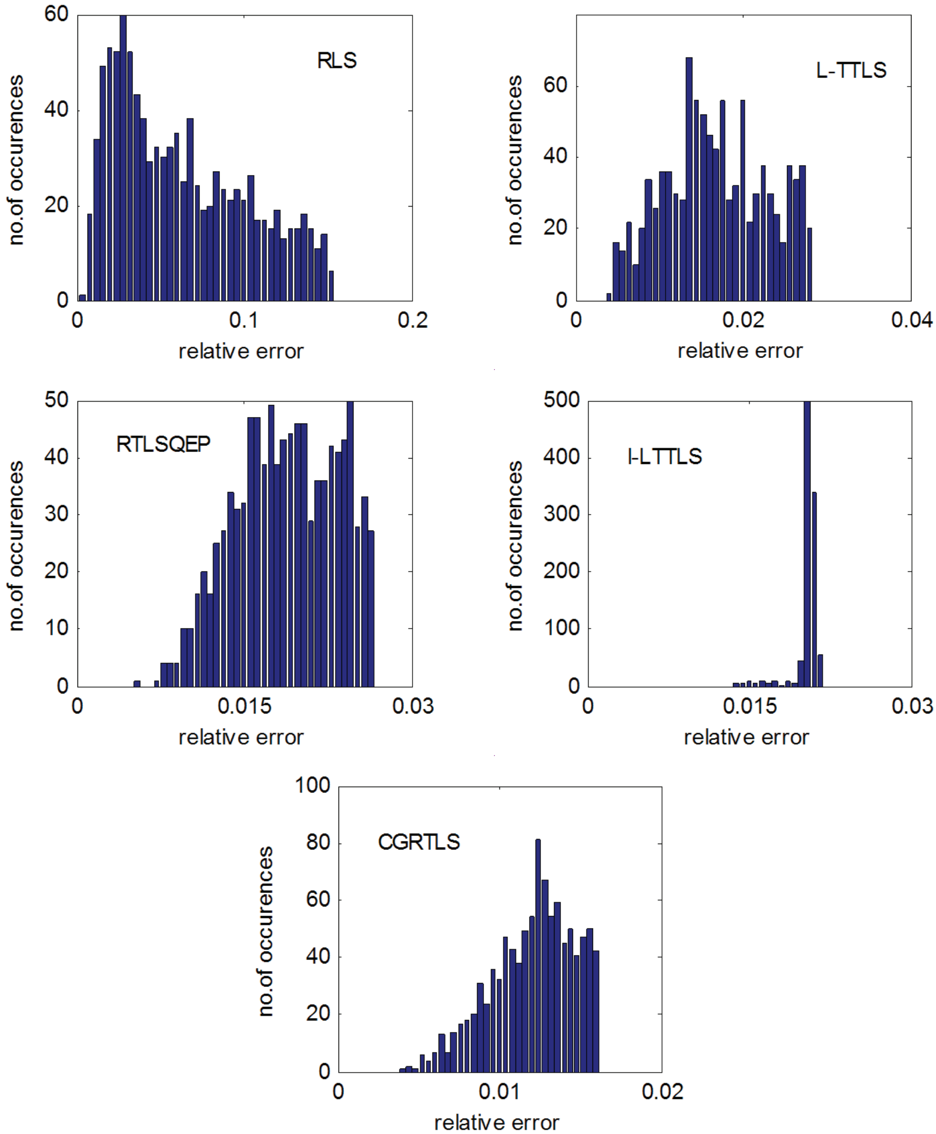

Figure 3: Histograms present the optimal relative errors of 1000 test problems solved by five different regularization methods for Example.1, with matrix dimensions $m_1 = m_2 = 100$, noise levels $\rho_1 = 1 \times 10^{-3}$

