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Tikhonov regularization for weighted total least squares problems[☆]

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Abstract

In this work, we study and analyze the regularized weighted total least squares (RWTLS) formulation. Our regularization of the weighted total least squares problem is based on the Tikhonov regularization. Numerical examples are presented to demonstrate the effectiveness of the RWTLS method.

Keywords: Tikhonov regularization; Total least squares; Weighted regularized total least squares; Matrix differentiation; Lagrange multiplier

1. Introduction

In this work, we study the regularized weighted total least squares (RWTLS) formulation. Our regularization of the weighted total least squares problem is based on the Tikhonov regularization [1].

For the total least squares (TLS) problem [2], the truncation approach has already been studied by Fierro et al. [3]. In [4], Golub et al. has considered the Tikhonov regularization approach for TLS problems. They derived a new regularization method in which stabilization enters the formulation in a natural way, and that is able to produce regularized solutions with superior properties for certain problems in which the perturbations are large. In the present work, we focus on RWTLS problems. We show that the RWTLS solution is closely related to the Tikhonov solution to the weighted least squares solution.

Our work is organized as follows. In Section 2, we introduce the RWTLS formulation and study its regularizing properties. Computational methods are described in Section 3. In Section 4, numerical examples are presented to demonstrate the RWTLS method.

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2. The regularized weighted total least squares

A general version of Tikhonov's formulation for the linear weighted total least squares (WTLS) problem takes the form [5]

$$\min_x \|U[(A,b)-(\tilde{A},\tilde{b})]V\|_F \quad \text{subject to} \quad \tilde{b}=\tilde{A}x, \quad \|Dx\|_S \le \delta, \tag{1}$$

where D is the regularization matrix, $V=\operatorname{diag}(W,\gamma)$ with γ being a non-zero constant, U and W are nonsingular matrices, S is a symmetric positive definite matrix with $\|y\|_S^2 = y^{\mathrm{T}}Sy$, and δ is a positive constant. By using the Lagrange multiplier formulation, this problem can be rewritten as follows:

$$\mathcal{L}(\tilde{A},x,\mu)=\|U[(A,b)-(\tilde{A},\tilde{b})]V\|_F^2+\mu(\|Dx\|_S^2-\delta^2), \quad \text{subject to} \quad \tilde{b}=\tilde{A}x, \tag{2}$$

where μ is the Lagrange multiplier, and μ is equal to zero if the inequality constraint becomes equality. The solution $\bar{x}_\delta$ to this problem is different from the solution x_{WTLS} to

$$\min_x \|U[(A,b)-(\tilde{A},\tilde{b})]V\|_F \quad \text{subject to} \quad \tilde{b}=\tilde{A}x, \tag{3}$$

for δ less than $\|Dx_{\mathrm{WTLS}}\|_2$.

Before we show the properties of the solution to (2), we have the following results about the matrix differentiation for the matrices A, $\tilde{A}$, W and U.

Lemma 1.

$$\begin{array}{llll}
\text{(i)} & \dfrac{\partial\, \mathrm{tr}(W^{\mathrm{T}}A^{\mathrm{T}}U^{\mathrm{T}}U\tilde{A}W)}{\partial\tilde{A}} = U^{\mathrm{T}}UAWW^{\mathrm{T}} & \text{(ii)} & \dfrac{\partial\, \mathrm{tr}(W^{\mathrm{T}}\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}UAW)}{\partial\tilde{A}} = U^{\mathrm{T}}UAWW^{\mathrm{T}} \\
\text{(iii)} & \dfrac{\partial\, \mathrm{tr}(W^{\mathrm{T}}\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}U\tilde{A}W)}{\partial\tilde{A}} = 2U^{\mathrm{T}}U\tilde{A}WW^{\mathrm{T}} & \text{(iv)} & \dfrac{\partial\, (b^{\mathrm{T}}U^{\mathrm{T}}U\tilde{A}x)}{\partial\tilde{A}} = U^{\mathrm{T}}Ubx^{\mathrm{T}} \\
\text{(v)} & \dfrac{\partial\, (x^{\mathrm{T}}\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}Ub)}{\partial\tilde{A}} = U^{\mathrm{T}}Ubx^{\mathrm{T}} & \text{(vi)} & \dfrac{\partial\, (x^{\mathrm{T}}\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}U\tilde{A}x)}{\partial\tilde{A}} = 2U^{\mathrm{T}}U\tilde{A}xx^{\mathrm{T}}.
\end{array}$$

Proof. Since (i) is equivalent to (ii), (iv) is equivalent to (v), and (vi) is a special case of (iii), we only give the proofs of (i) and (iii).

