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REGULARIZED TOTAL LEAST SQUARES: COMPUTATIONAL ASPECTS AND ERROR BOUNDS

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ABSTRACT. For solving linear ill-posed problems regularization methods are required when the right hand side and the operator are with some noise. In the present paper regularized approximations are obtained by regularized total least squares and dual regularized total least squares. We discuss computational aspects and provide order optimal error bounds that characterize the accuracy of the regularized approximations. The results extend earlier results where the operator is exactly given. We also present some numerical experiments, which shed a light on the relationship between RTLS, dual RTLS and the standard Tikhonov regularization.

1. **Introduction**

Ill-posed problems arise in several context and have important applications in science and engineering (see, e.g., [4, 6, 10, 18]). In this paper we consider ill-posed problems

$$A_0 x = y_0 \tag{1.1}$$

where $A_0 : X \to Y$ is a bounded linear operator between infinite dimensional real Hilbert spaces X and Y with non-closed range $\mathcal{R}(A_0)$. We shall denote the inner product and the corresponding norm on the Hilbert spaces by $(\cdot, \cdot)$ and $\|\cdot\|$ respectively. We assume throughout the paper that the operator A_0 is injective and that y_0 belongs to $\mathcal{R}(A_0)$ so that (1.1) has a unique solution $x^\dagger \in X$. We are interested in problems (1.1) where

(i) instead of the exact right hand side $y_0 \in \mathcal{R}(A_0)$ we have noisy data $y_\delta \in Y$ with

$$\|y_0 - y_\delta\| \le \delta, \tag{1.2}$$

(ii) instead of the exact operator $A_0 \in \mathcal{L}(X, Y)$ we have some noisy operator $A_h \in \mathcal{L}(X, Y)$ with

$$\|A_0 - A_h\| \le h. \tag{1.3}$$

Since $\mathcal{R}(A_0)$ is assumed to be non-closed, the solution $x^\dagger$ of problem (1.1) does not depend continuously on the data. Hence, the numerical treatment of problem (1.1), (1.2), (1.3) requires the application of special regularization methods.

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Tikhonov regularization. Tikhonov regularization [4, 6, 10, 18, 20] is known as one of the most widely applied methods for solving ill-posed problems. In this method a regularized approximation $x_\alpha^{\delta,h}$ is obtained by solving the minimization problem

$$\min_{x\in X} J_\alpha(x), \quad J_\alpha(x) = \|A_h x - y_\delta\|^2 + \alpha\|Bx\|^2 \tag{1.4}$$

where $B : \mathcal{D}(B) \subset X \to X$ is some unbounded densely defined self-adjoint strictly positive definite operator and $\alpha > 0$ is the regularization parameter to be chosen properly. Hence, in Tikhonov's method the regularized approximation is given by

$$x_\alpha^{\delta,h} = (A_h^* A_h + \alpha B^* B)^{-1} A_h^* y_\delta. \tag{1.5}$$

Regularized total least squares. In the classical total least squares problem (TLS problem) some estimate $(\hat{x}, \hat{y}, \hat{A})$ for $(x^\dagger, y_0, A_0)$ from given data (y_δ, A_h) is determined by solving the constrained minimization problem

$$\|A - A_h\|^2 + \|y - y_\delta\|^2 \to \min \quad \text{subject to} \quad Ax = y, \tag{1.6}$$

see [7]. Due to the ill-posedness of problem (1.1) it may happen that there does not exist any solution $\hat{x}$ of the TLS problem (1.6) in the space X. Furthermore, if there exists a solution $\hat{x} \in X$ of the TLS problem (1.6), this solution may be far away from the desired solution $x^\dagger$. Therefore, it is quite natural to restrict the set of admissible solutions by searching for approximations $\hat{x}$ that belong to some prescribed set K, which is the philosophy of regularized total least squares. The simplest case occurs when the set K is a ball $K = \left\{x \in X \,\middle|\, \|Bx\| \le R\right\}$ with prescribed radius R. This leads us to the regularized total least squares problem (RTLS problem) in which some estimate $(\hat{x}, \hat{y}, \hat{A})$ for $(x^\dagger, y_0, A_0)$ is determined by solving the constrained minimization problem

$$\|A - A_h\|^2 + \|y - y_\delta\|^2 \to \min \quad \text{subject to} \quad Ax = y, \ \ \|Bx\| \le R, \tag{1.7}$$

see [3, 14, 15]. In the special case of exactly given operators $A_h = A_0$, this philosophy leads us to the method of quasi-solution of Ivanov, see [8], in which $\hat{x}$ is determined by solving the constrained minimization problem $\|A_0 x - y_\delta\|^2 \to \min$ subject to $x \in K$. This approximation $\hat{x}$ is sometimes also called K-constrained least squares solution.

Dual regularized total least squares. One disadvantage of the RTLS problem (1.7) is that this method requires a reliable bound R for the norm $\|Bx^\dagger\|$. In many practical applications, however, such a bound is unknown. On the other hand, in different applications reliable bounds for the noise levels δ and h in (1.2) and (1.3) are known. In this case it makes sense to look for approximations $(\hat{x}, \hat{y}, \hat{A})$ which satisfy the side conditions $Ax = y$, $\|y - y_\delta\| \le \delta$ and $\|A - A_h\| \le h$. The solution set characterized by these three side conditions is non-empty. Selecting from the solution set the element which minimizes $\|Bx\|$ leads us to a problem in which some estimate $(\hat{x}, \hat{y}, \hat{A})$ for $(x^\dagger, y_0, A_0)$ is determined by solving the constrained minimization problem

$$\|Bx\| \to \min \quad \text{subject to} \quad Ax = y, \ \ \|y - y_\delta\| \le \delta, \ \ \|A - A_h\| \le h. \tag{1.8}$$

This problem is, in some sense, the dual of problem (1.7). Therefore, we propose to call this problem as the *dual regularized total least squares problem* (dual RTLS problem).