The I-LTLLS algorithm outperforms CGRTLS, L-TTLS, RTLSQEP, RLS in Fig.2. This is no surprise that there is a larger gap in the eigenvalue spectrum when the matrix dimensions satisfy $m_1 = m_2 = 20$. This feature denotes that it is easy to cut off a certain number of terms in the SVD of the coefficient matrix. And these certain terms can be considered as noises far away from the singular subspaces of true system energy. In this case, Tikhonov regularization method may be difficult to regularize both reliable and noise parts efficiently. In Fig.3, the CGRTLS algorithm is clearly superior to the other three methods since the singular values of matrix decay gradually to zero when the matrix dimensions satisfy $m_1 = m_2 = 100$. At this time, it is difficult to determine an appropriate truncation level for truncated TLS. And the smaller singular values which are truncated may be useful information. Therefore, distribution of singular values has a great impact on solving ill-posed problems when we employ regularization algorithms.

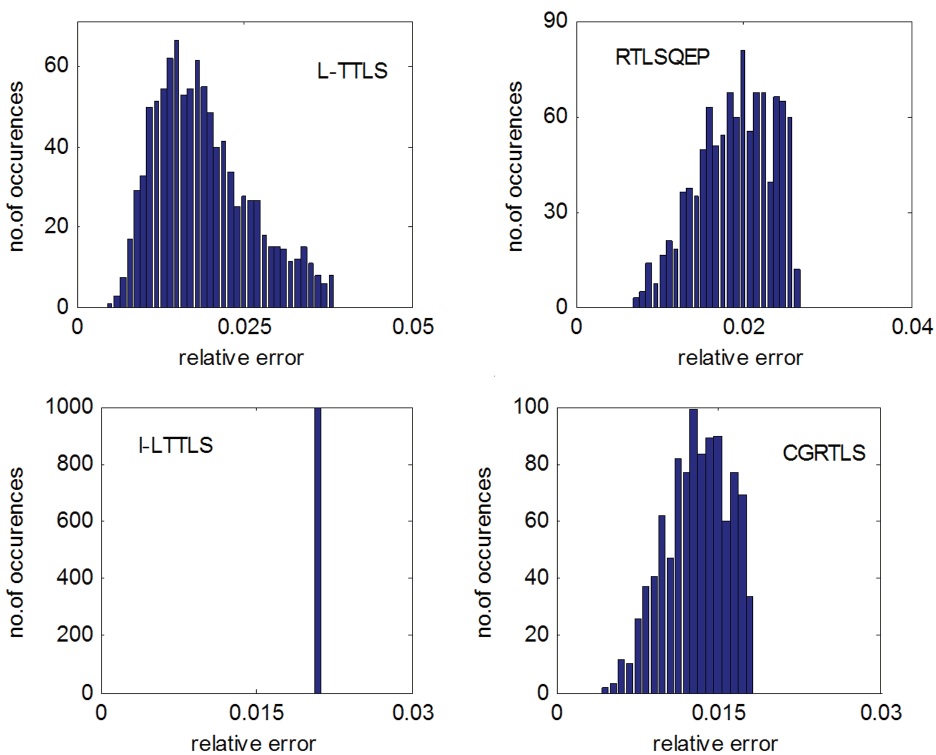

Figure 4: Histograms present the optimal relative errors of 1000 test problems solved by four different regularization methods for Example.2, with matrix dimensions $m_1 = 60, m_2 = 50$, noise levels $\rho_1 = 1 \times 10^{-3}$