Let Z be a $p\times q$ matrix of differentiable functions of the $m\times n$ matrix X. If

$$\frac{\partial Z}{\partial x_{ij}} = GE_{ij}^{(mn)}H + C(E_{ij}^{(mn)})^{\mathrm{T}}F, \quad i=1,\ldots,m,\ j=1,\ldots,n$$

then

$$\frac{\partial z_{ij}}{\partial X} = G^{\mathrm{T}}E_{ij}^{(pq)}H^{\mathrm{T}} + F(E_{ij}^{(pq)})^{\mathrm{T}}C, \quad i=1,\ldots,p,\ j=1,\ldots,q,$$

and the converse is also true (see p. 57, Theorem 7.1 in [6]), where $G=(g_{ij})$ is a $p\times m$ matrix, $H=(h_{ij})$ is an $n\times q$ matrix, $C=(c_{ij})$ is a $p\times n$ matrix, $F=(f_{ij})$ is an $m\times q$ matrix $E_{ij}^{(kl)}$ is a k-by-l zero matrix except the (i,j)-entry being equal to one.

For (i), we consider $Y = W^{\mathrm{T}}A^{\mathrm{T}}U^{\mathrm{T}}U$ and we have $\frac{\partial\, \mathrm{tr}(Y\tilde{A}W)}{\partial\tilde{A}} = \frac{\partial}{\partial\tilde{A}}\left(\sum_i (Y\tilde{A}W)_{ii}\right) = \sum_i \frac{\partial (Y\tilde{A}W)_{ii}}{\partial\tilde{A}}$. Since $\frac{\partial(Y\tilde{A}W)}{\partial\,\tilde{A}_{ij}} = YE_{ij}W$ and $\frac{\partial(Y\tilde{A}W)_{ij}}{\partial\tilde{A}} = Y^{\mathrm{T}}E_{ij}W^{\mathrm{T}}$, we obtain $\frac{\partial\, \mathrm{tr}(Y\tilde{A}W)}{\partial\,\tilde{A}} = \sum_i Y^{\mathrm{T}}E_{ii}W^{\mathrm{T}} = Y^{\mathrm{T}}W^{\mathrm{T}}$. The result follows.

For (iii), we find that $\frac{\partial[(U\tilde{A}W)^{\mathrm{T}}(U\tilde{A}W)]}{\partial\,\tilde{A}_{ij}} = W^{\mathrm{T}}E_{ij}^{\mathrm{T}}U^{\mathrm{T}}U\tilde{A}W + (U\tilde{A}W)^{\mathrm{T}}UE_{ij}W$, and therefore we have $\frac{\partial[(U\tilde{A}W)^{\mathrm{T}}(U\tilde{A}W)]_{ii}}{\partial\,\tilde{A}} = U^{\mathrm{T}}U\tilde{A}WE_{ii}^{\mathrm{T}}W^{\mathrm{T}} + U^{\mathrm{T}}U\tilde{A}WE_{ii}W^{\mathrm{T}}$. It follows that

$$\frac{\partial\ \mathrm{tr}[(U\tilde{A}W)^{\mathrm{T}}(U\tilde{A}W)]}{\partial\tilde{A}} = \sum_i \frac{\partial[(U\tilde{A}W)^{\mathrm{T}}(U\tilde{A}W)]_{ii}}{\partial\tilde{A}} = \sum_i U^{\mathrm{T}}U\tilde{A}WE_{ii}^{\mathrm{T}}W^{\mathrm{T}} + U^{\mathrm{T}}U\tilde{A}WE_{ii}W^{\mathrm{T}}$$
$$= 2U^{\mathrm{T}}U\tilde{A}WW^{\mathrm{T}}. \quad \square$$

