A REGULARIZED TOTAL LEAST SQUARES ALGORITHM*

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Abstract Error-contaminated systems $Ax \approx b$, for which A is ill-conditioned, are considered. Such systems may be solved using Tikhonov-like regularized total least squares (R-TLS) methods. Golub et al, 1999, presented a direct algorithm for the solution of the Lagrange multiplier formulation for the R-TLS problem. Here we present a parameter independent algorithm for the approximate R-TLS solution. The algorithm, which utilizes the shifted inverse power method, relies only on a prescribed estimate for the regularization constraint condition and does not require the specification of other regularization parameters. An extension of the algorithm for nonsmooth solutions is also presented.

Keywords: total least squares, ill-conditioned problem, regularization.

1. Introduction

We consider the development of algorithms for the solution of the Tikhonov type regularization of the total least squares (R-TLS) problem

$$\min \|(E,f)\|_F \quad \text{subject to} \quad (A+E)x = b+f \quad \|Lx\| \leq \delta. \tag{1.1}$$

Here δ is a regularization parameter, and $L \in R^{l\times n}$ defines a (semi)norm on the solution which is frequently chosen to approximate the first or second derivative operator. The utility of regularization for TLS, some of its properties, and its verification numerically via a parameter dependent direct algorithm was presented in [Golub et al., 1999]. Their algorithm, however, requires the development of a systematic approach for parameter selection. Here we develop a practical iterative algorithm utilizing the shifted inverse power method for which the only prescribed parameter, δ, should be determined *a priori* from

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knowledge of the underlying physical model. The algorithm then determines both the Lagrange multipliers and estimates a R-TLS solution concurrently.

In Section 2 we derive the algorithm which is then extended in Section 3 when regularization information on subdomains is available. Numerical results are presented in Section 4.

2. Derivation of the Algorithm

The Lagrange multiplier formulation for the R-TLS problem (1.1), given by

$$\mathcal{L}(E, f, x, \xi, \mu) = \|(E, f)\|_F^2 + \xi^T(Ax + Ex - b - f) + \mu(\|Lx\|^2 - \delta^2),$$

where ξ and μ are to be determined, [Luenberger, 1984], can be simplified by the Kuhn-Tucker conditions to yield the equations

$$\mu L^T Lx + A^T f - \|f\|^2 x = 0, \tag{2.2}$$

$$(1 + \|x\|^2) f = Ax - b, \tag{2.3}$$

$$\mu \geq 0, \;\; \mu(x^T L^T Lx - \delta^2) = 0. \tag{2.4}$$

Let x^* and μ^* denote the values of the solution x and parameter μ at the optimal solution of (1.1). If $\mu^* = 0$, the constraint $\|Lx\| \leq \delta$ is inactive, (e.g. see [Luenberger, 1984] Chapter 11.3), δ has been chosen too large, and $x^* = x_{TLS}$, where x_{TLS} is the solution of the TLS problem without regularization. Thus in the development of the algorithm we explicitly assume that the regularization parameter δ is provided such that $\|Lx\| \leq \delta$ is active. Equivalently, by (2.4), this requires

$$x^T L^T Lx - \delta^2 = 0, \tag{2.5}$$

and Theorem 2.1 of [Golub et al., 1999] can be applied to characterize the R-TLS solution.

Theorem 2.1 *For regularization problem* (1.1), *if the constraint is active, the solution x^* satisfies*

$$(A^T A + \lambda_I I + \lambda_L L^T L)x^* = A^T b, \tag{2.6}$$

$$\mu > 0, \; (x^*)^T L^T Lx^* - \delta^2 = 0, \tag{2.7}$$

where

$$\lambda_I = -\frac{\|Ax^* - b\|^2}{1 + \|x^*\|^2}, \tag{2.8}$$

$$\lambda_L = \mu(1 + \|x^*\|^2), \tag{2.9}$$

$$\mu = -\frac{1}{\delta^2}\left(\frac{b^T(Ax^* - b)}{1 + \|x^*\|^2} + \frac{\|Ax^* - b\|^2}{(1 + \|x^*\|^2)^2}\right). \tag{2.10}$$

This result can be further extended to characterize the R-TLS solution in terms of an eigenpair for an augmented system describing equations (2.2) - (2.4).