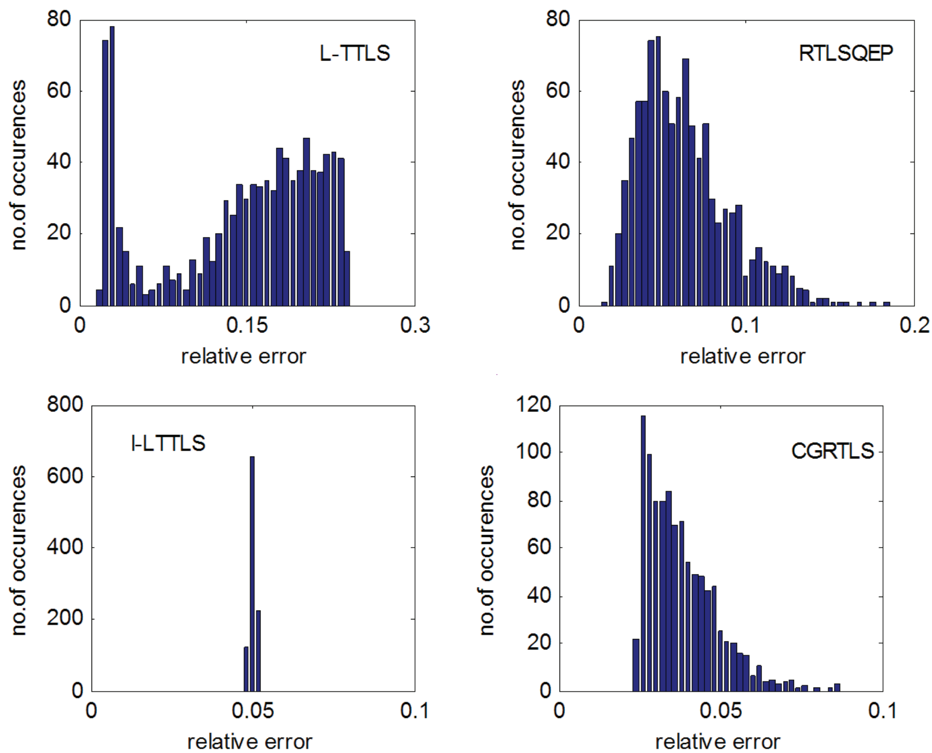

Figure 5: Histograms present the optimal relative errors of 1000 test problems solved by four different regularization methods for Example.2, with matrix dimensions $m_1 = 60, m_2 = 50$, noise levels $\rho_2 = 1 \times 10^{-2}$

Test 2. Our second test problem is generated by considering the Example.2. We consider the rectangle matrix with dimensions $m_1 = 60, m_2 = 50$, whose singular values decay gradually to zero and the condition number is 6.529×10^{16}. Therefore it is a typically ill-condition matrix. Our test is presented as histograms of the relative error, in the solution over 1000 independent simulations of the same example. Seeing numerical relative errors γ of all four TLS-based algorithms in the histograms Fig. 4 and Fig.5, where the noise levels are $\rho_1 = 1 \times 10^{-3}$ and $\rho_2 = 1 \times 10^{-2}$, respectively. It is obvious that for smaller noise level $\sigma_1 = 1 \times 10^{-3}$, the solutions of all four algorithms are not expected much difference. However, in Fig.5, the relative errors of all algorithms grow as noise level increases, and the I-LTTLS, CGRTLS and RTLSQEP algorithms increase lower than L-TTLS algorithms when the noise level increases to $\sigma_1 = 1 \times 10^{-2}$. The CGRTLS algorithm with adaptive selection of regularization parameter is turned out to be slightly superior to other TLS algorithms. We can also conclude that the results of relative error indicate that the I-LTTLS is not very sensitive to the random noises.

Next, several starting regularization parameters are used to initialize the CGRTLS algorithm, and the results average over 100 random simulations. The average regularization parameter $\bar{\lambda}$ and average relative error $\bar{\gamma}$ for various starting regularization parameters λ_0 are computed in Table.2. As we can see, the CGRTLS algorithm has low sensitivity to initial regularization parameter since the $\bar{\gamma}$ and $\bar{\lambda}$ are almost same at different initial parameter values. As a result, rather than using the parameter selection principles described in some of previous works, an adaptive principle of selecting regularization parameter can be applied to determine the optimum regularization parameters, which has a stronger robustness, higher accuracy and convergent rate.