Theorem 1. *The RWTLS solution to (1) with the inequality constraint replaced by equality is a solution to the problem*

$$(A^{\mathrm{T}}U^{\mathrm{T}}UA + \alpha W^{-T}W^{-1} + \beta D^{\mathrm{T}}SD)x = A^{\mathrm{T}}U^{\mathrm{T}}Ub, \tag{4}$$

where the parameters α and β are given by

$$\alpha = \frac{-\gamma^2\|b-Ax\|^2_{U^{\mathrm{T}}U}}{1+\gamma^2\|x\|^2_{W^{-T}W^{-1}}}, \qquad \beta = \frac{\mu}{\gamma^2}(1+\gamma^2\|x\|^2_{W^{-T}W^{-1}}) \tag{5}$$

and μ is the Lagrange multiplier in (2). The two parameters are related by

$$\beta\delta^2 = (Ub)^{\mathrm{T}}U(b-Ax) + \frac{1}{\gamma^2}\alpha, \tag{6}$$

and the weighted TLS residual satisfies

$$\|U[(A,b)-(\tilde{A},\tilde{b})]V\|_F^2 = -\alpha. \tag{7}$$

Proof. We characterize the solution to (1) by setting the partial derivatives of $\mathcal{L}(\tilde{A},x,\mu)$ to zero. Using Lemma 1, the differentiation of $\mathcal{L}(\tilde{A},x,\mu)$ with respect to $\tilde{A}$ yields

$$U\tilde{A}WW^{\mathrm{T}} - UAWW^{\mathrm{T}} - \gamma\tilde{r}x^{\mathrm{T}} = 0, \tag{8}$$

where $\tilde{r} = \gamma U(b-\tilde{A}x) = \gamma U(b-\tilde{b})$. Moreover, the differentiation of $\mathcal{L}(\tilde{A},x,\mu)$ with respect to the entries in x yields

$$-\gamma\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}\tilde{r} + \mu D^{\mathrm{T}}SDx = 0 \quad \text{or} \quad (\gamma^2\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}U\tilde{A} + \mu D^{\mathrm{T}}SD)x = \gamma^2\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}Ub. \tag{9}$$

By using (8) and (9), we have

$$\begin{aligned} A^{\mathrm{T}}U^{\mathrm{T}}UA &= (U\tilde{A} - \gamma\tilde{r}x^{\mathrm{T}}W^{-T}W^{-1})^{\mathrm{T}}(U\tilde{A} - \gamma\tilde{r}x^{\mathrm{T}}W^{-T}W^{-1}) \\ &= \tilde{A}^{\mathrm{T}}U^{\mathrm{T}}U\tilde{A} + \gamma^2\|\tilde{r}\|_2^2W^{-T}W^{-1}xx^{\mathrm{T}}W^{-T}W^{-1} \\ &\quad - \mu D^{\mathrm{T}}SDxx^{\mathrm{T}}W^{-T}W^{-1} - \mu W^{-T}W^{-1}xx^{\mathrm{T}}D^{\mathrm{T}}SD \end{aligned}$$

and $\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}Ub = A^{\mathrm{T}}U^{\mathrm{T}}Ub + \gamma W^{-T}W^{-1}x\tilde{r}^{\mathrm{T}}Ub$. By using the assumption that $\|Dx\|_S = \delta$ and gathering the above terms, we obtain (5) with

$$\alpha = \mu\delta^2 - \gamma^2\|\tilde{r}\|_2^2\|x\|^2_{W^{-T}W^{-1}} - \gamma\tilde{r}^{\mathrm{T}}Ub \quad \text{and} \quad \beta = \frac{\mu}{\gamma^2}(1+\gamma^2\|x\|^2_{W^{-T}W^{-1}}).$$

In order to obtain the expression for α, we first rewrite $\tilde{r}$ as

$$\tilde{r} = \gamma U(b-\tilde{A}x) = \gamma U(b - Ax - \gamma U^{-1}\tilde{r}x^{\mathrm{T}}W^{-T}W^{-1}x) = \gamma U(b-Ax) - \gamma^2\tilde{r}\|x\|^2_{W^{-T}W^{-1}}$$

from which we obtain the relation

$$\tilde{r} = \frac{\gamma U(b-Ax)}{1+\gamma^2\|x\|^2_{W^{-T}W^{-1}}}. \tag{10}$$

From (9), we have

$$\mu = \frac{\gamma x^{\mathrm{T}}\tilde{A}^{\mathrm{T}}U^{\mathrm{T}}\tilde{r}}{x^{\mathrm{T}}D^{\mathrm{T}}SDx} = \frac{(\gamma Ub - \tilde{r})^{\mathrm{T}}\tilde{r}}{\delta^2}. \tag{11}$$

By inserting (10) and (11) into the expression for α, we obtain (5). Eq. (6) is proved by multiplying β by δ^2 and inserting (10) and (11).