The paper is organized as follows. In Sections 2, 3 and 4 we discuss some computational aspects of the RTLS problem (1.7) and of the dual RTLS problem (1.8) in finite dimensional spaces. Main attention is devoted to the problem of eliminating the unknowns A and y in both problems (1.7) and (1.8). As a result, both problems lead in the general case $B \neq I$ to special multi-parameter regularization methods with two regularization parameters where one of the regularization parameters is negative. In Section 5 we discuss characterization results for generalized problems (1.7) and (1.8) in which the norm $\|A - A_h\|$ is replaced by $\|(A - A_h)G\|$. In Sections 6 and 7 we provide error bounds for the regularized approximations obtained by methods (1.7) and (1.8). In Section 6 we treat the special case $B = I$ and derive error bounds under the classical source condition $x^\dagger = A^* v$ with $v \in Y$ that show that the accuracy of the regularized approximations is of the order $O(\sqrt{\delta + h}\,)$. In the general case $B \neq I$ in Section 7 some link condition between A and B and some smoothness condition for $x^\dagger$ in terms of B are exploited for deriving error bounds. In our final Section 8 some numerical experiments are given, which shed a light on the relationship between RTLS, dual RTLS and the standard Tikhonov regularization.

2. **Computational aspects for RTLS**

Computational aspects are studied in the literature for discrete problems (1.1) in finite-dimensional spaces. Therefore we restrict our studies to the case when $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$, equipped with the Euclidian norm $\|\cdot\|_2$ and use as a matrix norm the Frobenius norm $\|\cdot\|_F$.

2.1. **Overview.** The TLS method which is problem (1.7) without the constraint $\|Bx\|_2 \leq R$ is a successful method for noise reduction in linear least squares problems in a number of applications. For an overview on computational aspects and analysis of TLS see the monograph [7]. The TLS method is suited for finite dimensional problems where both the coefficient matrix and the right-hand side are not precisely known and where the coefficient matrix is not very ill-conditioned. For discrete ill-posed problems where the coefficient matrix is very ill-conditioned and also for infinite dimensional ill-posed problems, some additional stabilization is necessary leading to the RTLS problem (1.7). The aim of our work in this section is to review properties of the RTLS problem (1.7) which serve as a basis for the development of practical computational algorithms.

Previous results about properties and computational aspects of RTLS problems may be found in [1, 3, 14, 15]. Let us summarize different alternative characterizations of the RTLS-solution that serve as a starting point for developing algorithms solving the RTLS problem (1.7) effectively. From [3] we have

Theorem 2.1. *If the constraint $\|Bx\|_2 \leq R$ of the RTLS problem (1.7) is active, then the RTLS solution $x = \hat{x}$ satisfies the equations*

$$(A_h^T A_h + \alpha B^T B + \beta I)x = A_h^T y_\delta \quad \text{and} \quad \|Bx\|_2 = R. \tag{2.1}$$

The parameters α and β satisfy

$$\alpha = \mu(1 + \|x\|_2^2) \quad \textit{and} \quad \beta = -\frac{\|A_h x - y_\delta\|_2^2}{1 + \|x\|_2^2} \tag{2.2}$$

and $\mu > 0$ is the Lagrange multiplier. Moreover,

$$\beta = \alpha R^2 - y_\delta^T (y_\delta - A_h x) = -\|A - A_h\|_F^2 - \|y - y_\delta\|_2^2. \tag{2.3}$$

The results of Theorem 2.1 allow a second characterization of the RTLS solution of the problem (1.7). The equations (2.1) and (2.3) show that the RTLS problem (1.7) can be reformulated as a special eigenvalue-eigenvector problem for a special augmented system, see [14, 15].

Theorem 2.2. *If the constraint $\|Bx\|_2 \le R$ of the RTLS problem (1.7) is active, then the RTLS solution $x = \hat{x}$ satisfies the eigenvalue-eigenvector problem*

$$\begin{pmatrix} A_h^T A_h + \alpha B^T B & A_h^T y_\delta \\ y_\delta^T A_h & -\alpha R^2 + y_\delta^T y_\delta \end{pmatrix} \begin{pmatrix} x \\ -1 \end{pmatrix} = -\beta \begin{pmatrix} x \\ -1 \end{pmatrix} \tag{2.4}$$

with α and β given by (2.2), (2.3).

The results of Theorem 2.1 allow a third characterization of the RTLS solution of problem (1.7). This characterization shows that the RTLS problem can be reformulated as a problem of minimizing the ratio of two quadratic functions subject to a norm constraint, see [1].

Theorem 2.3. *The RTLS solution $x = \hat{x}$ of the problem (1.7) is the solution of the constrained minimization problem*

$$\frac{\|A_h x - y_\delta\|_2^2}{1 + \|x\|_2^2} \to \min \quad \textit{subject to} \quad \|Bx\|_2 \le R. \tag{2.5}$$

2.2. **The standard form case B = I.** Let us discuss the standard form case $B = I$ in some detail. In this case the Theorem 2.1 is simplified as follows:

Corollary 2.4. *If the constraint $\|x\|_2 \le R$ of the RTLS problem (1.7) with $B = I$ is active, then the RTLS solution $x = \hat{x}$ is the solution of the equation*

$$(A_h^T A_h + \alpha I) x = A_h^T y_\delta \tag{2.6}$$

and α is the solution of the nonlinear equation $\|x\|_2 = R$.

The numerical computation of the RTLS solution $x = \hat{x}$ of problem (1.7) in the case $B = I$ can therefore effectively be done by following two steps:

(i) Compute the parameter $\alpha^* > 0$ by solving the nonlinear equation

$$f(\alpha) = \|x_\alpha^{\delta,h}\|_2^2 - R^2 = 0 \tag{2.7}$$

where $x_\alpha^{\delta,h}$ is the solution of the equation (2.6).

(ii) Solve the equation (2.6) with $\alpha = \alpha^*$ from step (i).

From our next proposition we conclude that f is monotonically decreasing and that equation (2.7) possesses a unique positive solution $\alpha^* > 0$ provided

$$R < \|x_{\delta,h}^\dagger\|_2. \tag{2.8}$$

Here $x^{\dagger}_{\delta,h}$ is the Moore-Penrose solution of the perturbed linear system $A_h x = y_\delta$ which is the least squares solution with the minimal norm.