Table 2: The average relative error $\bar{\gamma}$ and average regularization parameter $\bar{\lambda}$ for various λ_0

λ_0	0	1×10^{-6}	1×10^{-4}	1×10^{-2}	1×10^{0}	1×10^{1}
$\bar{\gamma}$	0.0312	0.0356	0.0385	0.0301	0.0290	0.0328
$\bar{\lambda}$	0.0156	0.0173	0.0157	0.0167	0.0151	0.0149

Example.3: Now we apply the two novel methods of TLS regularization to tackle inverse heat conduction problem. The one-dimensional heat conduction problem is described as

$$\frac{\partial u}{\partial t} = D^2 \frac{\partial^2 u}{\partial x^2}, (0 < x < L, t > 0) \tag{22}$$

$$u_x(0,t) = u_x(L,t) = 0$$

$$u(x,0) = f(x)$$

where $u(x,t)$ denotes temperature, x is spatial variable and t is time variable. $f(x)$ is initial condition, D denotes heat transfer coefficient.

The temperature distribution $u(x,t)$ of the heat conduction problem for a given initial condition is explicitly obtained using separation of variables

$$u(x,t) = \frac{a_0}{2} + \sum_{n=1}^{+\infty} a_n e^{-(\frac{n\pi D}{L})^2 t} \cos\frac{n\pi x}{L} \tag{23}$$

where

$$a_n = \frac{2}{L}\int_0^L f(y)\cos\frac{n\pi y}{L}dy$$

Then we can change Eq.(23) into the Fredholm integral equation of the first kind

$$u(x,t) = \int_0^L K(x,y,t) f(y) dy \tag{24}$$

where the integral operator $K(x,y,t) = \frac{1}{2} + \sum_{n=1}^{+\infty} \cos\frac{n\pi y}{L} \cos\frac{n\pi x}{L} e^{-(\frac{n\pi D}{L})^2 t}$

Thus the initial temperature $f(x)$ can be obtained by solving the inverse problem (24). As we know, the first step is to discretize the quadrature formula (24), and the interval$[0,L]$can be divided into equal intervals of width $\Delta L = \frac{L}{N}$(N=60). Finally, the Eq.(24) can be rewritten as ***Ax=b***, and the explicit discretization process is described in section 3.1. Here we set a finite number of expansion terms 100 for the operator K which guarantees the convergence of the series. The initial exact temperature is

$$f(x) = \begin{cases} 6x, & 0 \le x < 0.5 \\ 6(1-x), & 0.5 \le x \le 1 \end{cases}$$

To estimate the initial temperature, the temperature $u(x,t_1)$ can be firstly obtained by Eq.(24) at time t_1. We set t_1=1, D=0.06 and both the A and b are contaminated by random noises whose noise levels are $\rho_1 = 1\times10^{-3}$ and $\rho_2 = 1\times10^{-2}$. The condition number of the matrix $\boldsymbol{A} \in \mathrm{R}^{60\times60}$ is 4.571×10^{17}, and consequently the inverse problem of heat conduction is an seriously ill-posed linear problem.

The initial temperature distribution computed by LS method, compared with exact initial temperature distribution, is given in figure 6. It is obvious that there is a great error when the LS method is used to estimate the initial temperature. The constructed solutions of the I-LTTLS and CGRTLS algorithms apprehended from Fig.7 and Fig.8 are in good agreement with the exact solution. Therefore, the two novel methods of TLS regularization are efficient and accurate to solve backward heat conduction problem, even when both the measurement items $u(x,t_1)$ and the integral operator K are contaminated by some random noises. As we can see, the solution of CGRTLS algorithm is slightly superior to I-LTTLS algorithm. It is probably because the singular values of system matrix decay gradually to zero. Next, the initial temperature constructed by CGRTLS algorithm for several different starting regularization parameters are shown in Fig. 9, and we can still concluded that the CGRTLS algorithm has low sensitivity to starting regularization parameters.