Finally, we note from (8) that $UAW - U\tilde{A}W = -\gamma\tilde{r}x^{\mathrm{T}}W^{-T}$ and therefore we have $(UAW, \gamma Ub) - (U\tilde{A}W, \gamma U\tilde{A}x) = (-\gamma\tilde{r}x^{\mathrm{T}}W^{-T}, \tilde{r})$. It follows that

$$\begin{aligned}\|U[(A,b)-(\tilde{A},\tilde{b})]V\|_F^2 &= \|\gamma\tilde{r}x^{\mathrm{T}}W^{-T}\|_F^2 + \|\tilde{r}\|_2^2 \\ &= (1+\gamma^2\|x\|^2_{W^{-T}W^{-1}})\|\tilde{r}\|_2^2 = \frac{\gamma^2\|b-Ax\|^2_{U^{\mathrm{T}}U}}{1+\gamma^2\|x\|^2_{W^{-T}W^{-1}}} = -\alpha. \qquad \square\end{aligned}$$

The next theorem tells us the relationship between the RWTLS solution and the WTLS solution in (3) without the regularization.

Theorem 2. *For a given value of δ, the RWTLS solution $x_{RWTLS}(\delta)$ is related to the solution x_{WTLS} to the weighted total least squares problem without the regularization as follows:*

δ	solution	α	β
$\delta < \|Dx_{\mathrm{WTLS}}\|_S$	$x_{RWTLS}(\delta) \neq x_{\mathrm{WTLS}}$	$\alpha < 0$ and $\frac{\partial\alpha}{\partial\delta} > 0$	$\beta > 0$
$\delta \geq \|Dx_{\mathrm{WTLS}}\|_S$	$x_{RWTLS}(\delta) = x_{\mathrm{WTLS}}$	$\alpha = -\sigma_{\min}((UAW, \gamma Ub))^2$	$\beta = 0$

Here $\sigma_{\min}((UAW, \gamma Ub))$ is the smallest singular value of the matrix $(UAW, \gamma Ub)$.

Proof. For $\delta < \|Dx_{\mathrm{WTLS}}\|_S$, the inequality constraint is active and therefore the Lagrange multiplier μ is positive, since this is a necessary condition for optimality, see [7]. By (5), we know that β is positive. Since the optimal solutions for small values of δ are candidate solutions for large values of δ, the residual norm in (7) is monotonically decreasing when δ increases. This implies that α is monotonically increasing when δ increases (recall that α is always a negative number). For $\delta \geq \|Dx_{\mathrm{WTLS}}\|_S$, the Lagrange multiplier μ is equal to zero. The solution becomes the unconstrained minimizer x_{WTLS}. Hence the result follows.

For $\delta = \|Dx_{\mathrm{WTLS}}\|$, the Lagrange multiplier is zero, and the solution again becomes the unconstrained minimizer x_{WTLS}. The value of α is equal to the negative of the squares of the smallest singular value $(UAW, \gamma Ub)$ directly from Theorem 4.1 in [5]. We note that the constraint is never again active for large values of δ. Therefore the solution remains unchanged. $\square$

3. Computational method

Choosing α and β is not a trivial problem. If no a priori information is known, then it may be necessary to solve the linear systems for several values of α and β. On the basis of the computed solutions, we try to determine the values of α and β in a suitable manner. For example, the cross-validation technique [1] can be used, but its computational cost is high. In our numerical examples in the next section, we determine α and β such that the error between the true solution and the computed solution is small enough for the illustration only.