Proposition 2.5. *The function $f : \mathbb{R}^+ \to \mathbb{R}$ defined by (2.7) is continuous and possesses the properties*

$$\lim_{\alpha\to 0} f(\alpha) = \|x^{\dagger}_{\delta,h}\|_2^2 - R^2 \quad \text{and} \quad \lim_{\alpha\to\infty} f(\alpha) = -R^2. \tag{2.9}$$

In addition, $f : \mathbb{R}^+ \to \mathbb{R}$ is monotonically decreasing and convex. Let $v_\alpha^{\delta,h}$ be the solution of the equation $(A_h^T A_h + \alpha I)v_\alpha^{\delta,h} = x_\alpha^{\delta,h}$, then

$$f'(\alpha) = -2(v_\alpha^{\delta,h}, x_\alpha^{\delta}) < 0 \quad \text{and} \quad f''(\alpha) = 6\|v_\alpha^{\delta,h}\|_2^2 > 0. \tag{2.10}$$

Proof. For $\alpha \to 0$ we have $x_\alpha^{\delta,h} \to x^{\dagger}_{\delta,h}$. Hence, the first limit relation of (2.9) follows. For $\alpha \to \infty$ we have $x_\alpha^{\delta,h} \to 0$. Hence, the second limit relation of (2.9) follows. By the product rule we have

$$f'(\alpha) = 2\left(\frac{\mathrm{d}}{\mathrm{d}\alpha} x_\alpha^{\delta,h}, x_\alpha^{\delta,h}\right). \tag{2.11}$$

In addition, differentiating both sides of equation (2.6) by α provides the equation $x_\alpha^{\delta,h} + (A_h^T A_h + \alpha I)\frac{\mathrm{d}}{\mathrm{d}\alpha} x_\alpha^{\delta,h} = 0$, that is, $\frac{\mathrm{d}}{\mathrm{d}\alpha} x_\alpha^{\delta,h} = -v_\alpha^{\delta,h}$. We substitute this expression into (2.11) and obtain the first identity of (2.10). The proof of the second identity of (2.10) is similar. □

Due to properties (2.10) we conclude that Newton's method for $f(\alpha) = 0$ converges monotonically for arbitrary starting value $\alpha \in (0, \alpha^*)$.

Remark 2.6. Due to stability reasons it is desirable to iterate with regularization parameters $\alpha \geq \alpha^*$. This can be reached, e.g., by applying Newton's method to the equivalent equation

$$h(r) := f(r^{-1/2}) = 0. \tag{2.12}$$

The function h defined by (2.12) is monotonically increasing and concave on $\mathbb{R}^+$ and for the first and second derivative of h we have

$$h'(r) = r^{-3/2}(v_r^{\delta,h}, x_r^{\delta,h}) > 0 \quad \text{and} \quad h''(r) = -(3/2)r^{-5/2}\|Av_r^{\delta,h}\|_2^2 < 0, \tag{2.13}$$

where $x_r^{\delta,h}$ is the solution of the equation $(A_h^T A_h + r^{-1/2} I)x_r^{\delta,h} = A_h^T y_\delta$ and $v_r^{\delta,h}$ is the solution of the equation $(A_h^T A_h + r^{-1/2} I)v_r^{\delta,h} = x_r^{\delta,h}$. For the Newton iterates $r_{k+1} = r_k - h(r_k)/h'(r_k)$ the error representation

$$r_{k+1} - r^* = \frac{h''(\xi_k)}{2h'(r_k)}(r_k - r^*)^2 \quad \text{with} \quad \xi_k \in (r_k, r^*) \tag{2.14}$$

is valid. From (2.13) and (2.14) we conclude that Newton's method applied to the equation $h(r) = 0$ converges monotonically from below for arbitrary starting values $r \in (0, r^*)$. Rewriting Newton's method in terms of α leads to the iteration

$$\alpha_{k+1} = \varphi(\alpha_k) \quad \text{with} \quad \varphi(\alpha) = \left(\frac{\alpha^3 (v_\alpha^{\delta,h}, x_\alpha^{\delta,h})}{\alpha(v_\alpha^{\delta,h}, x_\alpha^{\delta,h}) + R^2 - \|x_\alpha^{\delta,h}\|_2^2}\right)^{1/2} \tag{2.15}$$

that converges monotonically from above for arbitrary starting values $\alpha \in (\alpha^*, \infty)$.

Due to noise amplification, the Moore-Penrose solution $x^\dagger_{\delta,h}$ of the discretized ill-posed problem $A_h x = y_\delta$ with noisy data (y_δ, A_h) is generally highly oscillating with large norm $\|x^\dagger_{\delta,h}\|_2$. Therefore it makes no sense to choose the constant R of the RTLS problem (1.7) larger than $\|x^\dagger_{\delta,h}\|_2$ since the unknown solution $x^\dagger$ of the unperturbed system $A_0 x = y_0$ is expected to satisfy $\|x^\dagger\|_2 < \|x^\dagger_{\delta,h}\|_2$. Hence, one will choose R sufficiently small such that (2.8) holds. In this case the constraint $\|x\|_2 \le R$ of the RTLS problem (1.7) is active and Corollary 2.4 applies. This corollary tells us that the RTLS solution is equivalent to the Tikhonov solution $x_\alpha^{\delta,h} = (A_h^T A_h + \alpha I)^{-1} A_h^T y_\delta$ with α chosen from the nonlinear equation $\|x_\alpha^{\delta,h}\|_2 = R$. This solution $x = x_\alpha^{\delta,h}$ can be obtained by following algorithm.

Algorithm 1 Solving the RTLS problem (1.7) in the standard form case

Input: $\varepsilon > 0$, y_δ, A_h and R satisfying (2.8).

1: Choose some starting value $\alpha \ge \alpha^*$.
2: Solve $(A_h^T A_h + \alpha I)x = A_h^T y_\delta$.
3: Solve $(A_h^T A_h + \alpha I)v = x$.
4: Update $\alpha_{\text{new}} := \left(\dfrac{\alpha^3 (v,x)}{\alpha(v,x) + R^2 - \|x\|_2^2} \right)^{1/2}$.
5: **if** $|\alpha_{\text{new}} - \alpha| \ge \varepsilon|\alpha|$ **then** $\alpha := \alpha_{\text{new}}$ and **goto** 2
6: **else** solve $(A_h^T A_h + \alpha_{\text{new}} I)x = A_h^T y_\delta$.