3.2 two-dimensional Fredholm integral equation of the first kind

Consider the following two-dimensional Fredholm integral equations of the first kind

$$T(u,v) = \int_a^b \int_c^d K(u,v,s,t) f(s,t) ds dt \tag{25}$$

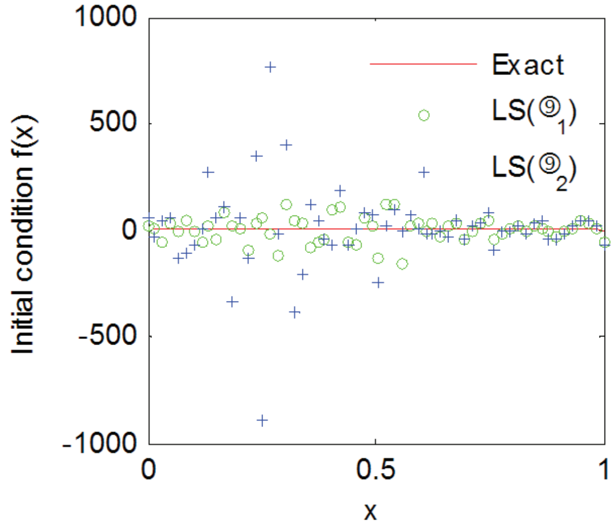

Figure 6: Comparison between the exact and the LS algorithm results

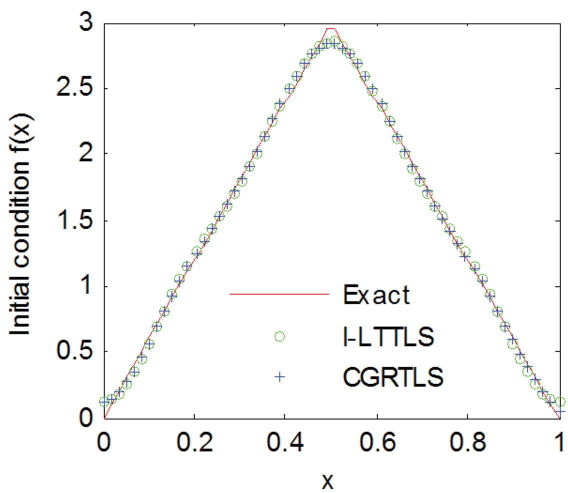

Figure 7: Comparison between the exact and the TLS algorithm results at $\rho_1 = 1 \times 10^{-3}$

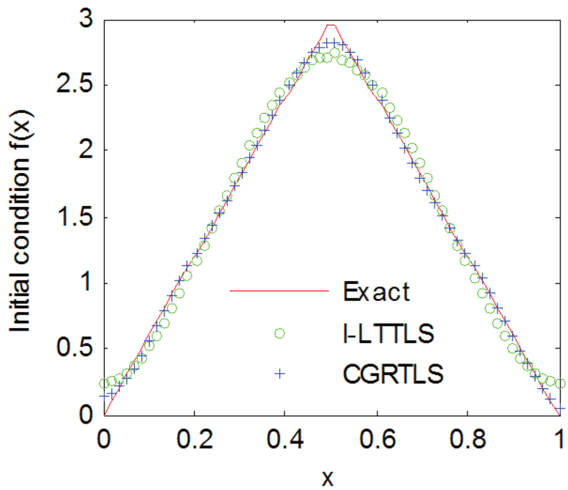

Figure 8: Comparison between the exact and TLS algorithm results at $\rho_1 = 1 \times 10^{-2}$