Let us discuss how to solve (4) efficiently for many values of α and β. We notice that the equation is equivalent to the augmented system

$$\begin{pmatrix} I & 0 & UAW \\ 0 & I & \beta^{1/2}S^{1/2}DW \\ (UAW)^{\mathrm{T}} & \beta^{1/2}W^{\mathrm{T}}D^{\mathrm{T}}S^{1/2} & -\alpha I \end{pmatrix} \begin{pmatrix} r \\ s \\ W^{-1}x \end{pmatrix} = \begin{pmatrix} Ub \\ 0 \\ 0 \end{pmatrix}, \tag{12}$$

where $r = Ub - UAx$ and $s = -\beta^{1/2}S^{1/2}Dx$. Here we assume that the matrix D is a banded matrix, which usually represents a finite difference matrix, and both W and S are diagonal weighting matrices. We first reduce UAW to a bidiagonal form B by means of orthogonal transformations: $H^{\mathrm{T}}(UAW)K = B$. Since $S^{1/2}DW$ is still a banded matrix, we use a sequence of Givens transformations to retain its banded form, i.e., $C = J^{\mathrm{T}}(S^{1/2}DW)K$. Once B and C have been computed, we can recast the augmented system in (12) in the following form:

$$\begin{pmatrix} I & 0 & B \\ 0 & I & \beta^{1/2}C \\ B^{\mathrm{T}} & \beta^{1/2}C^{\mathrm{T}} & -\alpha I \end{pmatrix} \begin{pmatrix} H^{\mathrm{T}}r \\ J^{\mathrm{T}}s \\ K^{\mathrm{T}}W^{-1}x \end{pmatrix} = \begin{pmatrix} H^{\mathrm{T}}Ub \\ 0 \\ 0 \end{pmatrix}. \tag{13}$$

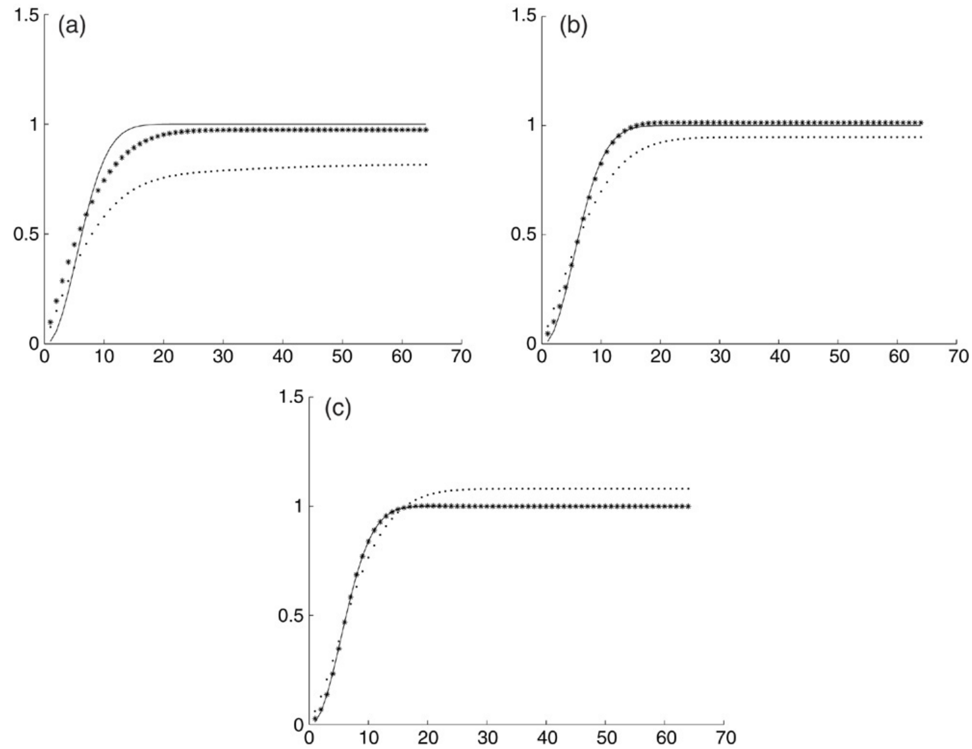

Fig. 1. Numerical solutions for different methods, (a) $\sigma = 0.1$, $\hat{\alpha} = -2.0047\text{e–}5$ and $\hat{\beta} = 36.6941$; (b) $\sigma = 0.01$, $\hat{\alpha} = -2.02925\text{e–}7$ and $\hat{\beta} = 312.4827$, and (c) $\sigma = 0.001$, $\hat{\alpha} = -9.4536\text{e–}9$ and $\hat{\beta} = 1324.7325$.