Theorem 2.2 *If the constraint is active, the solution x^* of regularization problem (1.1) satisfies:*

$$B(x^*)\begin{pmatrix} x^* \\ -1 \end{pmatrix} = -\lambda_I \begin{pmatrix} x^* \\ -1 \end{pmatrix}, \tag{2.11}$$

where

$$B(x^*) = \begin{pmatrix} A^TA + \lambda_L(x^*)L^TL, & A^Tb \\ b^TA, & -\lambda_L(x^*)\delta^2 + b^Tb \end{pmatrix},$$

and λ_L is determined by (2.9) *and (2.10).*

Conversely, if the pair $(\hat{x}^T, -1), -\hat{\lambda}$ is an eigenvector-eigenvalue pair for matrix $B(\hat{x})$,

$$B(\hat{x})\begin{pmatrix} \hat{x} \\ -1 \end{pmatrix} = -\hat{\lambda} \begin{pmatrix} \hat{x} \\ -1 \end{pmatrix} \tag{2.12}$$

and $\mu(\hat{x}) \neq 0$, then

$$\hat{x}^TL^TL\hat{x} = \delta^2, \;\; \hat{\lambda} = -\frac{\|A\hat{x} - b\|^2}{1 + \|\hat{x}\|^2},$$

and, furthermore, $\hat{x}$ satisfies (2.6)

Now, as in [Golub et al., 1999], we observe, from the relation $(E, f) = (-fx^T, f) = f(-x^T, 1)$ and (2.3), that

$$\|(E, f)\|_F^2 = \|f\|^2(1 + \|x\|^2) = \frac{\|Ax - b\|^2}{1 + \|x\|^2} = -\lambda_I.$$

Thus determining the minimum $\hat{\lambda}(\hat{x})$ which satisfies the eigenvalue equation (2.11) and $\mu(\hat{x}) > 0$ is equivalent to solving (1.1). Moreover, the Lagrange parameters are explicitly prescribed provided that an estimate for δ has been made available. In particular, because of the continuous dependence of the matrix spectrum on its entries, we have shown, by including the constraint within (2.11), that the R-TLS solution may be obtained utilizing a approach similar to Rayleigh quotient iteration (RQI) for the TLS problem [Bjiörck et al., 2000], modified for matrix $B = B(x)$.

Our initial results use the shifted inverse power method to obtain an approximate value for $\lambda_I(x^*)$ and x^*. We denote by $\lambda_I^{(k)}$, $\lambda_L^{(k)}$, the values for $\lambda_I(x)$, $\lambda_L(x)$, given by (2.8) and (2.9), respectively, with $x = x^{(k)}$, where throughout the superscript k denotes the values at the k^{th} iteration. The estimate of the normalized eigenvector of B is given by

$$z^{(k)} = ((x^{(k)})^T, -1)/\sqrt{1 + \|x^{(k)}\|^2}, \tag{2.13}$$

and we define the residual at step k by $\rho^{(k)} = \|B(x^{(k)})z^{(k)} + \lambda_I(x^{(k)})z^{(k)}\|$. We set a tolerance τ, on the residual ρ such that the iteration stops when $\frac{\rho^{(k)}}{|\lambda_I^{(k)}|} < \tau$ is obtained. In fact, by the Cauchy-Schwartz inequality, and $\|z^{(k)}\| = 1$,

$$\begin{aligned} \rho^{(k)} &\geq |(z^{(k)})^T(B(x^{(k)}) + \lambda_I(x^{(k)}))z^{(k)}| \\ &= |\mu(x^{(k)})(\|Lx^{(k)}\|^2 - \delta^2)|. \end{aligned} \tag{2.14}$$

Thus, the residual $\rho^{(k)}$ also provides an upper estimate for the violation of the constraint condition (2.4) and, if $z^{(k)}$ is sufficiently close to an eigenvector of $B(x^{(k)})$, then the inequality in (2.14) is replaced by equality.