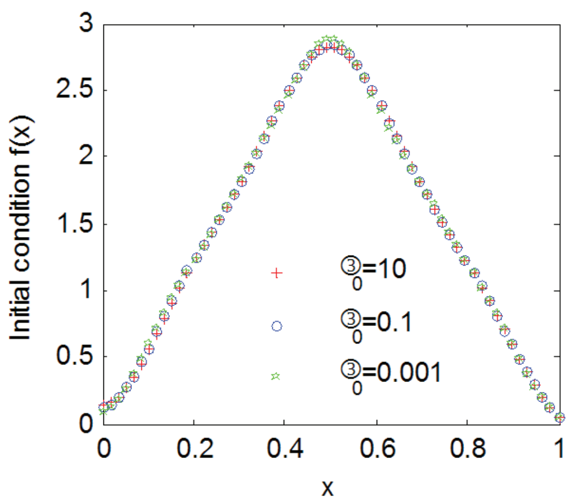

Figure 9: The constructed initial temperature for various λ_0

whose exact solution is $f(s,t) = s+t$
with the kernel

$$K(u,v,s,t) = \frac{u}{1+\sqrt{(s-u)^2+(t-v)^2}}$$

where $s,t \in \Omega_1 \subset R^2$, $u,v \in \Omega_2 \subset R^2$, we set $\Omega_1 = \Omega_2 = \Omega = [-5,5]\times[-5,5]$, let us discretize the intervals Ω_1 and Ω_2 into $m_1 \times n_1$ and $m_2 \times n_2$ respectively. The two-dimensional Fredholm integral Eq. (25) can then be replaced by a set of numerical equations

$$\begin{aligned} T(u_p,v_q) &= \int_a^b \int_c^d K(u_p,v_q,s,t)f(s,t)dsdt \\ &\approx \sum_{j=1}^{n_1}\sum_{i=1}^{m_1} K(u_p,v_q,s_i,t_j)w_i w_j^{'} \end{aligned}$$

where $p = 1,2,\cdots,m_2$, $q = 1,2,\cdots,n_2$, the above equations may be scattered concretely as

$$\begin{aligned} &K(u_p,v_q,s_1,t_1)f(s_1,t_1)w_1w_1^{'} + K(u_p,v_q,s_2,t_1)f(s_2,t_1)w_2w_1^{'} \\ &+\cdots+K(u_p,v_q,s_{m_1},t_1)f(s_{m_1},t_1)w_{m_1}w_1^{'} + K(u_p,v_q,s_1,t_2)f(s_1,t_2)w_1w_2^{'} \\ &+\cdots+K(u_p,v_q,s_2,t_2)f(s_2,t_2)w_2w_2^{'} + K(u_p,v_q,s_{m_1},t_2)f(s_{m_1},t_2)w_{m_1}w_2^{'} \\ &+\cdots+K(u_p,v_q,s_{m_1},t_{n_1})f(s_{m_1},t_{n_1})w_{m_1}w_{n_1}^{'} \end{aligned} \qquad (26)$$

Eq. (26) can be rewritten as

$$\boldsymbol{Ax} = \boldsymbol{b}$$

where $\boldsymbol{A}(m_2\cdot(q-1)+p, m_1\cdot(j-1)+i) = K(u_p,v_q,s_i,t_j)w_iw_j^{'}$ is a rectangular matrix with dimensions $(m_2\cdot n_2)\times(m_1\cdot n_1)$, vectors $\boldsymbol{x} = f(s_i,t_j)$, $\boldsymbol{b} = \boldsymbol{Ax}$ is respectively $(m_1\cdot n_1)\times 1$ and $(m_2\cdot n_2)\times 1$ column vector, with $i = 1,2,\cdots,m_1$, $j = 1,2,\cdots,n_1$ and $p = 1,2,\cdots,m_2$, $q = 1,2,\cdots,n_2$.

Test 3. Fix matrix dimensions $m_1 = n_1 = m_2 = n_2 = 20$. The noise level is $\rho_1 = 1\times 10^{-3}$, and average results for 500 random simulations. The condition number of the matrix $\boldsymbol{A} \in \mathrm{R}^{400\times 400}$ is 3.804×10^3, and consequently the Eq.(26) is an ill-posed linear problem. The singular values of the matrix $(\boldsymbol{A},\boldsymbol{b})$ decay gradually to zero. In the histograms Fig.10, we compare the relative errors obtained by the L-TTLS, I-LTTLS, CGRTLS and RTLSQEP algorithms. We can conclude that the results of the CGRTLS method outperforms other three algorithms i.e., the higher accuracy is obtained, and moreover, the robustness of the I-LTTLS algorithm perfects best of these methods.