Following the approach in [4], we use Givens rotations to get the following result:

$$\begin{pmatrix} B \\ \beta^{1/2} C \end{pmatrix} = G \begin{pmatrix} \widehat{B} \\ 0 \end{pmatrix} = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} \begin{pmatrix} \widehat{B} \\ 0 \end{pmatrix}.$$

Then we insert this G into the augmented system (12); it becomes

$$\begin{pmatrix} I & 0 & \widehat{B} \\ 0 & I & 0 \\ \widehat{B}^{\mathrm{T}} & 0 & -\alpha I \end{pmatrix} \begin{pmatrix} \hat{r} \\ \hat{s} \\ K^{\mathrm{T}} W^{-1} x \end{pmatrix} = \begin{pmatrix} G_{11}^{\mathrm{T}} H^{\mathrm{T}} U b \\ G_{12}^{\mathrm{T}} H^{\mathrm{T}} U b \\ 0 \end{pmatrix},$$

where $\hat{r} = G_{11}^{\mathrm{T}} H^{\mathrm{T}} r + G_{21}^{\mathrm{T}} J^{\mathrm{T}} s$ and $\hat{s} = G_{12}^{\mathrm{T}} H^{\mathrm{T}} r + G_{22}^{\mathrm{T}} J^{\mathrm{T}} s$. After a suitable permutation, the system becomes a tridiagonal system that can be solved by a general tridiagonal solver.

4. Numerical examples

In this section, we present numerical results that illustrate the usefulness of the RWTLS method. Our computations are carried out in MATLAB. We consider an example in [4].

This test problem is a discretization by means of Gauss–Laguerre quadrature of the inverse Laplace transform

$$\int_0^\infty \exp(-st) f(t) \mathrm{d}t = \frac{1}{s} - \frac{1}{s + 4/25}, \quad s > 0. \tag{14}$$

The exact solution of (14) is known as $f(t) = 1 - \exp(-4t/25)$. This example has been implemented in the function *ilaplace*$(n, 2)$ in Hansen's regularization toolbox [8].

In the tests, we consider that the size of the coefficient matrix is 64, and the perturbed part of the coefficient matrix is E and its elements are generated from a normal distribution with zero mean and the unit standard deviation. The perturbed right-hand side is generated as $b = (A + \sigma \|E\|_F^{-1} E)x^* + \sigma \|e\|_2^{-1} e$, where the elements of e are from normal distributions with zero mean and the unit standard deviation, x^* is the reference solution and σ is the magnitude of noise. We use different values of α and β to compute the solutions and then choose the optimal $\hat{\alpha}$ and $\hat{\beta}$ such that the error between the true solution and the computed solution is minimal.

In Fig. 1, we show the results for different $\sigma = 0.001, 0.01, 0.1$. The solid line is the exact solution derived from $f(t)$ directly with $t \in [0,\ 64]$ (which is for the discretized 64×64 problem) while the line with "*" is the solution of RWTLS computed by the method we mentioned in (12) and the dotted line is the solution of RTLS computed from (22) in [4] (i.e., the regularized TLS solution without the weighting). The optimal values of $\hat{\alpha}$ and $\hat{\beta}$ for different σ are given in Fig. 1. In the RWTLS method, we select U to be a diagonal matrix whose elements are $1/\sigma$ for the first 16 elements and the last 16 elements are 3σ which are not larger than 0.1—otherwise divide them by 10 until the condition is satisfied; the other elements are equal to 1. The first half elements of W are ones while the last half ones are equal to σ. The matrix S is the identity matrix and the matrix D is the first-order finite difference matrix. At the same time we let $\gamma = 1$. In each case, the optimal regularization parameter μ is selected. We see from the figures that the solutions provided by the RWTLS method are better than those from the RTLS method.

One of the future research projects is studying how to choose the weighting matrices W and S without knowing the noise. We expect some optimization models should be incorporated into the objective function and the weighting can be determined by the optimization process; see for instance [9].

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