In order to start the iteration we shall assume the calculation of an initial estimate $x^{(0)}$ from the regularized LS problem with a small regularization parameter, [Hansen, 1994]. While it remains to determine a strategy for finding the optimal initial estimate of x, the choice $x^{(0)} = x_{RLS}$ is sufficient for the purposes of the verification of the algorithm when $L \neq I$. In the latter case, we note by [Golub et al., 1999], that the regularized LS and TLS solutions are identical for $\delta < ||x_{LS}||$ and thus this initial choice is inappropriate.

Algorithm 1

1 Given $x^{(0)}$, calculate $\lambda_I^{(0)}$,$\lambda_L^{(0)}$ and $z^{(0)}$ from (2.8), (2.9) and (2.13).

2 Iterate to convergence, for k=0,1,2,...

   (a) solve $(B(x^{(k)}) + \lambda_I^{(k)} I)y = z^{(k)}$.
   (b) $x^{(k+1)} = -y(1:n)/y(n+1)$.
   (c) Update $\lambda_I^{(k+1)}$ and $\lambda_L^{(k+1)}$.
   (d) $z^{(k+1)} = y/\|y\|$.
   (e) Update $\rho^{(k+1)}$.
   (f) If $\frac{\rho^{(k+1)}}{|\lambda_I^{(k+1)}|} < \tau$ and $\mu(x^{k+1}) > 0$, break.

   end for.

Remark 2.1

If $y(n+1) = 0$, we can not update x. In this case, we generate a new $z^{(k)}$ by combining $z^{(k)}$ and y, e.g. $y = y/\|y\|_2, z^{(k)} = (z^{(k)} + y)/\|z^{(k)} + y\|_2$.

Remark 2.2

The reduced conditions, (2.2)-(2.4), are only necessary, and uniqueness of the solution is not guaranteed. Clearly, should a different starting value generate an alternative solution, then the one with minimal eigenvalue is chosen for the R-TLS problem. We note that this difficulty with convergence is also encountered with the RQI for the TLS problem, [Bjiörck et al., 2000].

Remark 2.3

The efficiency of the algorithm clearly depends on the cost of solving the system

$$(B(x^{(k)}) + \lambda_I^{(k)} I)y = z^{(k)}. \tag{2.15}$$

3. Non-smooth solutions

We now suppose that the global problem domain can be decomposed such that known local constraints can be provided for each subdomain. Specifically, we suppose that the domain is partitioned as

$$x^T = ({x^{(1)}}^T, {x^{(2)}}^T, \cdots, {x^{(p)}}^T),$$

and that

$$\|L_i x^{(i)}\| \le \delta_i, \ i = 1, 2, \cdots, p,$$

where $\|L_i x^{(i)}\| \le \delta_i$, and L is a block-diagonal matrix,

$$L = \mathrm{diag}(L_1, L_2, \cdots, L_p).$$

This may well provide for a more accurate estimate of the global TLS solution, particularly in cases for which the solution is smooth on some region, but less smooth on another and may be especially significant when there are jumps between subdomains.

We define the set of active constraints via $\mathcal{S} = \{i : \|L_i x^{(i)}\| \le \delta_i$ *is active constraint*$\}$, and denote the local solution by ${\overline{x^{(i)}}}^T = (0, \cdots, {x^{(i)}}^T, \cdots, 0)$. Then we have

$$(A^T A + \lambda_I I + \lambda_L L^T L)x = A^T b,$$
$$\mu_i \ge 0, \ \ \sum_{i=1}^{p} \mu_i (x^{(i)T} L_i^T L_i x^{(i)} - \delta_i^2) = 0,$$

where

$$\lambda_I = -\frac{\|Ax - b\|^2}{1 + \|x\|^2},$$

$$\lambda_L = \mathrm{diag}(\lambda_L^{(i)}) \in R^{n\times n},\ \ \lambda_L^{(i)} = \mu_i(1+\|x\|^2), i = 1,2,\cdots,p,$$
$$\mu_i(1+\|x\|^2)\delta_i^2 = \overline{x^{(i)}}^T A^T b - \lambda_I\|x^{(i)}\|^2 - \overline{x^{(i)}}^T A^T Ax,\ if\ i \notin \mathcal{S},$$
$$\mu_i = 0,\ if\ i \in \mathcal{S}.$$