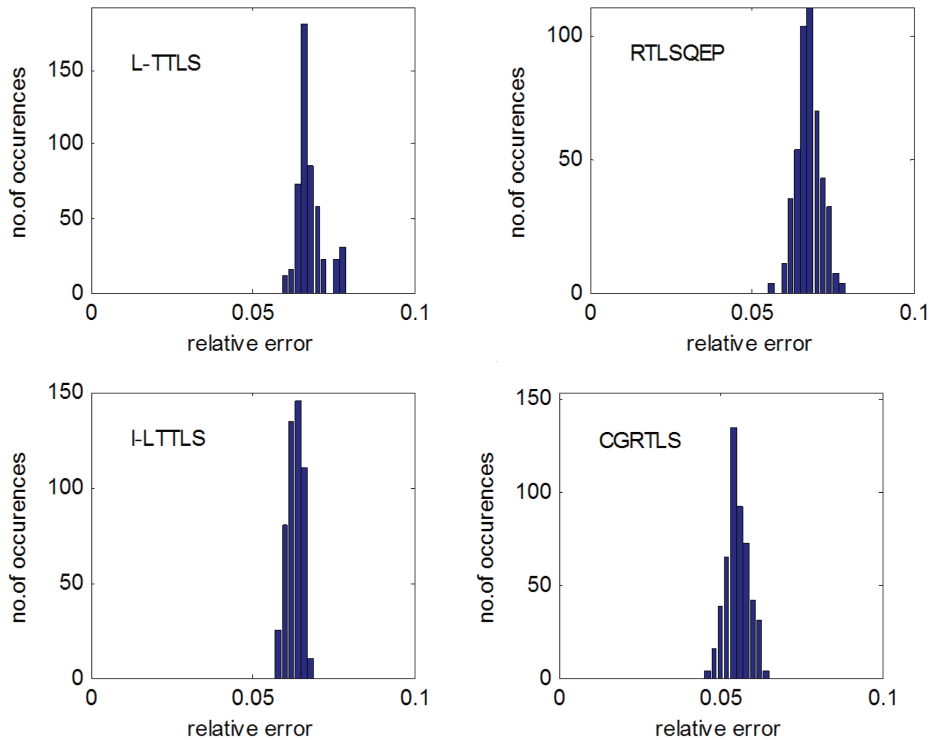

Figure 10: The four histograms illustrate the statistical distribution of relative error for two-dimensional Fredholm integral equation with $m_1 = n_1 = m_2 = n_2 = 20$ and a noise level $\rho_1 = 1 \times 10^{-3}$

Finally, a sample solution of two-dimensional Fredholm integral equations computed by the CGRTLS, I-LTTLS and RLS schemes is compared with the exact solutions apprehended from Fig.11. The constructed solutions of the I-LTTLS and CGRTLS schemes perform better than RLS scheme. This is due to the fact that the errors in both the system matrix and the right-hand side may produce large errors in the computed results. Consequently, the constructed solutions by the regularized TLS schemes which can consider both errors are much accurate than LS-based methods. It can be seen that the constructed solution using the CGRTLS algorithm is slightly superior to the solutions computed by the I-LTTLS algorithm i.e., the former solution match the exact solution well. Therefore, we prove that the CGRTLS algorithm generate more accurate solutions than the I-LTTLS algorithm when the singular values decay gradually to zero yet again.