3. Computational aspects for dual RTLS

In our knowledge, the dual RTLS problem (1.8) has not been studied in the literature so far except in the special case $h = 0$. In this special case method (1.8) reduces to Tikhonov regularization with α chosen by the discrepancy principle, see [12, 4]. In the case $h \ne 0$ the situation is more complicated. Let us start by collecting some properties which can be shown by straight forward computations.

Proposition 3.1. *Let $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$, $A, A_h \in \mathcal{L}(\mathbb{R}^n, \mathbb{R}^m)$ and $G \in \mathcal{L}(\mathbb{R}^k, \mathbb{R}^n)$. Then,*

(i) $\|y^T x\|_F = \|y\|_2 \|x\|_2$, (ii) $\frac{\partial}{\partial x}\|Ax - y\|_2^2 = 2A^T(Ax - y)$,

(iii) $\frac{\partial}{\partial A}(y, Ax) = yx^T$, (iv) $\frac{\partial}{\partial A}\|(A - A_h)G\|_F^2 = 2(A - A_h)GG^T$.

In the following theorem we provide a different characterization of the dual RTLS solution that serves for effective solving the dual RTLS problem (1.8).

Theorem 3.2. *If the two constraints $\|y - y_\delta\|_2 \le \delta$ and $\|A - A_h\|_F \le h$ of the dual RTLS problem (1.8) are active, then the dual RTLS solution $x = \hat{x}$ of problem (1.8) is a solution of the equation*

$$(A_h^T A_h + \alpha B^T B + \beta I)x = A_h^T y_\delta. \tag{3.1}$$

The parameters α and β satisfy

$$\alpha = \frac{\nu + \mu\|x\|_2^2}{\nu\mu} \quad \text{and} \quad \beta = -\frac{\mu\|A_h x - y_\delta\|_2^2}{\nu + \mu\|x\|_2^2} \tag{3.2}$$

where $\mu > 0$, $\nu > 0$ are the Lagrange multipliers. Moreover,

$$\|A_h x - y_\delta\|_2 = \delta + h\|x\|_2 \quad \textit{and} \quad \beta = -\frac{h(\delta + h\|x\|_2)}{\|x\|_2}. \tag{3.3}$$

Proof. We eliminate y in problem (1.8) and use the classical Lagrange multiplier formulation with the Lagrange function

$$\mathcal{L}(x, A, \mu, \nu) = \|Bx\|_2^2 + \mu\left(\|Ax - y_\delta\|_2^2 - \delta^2\right) + \nu\left(\|A - A_h\|_F^2 - h^2\right) \tag{3.4}$$

where μ and ν are the Lagrange multipliers which are non-zero since the constraints are assumed to be active. We characterize the solution to the dual RTLS problem (1.8) by setting the partial derivatives of the Lagrange function (3.4) equal to zero. Applying Proposition 3.1 we obtain

$$\mathcal{L}_x = 2B^T Bx + 2\mu A^T(Ax - y_\delta) = 0, \tag{3.5}$$

$$\mathcal{L}_A = 2\mu(Ax - y_\delta)x^T + 2\nu(A - A_h) = 0, \tag{3.6}$$

$$\mathcal{L}_\mu = \|Ax - y_\delta\|_2^2 - \delta^2 = 0, \tag{3.7}$$

$$\mathcal{L}_\nu = \|A - A_h\|_F^2 - h^2 = 0. \tag{3.8}$$

From (3.6) we have $A(\mu x x^T + \nu I) = \nu A_h + \mu y_\delta x^T$, or equivalently,

$$\begin{aligned} A &= \left(\nu A_h + \mu y_\delta x^T\right)\left(\mu x x^T + \nu I\right)^{-1} \\ &= \left(\nu A_h + \mu y_\delta x^T\right)\left(\frac{1}{\nu} I - \frac{\mu}{\nu(\nu + \mu\|x\|_2^2)}\, x x^T\right) \\ &= A_h - \frac{\mu}{\nu + \mu\|x\|_2^2}\left(A_h x - y_\delta\right) x^T. \end{aligned} \tag{3.9}$$

We substitute (3.9) into (3.5), rearrange terms and obtain the equation

$$B^T Bx + \frac{\mu\nu}{\nu + \mu\|x\|_2^2}\left(A_h^T - \frac{\mu}{\nu + \mu\|x\|_2^2}\, x(A_h x - y_\delta)^T\right)(A_h x - y_\delta) = 0.$$

We multiply this equation by $(\nu + \mu\|x\|_2^2)/(\mu\nu)$, rearrange terms and obtain the equivalent equation (3.1) with α and β given by (3.2). It remains to prove (3.3). We substitute (3.9) into (3.7), rearrange terms and obtain the equation

$$\|A_h x - y_\delta\|_2 = \frac{\delta}{\nu}\left(\nu + \mu\|x\|_2^2\right). \tag{3.10}$$

We substitute (3.9) into (3.8) and obtain $\|(A_h x - y_\delta)x^T\|_F = \frac{h}{\mu}(\nu + \mu\|x\|_2^2)$. Due to property (i) of the Proposition 3.1, this equation is equivalent to

$$\|A_h x - y_\delta\|_2 = \frac{h}{\mu\|x\|_2}\left(\nu + \mu\|x\|_2^2\right). \tag{3.11}$$

From (3.10) and (3.11) we obtain the two equations

$$\frac{\delta}{\nu} = \frac{h}{\mu\|x\|_2} \quad \text{and} \quad \|A_h x - y_\delta\|_2 = \delta + h\|x\|_2. \tag{3.12}$$

From (3.11) we have $\mu\|A_hx-y_\delta\|_2/(\nu+\mu\|x\|_2^2) = h/\|x\|_2$. Hence, from the second equation of (3.2) we have $\beta = -h\|A_hx - y_\delta\|_2/\|x\|_2$. From this equation and the second equation of (3.12) we obtain $\beta = -h(\delta + h\|x\|_2)/\|x\|_2$. □

Remark 3.3. We note that due to (3.9) and (3.11) the coefficient matrix A in the dual RTLS problem (1.8) is given by

$$A = A_h - \frac{h}{\|(A_hx - y_\delta)x^T\|_F}\,(A_hx - y_\delta)\,x^T,$$

and that due to this equation and the second equation of (3.12) the vector y in the dual RTLS-problem (1.8) is given by

$$y = y_\delta + \frac{\delta}{\|A_hx - y_\delta\|_2}\,(A_hx - y_\delta)\,,$$

where $x = \widehat{x}$.