From
$$\lambda_I\|x\|^2 = b^T Ax - \|Ax\|^2 - \sum_{i\in\mathcal{S}} \lambda_L^{(i)}\delta_i^2,$$
and
$$\lambda_I(1+\|x\|^2) = -b^T b - \|Ax\|^2 + 2b^T Ax,$$
we have
$$\lambda_I = b^T Ax - b^T b + \sum_{i\in\mathcal{S}} \lambda_L^{(i)}\delta_i^2.$$

Thus again (2.11) is satisfied for matrix
$$B = \begin{pmatrix} A^T A + \lambda_L(x)L^T L, & A^T b \\ b^T A, & b^T b - \sum_{i\in\mathcal{S}} \lambda_L^{(i)}\delta_i^2 \end{pmatrix},$$
and a similar algorithm can be constructed.

4. Numerical Results

It has already been demonstrated in [Golub et al., 1999] that R-TLS is able to compute better results than Tikhonov's method. Moreover, it is generally accepted that the ordinary TLS solution does not differ significantly from the ordinary LS solution for *small* levels of noise, [Fierro et al., 1997], [Stewart, 1984]. Thus, the purpose of our numerical experiments is not to compare the effectiveness of the R-TLS concept with the Tikhonov or LS solutions. Rather, we seek to validate the presented parameter-independent R-TLS algorithm. We report results for three examples; one of these, *ilaplace* is taken from the regularization tools package, [Hansen, 1994], and is tested statistically. The second example is designed to evaluate the behavious of the algorithm subject to different choices for the parameter δ, and the last is designed to evaluate the modified R-TLS algorithm which was presented in Section 3 for the case of a non-smooth solution. Moreover, since the purpose of the presentation is validation rather than efficiency, for all calculations we have used the Matlab operator "\" to solve $(B + \lambda_I(x)I)y = z$.

In the design of our experiments we wish to test the robustness of the algorithm to perturbations in both the system matrix and the right hand side. In particular, we note that in most cases, the condition of the TLS problem is mainly determined by the perturbation of the system matrix, rather than the perturbation of the right hand side. Thus we suppose that the exact system

$Ax^* = b$ is perturbed such that we solve the system

$$\overline{A}x_{RTLS} = \overline{b},\ \overline{A} = A + \sigma E,\ \overline{b} = b + \sigma e. \tag{4.16}$$

Here the entries in the error matrices E and e, obtained using the Matlab function *randn*, are normally distributed with zero mean and unit standard variation, and are normalized such that $\|E\|_F = \|e\|_2 = 1$. Different error levels are considered by chosing the parameter σ to be $1,\ 0.1,\ 0.01,\ 0.001$, *cf.* [Golub et al., 1999]. It is obvious that the solution of the perturbed system, (4.16), x_{RTLS} depends on the choice for E and e, and that agreement with the exact solution x^* for a single case does not predict the overall behaviour of the algorithm. Thus, our results are presented as histograms for the relative error, $\|x_{RTLS} - x^*\|/\|x^*\|$, in the solution over 500 independent simulations of the same example.

Example 4.1

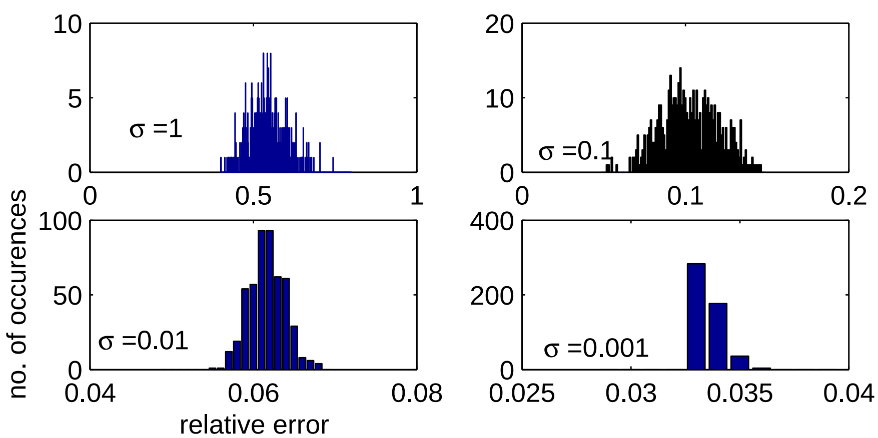

Figure 1. Example 4.1: The four histograms illustrate the statistical distribution of relative error. $\frac{\|x_{RTLS}-x^*\|}{\|x^*\|}$.