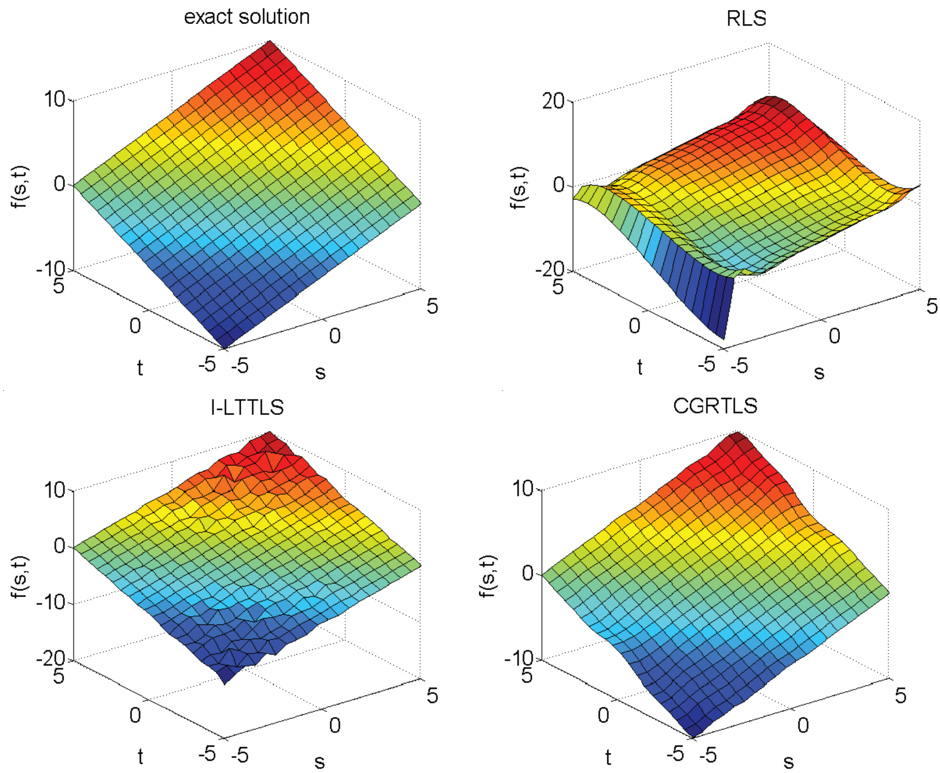

Figure 11: Approximated solution for different regularization solvers i.e., RLS, I-LTTLS and CGRTLS

4 Conclusions

We have proposed two novel iterative algorithms to incorporation of regularization and stabilization into the TLS setting. The two algorithms named I-LTTLS and CGRTLS are analogous to the truncated SVD and Tikhonov regularization approaches based on LS, respectively. The I-LTTLS algorithm overcomes the deficiencies of the Lanczos-TTLS algorithm which are difficult to obtain the truncate index k and get maximal truncate index $k_{\max}$ regarded as a critical precondition. The CGRTLS algorithm is able to choose the regularization parameter adaptively which gets higher efficiency than other famous methods, and moreover, converge to a global minimum point. Both algorithms aren't necessary to obtain any priori knowledge about noise level and exact solution.

We have demonstrated that the two novel algorithms are highly suitable for tackling Fredholm integral equations of the first kind which are known to be typically ill-posed problems. The I-LTLLS algorithm outperforms the CGRTLS algorithm slightly when the eigenvalues spectrum of the augmented matrix $(\boldsymbol{A},\boldsymbol{b})$ has a larger gap. It is because we can easily cut off a certain number of terms in the SVD which are considered as noises far away from the singular subspaces of true system energy. In this case, Tikhonov regularization may be difficult to regularize both reliable and noise parts efficiently. However, the CGRTLS algorithm is clearly superior to the I-LTTLS when the singular values decay gradually to zero. Because it is difficult to determine an appropriate truncation level for truncated TLS, and the smaller singular values which are truncated may be useful information. In all tests, the CGRTLS algorithm with adaptive selection of regularization parameter is turned out to be slightly superior to other TLS algorithms such as Lanczos TTLS and the state-of-the-art RTLSQEP algorithms. The results of relative error indicate that the I-LTTLS is not very sensitive to the random noise. We can also present that the TLS-based regularization algorithms under certain noise level are able to yield more accurate regularized solutions than LS-based method.

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