Remark 3.4. If the two constraints $\|y - y_\delta\|_2 \le \delta$ and $\|A - A_h\|_F \le h$ of the dual RTLS problem (1.8) are active, then we obtain from the results of Theorem 3.2 that the solution $x = \hat{x}$ of the dual RTLS problem can also be characterized either by the constrained minimization problem

$$\|Bx\|_2 \to \min \quad \text{subject to} \quad \|A_hx - y_\delta\|_2 = \delta + h\|x\|_2$$

or by the minimization problem

$$\|A_hx - y_\delta\|_2^2 + \alpha\|Bx\|_2^2 - (\delta + h\|x\|_2)^2 \to \min$$

with α chosen by the nonlinear equation $\|A_hx - y_\delta\|_2 = \delta + h\|x\|_2$.

4. Special cases for dual RTLS

4.1. **The case $\mathbf{h = 0}$.** In our first special case we assume that in the dual RTLS problem (1.8) we have $h = 0$, that is, the coefficient matrix $A_h = A_0$ is exactly given. In this special case the dual RTLS problem (1.8) reduces to

$$\|Bx\|_2 \to \min \quad \text{subject to} \quad A_0x = y,\ \ \|y - y_\delta\|_2 \le \delta \tag{4.1}$$

and the Lagrange function attains the form

$$\mathcal{L}(x,\mu) = \|Bx\|_2^2 + \mu(\|A_0x - y_\delta\|_2^2 - \delta^2).$$

Corollary 4.1. *If the constraint $\|y - y_\delta\|_2 \le \delta$ of the dual RTLS problem (4.1) is active, then the solution $x = \hat{x}$ of problem (4.1) satisfies*

$$(A_0^TA_0 + \alpha B^TB)x = A_0^Ty_\delta \quad \text{and} \quad \|A_0x - y_\delta\|_2 = \delta. \tag{4.2}$$

The parameter α and the Lagrange multiplier $\mu > 0$ are related by $\alpha = 1/\mu$.

Proof. Setting the partial derivatives of the Lagrange function equal to zero we obtain

$$\mathcal{L}_x = 2B^TBx + 2\mu A_0^T(A_0x - y_\delta) = 0,$$
$$\mathcal{L}_\mu = \|A_0x - y_\delta\|_2^2 - \delta^2 = 0.$$

These equations give (4.2). □

The numerical computation of the dual RTLS solution $x = \hat{x}$ of problem (4.1) can effectively be done in the following two steps:

(i) Compute the parameter $\alpha^* > 0$ by solving the nonlinear equation
$$f(\alpha) = \|A_0 x_\alpha^\delta - y_\delta\|_2^2 - \delta^2 = 0 \tag{4.3}$$
where x_α^δ is the solution of the first equation of (4.2).

(ii) Solve the first equation of (4.2) with $\alpha = \alpha^*$ from step (i).

From our next proposition we conclude that f is monotonically increasing and that equation (4.3) possesses a unique positive solution $\alpha^* > 0$ provided
$$\|Py_\delta\|_2 < \delta < \|y_\delta\|_2.$$
Here P denotes the orthogonal projector onto $\mathcal{R}(A_0)^\perp$.

Proposition 4.2. *The function $f : \mathbb{R}^+ \to \mathbb{R}$ defined by (4.3) is continuous and possesses the properties*
$$\lim_{\alpha\to 0} f(\alpha) = \|Py_\delta\|_2^2 - \delta^2 \quad \text{and} \quad \lim_{\alpha\to\infty} f(\alpha) = \|y_\delta\|_2^2 - \delta^2. \tag{4.4}$$
In addition, $f : \mathbb{R}^+ \to \mathbb{R}$ is monotonically increasing. Let v_α^δ be the solution of the equation $(A_0^T A_0 + \alpha B^T B)v_\alpha^\delta = B^T B x_\alpha^\delta$, then
$$f'(\alpha) = 2\alpha(v_\alpha^\delta, B^T B x_\alpha^\delta) > 0 \quad \text{and} \quad f''(\alpha) = 2(v_\alpha^\delta, B^T B x_\alpha^\delta) - 6\alpha\|Bv_\alpha^\delta\|_2^2. \tag{4.5}$$

Proof. For $\alpha \to 0$ we have $y_\delta - A_0 x_\alpha^\delta \to Py_\delta$. Hence, the first limit relation of (4.4) follows. For $\alpha \to \infty$ we have $x_\alpha^\delta \to 0$. Hence, the second limit relation of (4.4) follows. By the product rule and the first equation of (4.2) we have
$$f'(\alpha) = 2\left(\frac{\mathrm{d}}{\mathrm{d}\alpha}x_\alpha^\delta, A_0^T(A_0 x_\alpha^\delta - y_\delta)\right) = -2\alpha\left(\frac{\mathrm{d}}{\mathrm{d}\alpha}x_\alpha^\delta, B^T B x_\alpha^\delta\right). \tag{4.6}$$
In addition, differentiating both sides of the first equation of (4.2) by α provides the equation $B^T B x_\alpha^\delta + (A_0^T A_0 + \alpha B^T B)\frac{\mathrm{d}}{\mathrm{d}\alpha}x_\alpha^\delta = 0$, that is, $\frac{\mathrm{d}}{\mathrm{d}\alpha}x_\alpha^\delta = -v_\alpha^\delta$. We substitute this expression into (4.6) and obtain the first identity of (4.5). The proof of the second identity of (4.5) is similar. □

From the second identity of (4.5) it follows that the function f defined by (4.3) is convex for small α-values, but concave for large α-values. Hence, global and monotone convergence of Newton's method for solving equation (4.3) cannot be guaranteed. Therefore we propose to determine the solution r^* of the equivalent equation
$$h(r) := f(1/r) = 0 \tag{4.7}$$
by Newton's method. This function possesses the following properties:

(1) For $r > 0$ the function h is monotonically decreasing and we have
$$h'(r) = -2r^{-3}(v_r^\delta, B^T B x_r^\delta) < 0$$
where x_r^δ is the solution of the equation $(A_0^T A_0 + r^{-1}B^T B)x_r^\delta = A_0^T y_\delta$ and v_r^δ is the solution of the equation $(A_0^T A_0 + r^{-1}B^T B)v_r^\delta = B^T B x_r^\delta$.