Function *ilaplace* [Golub et al., 1999], [Hansen, 1994], the inverse Laplace transform problem, is used to generate matrix A with order 65×64, and vectors x^*, $b = Ax^*$, but modified such that the scaling $\|A\|_F = \|Ax^*\|_2 = 1$ is adopted. The operator $L \in R^{(n-1)\times n}$ approximates the first-derivative operator, $\delta = 0.9\|Lx^*\|$ bounds $\|Lx\|$, and we chose tolerance $\tau = 10^{(-4)}$ in the algorithm. Numerical results shown in Figure 1 demonstrate that the solutions are reasonable.

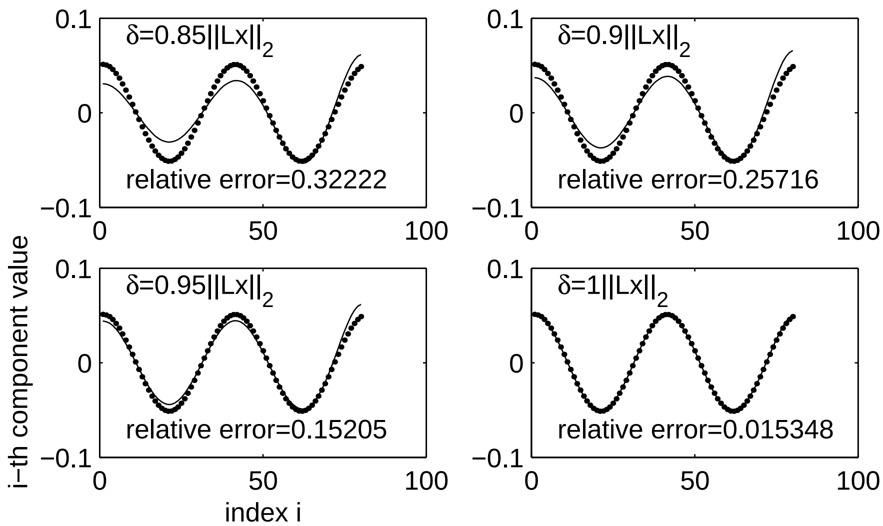

Figure 2. Example 4.2: The exact TLS solutions and RTLS solutions are given by the dotted lines and solid lines, respectively.

Example 4.2

In the former example the exact TLS solution is not known and it is therefore not possible to compare the regularized solution and non-regularized solution. Thus to evaluate the effect of the regularization we construct an ill-conditioned system with known TLS solution, and measure the difference between x_{TLS} and x_{RTLS} as the parameter δ is taken closer to the exact value for $\|Lx_{TLS}\|$. The $m \times (n+1)$ matrix $[A, b]$ is constructed as follows:

$$\begin{aligned} [A, b] &= U\Sigma V^T,\ \Sigma^T = (\ \Sigma_1,\quad 0\ ) \\ U &= I_m - 2xx^T,\ V = I_n - 2yy^T, \end{aligned}$$

where vectors x and y are normalized to size 1, $\|x\|_2 = \|y\|_2 = 1$, with entries $x(i) = sin(4\pi i/m), i = 0, 1, \cdots, m-1$ and $y(j) = cos(4\pi j/n), j = 0, 1, \cdots, n-1$. We use $m = 100, n = 80$ and take the singular values in the diagonal matrix of ordered singular values, Σ_1 to be geometrically spaced between 1 and 10^{-40}, [Fierro et al., 1997]. The operator L again approximates the first order derivative and we again use tolerance $\tau = 10^{-4}$. Figure 2 illustrates the results x_{RTLS} as compared to $x_{TLS} = -V(1:n, n+1)/V(n+1, n+1)$ for the regularization choices $\delta = \mu\|Lx_{TLS}\|$, $\mu = 0.8, 0.85, 0.9$ and 1.0. We see that as μ becomes closer to 1.0, so that δ is closer to $\|Lx_{TLS}\|$, the solution x_{RTLS} tends to x_{TLS}.

Example 4.3

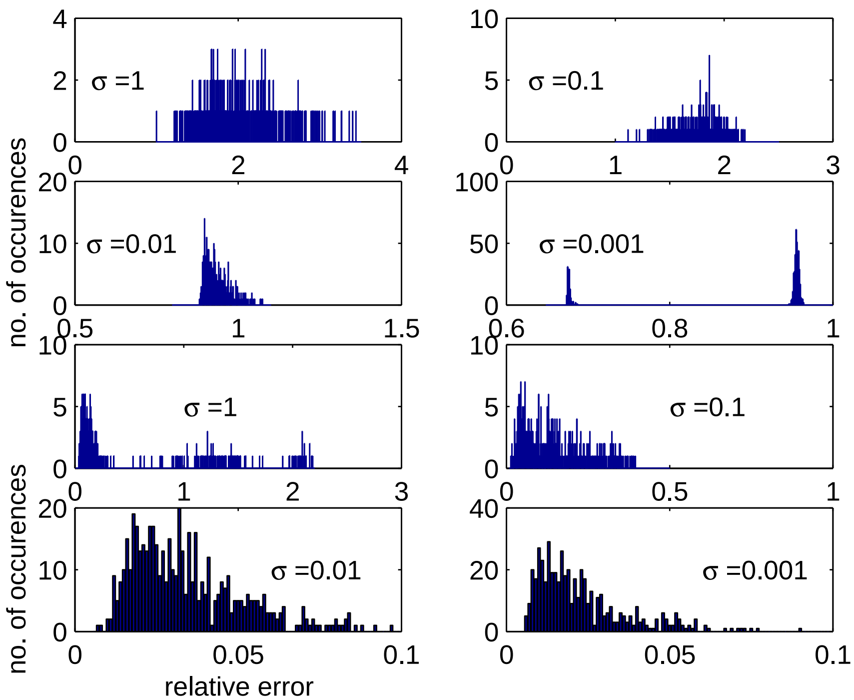

Figure 3. Example 4.3: upper and lower histograms show results for global constraint $\|Lx\| \leq \delta$, and subdomain constraints $\|L_i x\| \leq \delta_i$, resp..

This example is designed to test the modified algorithm for the case in which the solution is not expected to be smooth and we have information about the positions at which a lack of smoothness will occur. This example uses the system matrix defined from *shaw*, [Hansen, 1994], but with exact solution x^* given by

$$x^*(i) = \begin{cases} cos((i-1)*\pi/32) & 1 \leq i \leq 32, \\ cos((i-33)*\pi/32) & 33 \leq i \leq 64, \end{cases}$$

and the scaling such that $b = \|Ax^*\|_2 = 1$. The global algorithm which uses $\delta = \|Lx^*\|_2$, and tolerance $\tau = 10^{(-8)}$, and is illustrated in the upper four histograms of Figure 3, cannot provide an accurate estimate for x^*. On the other hand, with the subdomain parameters defined according to the values on each subdomain, $\delta_i = \|L_i x_i^*\|_2, i = 1, 2$, where L_1 and L_2 are first-derivative operators for each subdomain, and the tolerance is just $\tau = 10^{(-4)}$, we see from the lower four histograms of Figure 3 that better results are obtained. Note that for the modified algorithm the figure presents the difference between the exact and the RTLS solutions because they are too close to distinguish if overlaid on one figure.

5. Conclusions

The presented parameter independent algorithm for solving the regularized TLS problem works well for ill-conditioned problems with moderate error, provided only that an estimate for the degree of smoothness of the solution can be prescribed based on expected physical behaviour of the solution. Future work to make the algorithm practical, to study the convergence behaviour and to take advantage of system structure is planned.

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