(2) For $r > 0$ the function h is convex and we have
$$h''(r) = 6r^{-4}\|A_0 v_r^\delta\|_2^2 > 0.$$

From (2.14) and the two properties (1) and (2) we conclude that Newton's method applied to the equation $h(r) = 0$ converges monotonically for arbitrary starting values $r \in (0, r^*)$. Rewriting Newton's method $r_{k+1} = r_k - h(r_k)/h'(r_k)$ in terms of $\alpha_k := 1/r_k$ leads us to the iteration method

$$\alpha_{k+1} = \varphi(\alpha_k) \quad \text{with} \quad \varphi(\alpha) = \frac{2\alpha^3 (v_\alpha^\delta, B^T B x_\alpha^\delta)}{2\alpha^2 (v_\alpha^\delta, B^T B x_\alpha^\delta) + \|A_0 x_\alpha^\delta - y_\delta\|_2^2 - \delta^2}$$

where v_α^δ is the solution of $(A_0^T A_0 + \alpha B^T B) v_\alpha^\delta = B^T B x_\alpha^\delta$. This iteration method converges monotonically from above for arbitrary starting values $\alpha \in (\alpha^*, \infty)$. Summarizing, in the special case $h = 0$ the dual RTLS solution $x = x_\alpha^\delta$ can be obtained by following algorithm.

Algorithm 2 Solving the dual RTLS problem (1.8) in the case $h = 0$

Input: $\varepsilon > 0$, y_δ, A_0, B and δ satisfying $\|P y_\delta\|_2 < \delta < \|y_\delta\|_2$.

1: Choose some starting value $\alpha \geq \alpha^*$.
2: Solve $(A_0^T A_0 + \alpha B^T B) x = A_0^T y_\delta$.
3: Solve $(A_0^T A_0 + \alpha B^T B) v = B^T B x$.
4: Update $\alpha_{\text{new}} := \dfrac{2\alpha^3 (v, B^T B x)}{2\alpha^2 (v, B^T B x) + \|A_0 x - y_\delta\|_2^2 - \delta^2}$.
5: **if** $|\alpha_{\text{new}} - \alpha| \geq \varepsilon |\alpha|$ **then** $\alpha := \alpha_{\text{new}}$ and **goto** 2
6: **else** solve $(A_0^T A_0 + \alpha_{\text{new}} I) x = A_0^T y_\delta$.

4.2. **The case $\delta = 0$.** In our second special case we assume that in the dual RTLS problem (1.8) we have $\delta = 0$, that is, the vector $y_\delta = y_0$ is exactly given. In this case the dual RTLS problem (1.8) reduces to

$$\|Bx\|_2 \to \min \quad \text{subject to} \quad Ax = y_0, \ \|A - A_h\|_F \leq h \tag{4.8}$$

and the Lagrange function has the form

$$\mathcal{L}(x, A, \lambda, \nu) = \|Bx\|_2^2 + (\lambda, Ax - y_0) + \nu(\|A - A_h\|_F^2 - h^2).$$

Corollary 4.3. *If the constraint $\|A - A_h\|_F \leq h$ of the dual RTLS problem (4.8) is active, then the dual RTLS solution $x = \hat{x}$ of problem (4.8) is a solution of the equation*

$$(A_h^T A_h + \alpha B^T B + \beta I) x = A_h^T y_0. \tag{4.9}$$

The parameters α and β satisfy

$$\alpha = \frac{\|x\|_2^2}{\nu} \quad \textit{and} \quad \beta = -\frac{\|A_h x - y_0\|_2^2}{\|x\|_2^2} \tag{4.10}$$

where $\nu > 0$ is the Lagrange multiplier. Moreover,

$$\|A_h x - y_0\|_2 = h \|x\|_2 \quad \textit{and} \quad \beta = -h^2. \tag{4.11}$$

Proof. Setting the partial derivatives of the Lagrange function equal to zero gives

$$\mathcal{L}_x = 2B^T Bx + A^T\lambda = 0, \tag{4.12}$$

$$\mathcal{L}_A = \lambda x^T + 2\nu(A - A_h) = 0, \tag{4.13}$$

$$\mathcal{L}_\lambda = Ax - y_0 = 0, \tag{4.14}$$

$$\mathcal{L}_\nu = \|A - A_h\|_F^2 - h^2 = 0. \tag{4.15}$$

From (4.13) we have $A = A_h - \frac{1}{2\nu}\lambda x^T$. We substitute it into (4.14) and obtain $A_h x - \frac{\|x\|_2^2}{2\nu}\lambda = y_0$, that is,

$$\lambda = \frac{2\nu}{\|x\|_2^2}(A_h x - y_0). \tag{4.16}$$

From (4.16) and (4.13) we obtain that A has the representation

$$A = A_h - \frac{1}{\|x\|_2^2}(A_h x - y_0)x^T. \tag{4.17}$$

We substitute (4.16) and (4.17) into (4.12) and obtain

$$B^T Bx + \frac{\nu}{\|x\|_2^2}\left(A_h^T - \frac{1}{\|x\|_2^2}x(A_h x - y_0)^T\right)(A_h x - y_0) = 0.$$

We multiply this equation by $\|x\|_2^2/\nu$, rearrange terms and obtain the equivalent equation (4.9) with α and β given by (4.10). It remains to prove (4.11). We substitute (4.17) into (4.15) and obtain $\|(A_h x - y_0)x^T\|_F = h\|x\|_2^2$ which is equivalent to the first equation of (4.11). Finally, the second equation of (4.11) follows from the first equation of (4.11) and the second equation of (4.10). □

4.3. **The case B = I.** In the standard form case $B = I$ from the Theorem 3.2 one can obtain the following characterization of the solution of (1.8).

Corollary 4.4. *If the two constraints $\|y - y_\delta\|_2 \le \delta$ and $\|A - A_h\|_F \le h$ of the dual RTLS problem (1.8) are active, then the dual RTLS solution $x = \hat{x}$ of problem (1.8) with $B = I$ is the solution of the equation*

$$(A_h^T A_h + \alpha I)x = A_h^T y_\delta, \tag{4.18}$$

and α is the solution of the nonlinear equation $\|A_h x - y_\delta\|_2 = \delta + h\|x\|_2$.

The numerical computation of the dual RTLS solution of the problem (1.8) in the standard form case $B = I$ can therefore effectively be done in two steps:

(i) Compute the parameter $\alpha^* > 0$ by solving the nonlinear equation

$$f(\alpha) = \|A_h x_\alpha^{\delta,h} - y_\delta\|_2^2 - (\delta + h\|x_\alpha^{\delta,h}\|_2)^2 = 0, \tag{4.19}$$

where $x_\alpha^{\delta,h}$ is the solution of the equation (4.18).

(ii) Solve equation (4.18) with $\alpha = \alpha^*$ from step (i).

From our next proposition we conclude that f is monotonically increasing and that equation (4.19) possesses a unique positive solution $\alpha^* > 0$ provided

$$\|Py_\delta\|_2 - h\|x_{\delta,h}^\dagger\|_2 < \delta < \|y_\delta\|_2,$$

where $x^\dagger_{\delta,h} = A^\dagger_h y_\delta$ is the Moore-Penrose solution of the perturbed linear system $A_h x = y_\delta$ (which is the least squares solution of the minimal norm) and P is the orthogonal projector onto $\mathcal{R}(A_h)^\perp$.

Proposition 4.5. *The function $f : \mathbb{R}^+ \to \mathbb{R}$ defined by (4.19) is continuous and possesses the properties*

$$\lim_{\alpha\to 0} f(\alpha) = \|Py_\delta\|_2^2 - (\delta + h\|x^\dagger_{\delta,h}\|_2)^2 \quad \text{and} \quad \lim_{\alpha\to\infty} f(\alpha) = \|y_\delta\|_2^2 - \delta^2. \tag{4.20}$$

Let $v^{\delta,h}_\alpha = (A_h^T A_h + \alpha I)^{-1} x^{\delta,h}_\alpha$, then

$$f'(\alpha) = 2\left(\alpha + h^2 + h\delta/\|x^{\delta,h}_\alpha\|_2\right)(v^{\delta,h}_\alpha, x^{\delta,h}_\alpha) > 0. \tag{4.21}$$

Proof. For $\alpha \to 0$ we have $x^{\delta,h}_\alpha \to x^\dagger_{\delta,h}$. In addition, $y_\delta - A_h x^\dagger_{\delta,h} = y_\delta - A_h A^\dagger_h y_\delta = Py_\delta$. Hence, the first limit relation of (4.20) follows. For $\alpha \to \infty$ we have that $x^{\delta,h}_\alpha \to 0$. Hence, the second limit relation of (4.20) follows. We use that f is given by $f(\alpha) = \|A_h x^{\delta,h}_\alpha - y_\delta\|_2^2 - h^2\|x^{\delta,h}_\alpha\|_2^2 - 2\delta h\|x^{\delta,h}_\alpha\|_2 - \delta^2$, apply the chain rule and the product rule, exploit equation (4.18) and obtain

$$f'(\alpha) = -2\left(\alpha + h^2 + \frac{h\delta}{\|x^{\delta,h}_\alpha\|_2}\right)\left(\frac{\mathrm{d}}{\mathrm{d}\alpha}x^{\delta,h}_\alpha, x^{\delta,h}_\alpha\right). \tag{4.22}$$

In addition, differentiating both sides of the equation (4.18) by α provides the equation $x^{\delta,h}_\alpha + (A_h^T A_h + \alpha I)\frac{\mathrm{d}}{\mathrm{d}\alpha}x^{\delta,h}_\alpha = 0$, that is, $\frac{\mathrm{d}}{\mathrm{d}\alpha}x^{\delta,h}_\alpha = -v^{\delta,h}_\alpha$. From this identity and (4.22) we obtain (4.21). □

The function f defined by (4.19) is convex for small α-values, but concave for large α-values. Hence, global and monotone convergence of Newton's method for solving equation (4.19) cannot be guaranteed. Therefore we propose to determine the solution r^* of the equivalent equation

$$h(r) := f(r^{-1/2}) = 0 \tag{4.23}$$

by Newton's method. This function possesses the following properties.

Proposition 4.6. *Let h be defined by (4.23) with f given by (4.19), let $x^{\delta,h}_r$ be the solution of the equation $(A_h^T A_h + r^{-1/2} I)x^{\delta,h}_r = A_h^T y_\delta$ and $v^{\delta,h}_r$ be the solution of the equation $(A_h^T A_h + r^{-1/2} I)v^{\delta,h}_r = x^{\delta,h}_r$.*

(i) *$h : \mathbb{R}^+ \to \mathbb{R}$ is monotonically decreasing and*

$$h'(r) = -r^{-3/2}\left(r^{-1/2} + h^2 + \delta h/\|x^{\delta,h}_r\|_2\right)(v^{\delta,h}_r, x^{\delta,h}_r) < 0. \tag{4.24}$$

(ii) *$h : \mathbb{R}^+ \to \mathbb{R}$ is convex and*

$$\begin{aligned} h''(r) = {} & \frac{(v^{\delta,h}_r, x^{\delta,h}_r) + 3\|Av^{\delta,h}_r\|_2^2}{2r^3} + h^2\frac{3\|Av^{\delta,h}_r\|_2^2}{2r^{5/2}} \\ & + 2\delta h\frac{3r^{1/2}\|x^{\delta,h}_r\|_2^2 + |(v^{\delta,h}_r, x^{\delta,h}_r)|^2}{4r^3\|x^{\delta,h}_r\|_2^2} > 0. \end{aligned} \tag{4.25}$$

Proof. Using the relation $h'(r) = -\frac{1}{2}r^{-3/2}f'(r^{-1/2})$ together with (4.21) we obtain (4.24). The proof of (4.25) is similar. □

From (2.14) and Proposition 4.6 we conclude that Newton's method applied to the equation $h(r) = 0$ converges monotonically from below for arbitrary starting values $r \in (0, r^*)$. Rewriting Newton's method $r_{k+1} = r_k - h(r_k)/h'(r_k)$ in terms of $\alpha_k := r_k^{-1/2}$ leads us to the iteration method

$$\alpha_{k+1} = \varphi(\alpha_k) \quad \text{with} \quad \varphi(\alpha) = \left(\frac{\alpha^3 f'(\alpha)}{\alpha f'(\alpha) + 2f(\alpha)} \right)^{1/2}$$

where f and f' are given by (4.19) and (4.21), respectively. This iteration method converges monotonically from above for arbitrary starting values $\alpha \in (\alpha^*, \infty)$. Summarizing, in the special case $B = I$ the dual RTLS solution $x = x_\alpha^{\delta,h}$ can be obtained by following algorithm.

Algorithm 3 Solving the dual RTLS problem (1.8) in the standard form case

Input: $\varepsilon > 0$, y_δ, A_h, δ and h satisfying $\|Py_\delta\|_2 - h\|x^\dagger_{\delta,h}\|_2 < \delta < \|y_\delta\|_2$.

1: Choose some starting value $\alpha \geq \alpha^*$.
2: Solve $(A_h^T A_h + \alpha I)x = A_h^T y_\delta$.
3: Solve $(A_h^T A_h + \alpha I)v = x$.
4: Update $\alpha_{\text{new}} := \left(\frac{\alpha^3 f'(\alpha)}{\alpha f'(\alpha) + 2f(\alpha)} \right)^{1/2}$ with f from (4.19).
5: **if** $|\alpha_{\text{new}} - \alpha| \geq \varepsilon|\alpha|$ **then** $\alpha := \alpha_{\text{new}}$ and **goto** 2
6: **else** solve $(A_h^T A_h + \alpha_{\text{new}} I)x = A_h^T y_\delta$.

5. Revisiting RTLS and dual RTLS

In this section we generalize the regularized total least squares problem (1.7) by solving the constrained minimization problem

$$\|(A - A_h)G\|_F^2 + \|y - y_\delta\|_2^2 \to \min \quad \text{subject to} \quad Ax = y, \ \|Bx\|_2 \leq R, \tag{5.1}$$

and generalize the dual regularized total least squares problem (1.8) by solving the constrained minimization problem

$$\|Bx\|_2 \to \min \quad \text{subject to} \quad Ax = y, \ \|y - y_\delta\|_2 \leq \delta, \ \|(A - A_h)G\|_F \leq h. \tag{5.2}$$

In (5.1) and (5.2), respectively, G is a given (n, k)-matrix. The introduction of the additional matrix G can be motivated by an additional scaling in the constrained minimization problems (5.1) and (5.2), respectively. Considering the estimate

$$\|Ax\|_2 \leq \|A(B^T B)^{-1/2}\|_F \|Bx\|_2,$$

which corresponds to the estimate $\|Ax\|_Y \leq \|A(B^T B)^{-1/2}\|_{X \to Y} \|Bx\|_X$ in the infinite dimensional case, we conclude that

$$G = (B^T B)^{-1/2} \tag{5.3}$$

is one appropriate choice of treating the two problems (5.1) and (5.2). Using the proof ideas from [3, Theorem 2.1] we obtain that for arbitrary G the RTLS solution of the problem (5.1) can be characterized as follows.

Theorem 5.1. *Let G be an arbitrary (n,k)-matrix with rank $r(G) = n$. If the constraint $\|Bx\|_2 \le R$ of the RTLS problem (5.1) is active, then the RTLS solution $x = \hat{x}$ satisfies the equations*

$$(A_h^T A_h + \alpha B^T B + \beta (GG^T)^{-1})x = A_h^T y_\delta \quad \text{and} \quad \|Bx\|_2 = R. \tag{5.4}$$

The parameters α and β satisfy

$$\alpha = \mu(1 + \|(GG^T)^{-1/2}x\|_2^2) \quad \text{and} \quad \beta = -\frac{\|A_h x - y_\delta\|_2^2}{1 + \|(GG^T)^{-1/2}x\|_2^2}, \tag{5.5}$$

and $\mu > 0$ is the Lagrange multiplier. Moreover,

$$\beta = \alpha R^2 - y_\delta^T(y_\delta - A_h x) = -\|(A - A_h)G\|_F^2 - \|y - y_\delta\|_2^2. \tag{5.6}$$

For the special choice $G = (B^T B)^{-1/2}$ we obtain from Theorem 5.1 that the RTLS solution of the problem (5.1) can be characterized as follows.

Corollary 5.2. *Let G be chosen by (5.3). If the constraint $\|Bx\|_2 \le R$ of the RTLS problem (5.1) is active, then the RTLS solution satisfies the equations*

$$(A_h^T A_h + \alpha B^T B)x = A_h^T y_\delta \quad \text{and} \quad \|Bx\|_2 = R. \tag{5.7}$$

Now let us consider the dual RTLS problem (5.2). Extending the proof of Theorem 3.2 to the more general dual RTLS problem (5.2) with arbitrary G leads to following result.

Theorem 5.3. *Let G be an arbitrary (n,k)-matrix with rank $r(G) = n$. If the two constraints $\|y - y_\delta\|_2 \le \delta$ and $\|(A - A_h)G\|_F \le h$ of the dual RTLS problem (5.2) are active, then the dual RTLS solution is a solution of the equation*

$$(A_h^T A_h + \alpha B^T B + \beta (GG^T)^{-1})x = A_h^T y_\delta. \tag{5.8}$$

The parameters α and β satisfy

$$\alpha = \frac{\nu + \mu\|(GG^T)^{-1/2}x\|_2^2}{\nu\mu} \quad \text{and} \quad \beta = -\frac{\mu\|A_h x - y_\delta\|_2^2}{\nu + \mu\|(GG^T)^{-1/2}x\|_2^2}, \tag{5.9}$$

where $\mu > 0$, $\nu > 0$ are the Lagrange multipliers. Moreover,

$$\|A_h x - y_\delta\|_2 = \delta + h\|(GG^T)^{-1/2}x\|_2 \quad \text{and} \quad \beta = -\frac{h(\delta + h\|(GG^T)^{-1/2}x\|_2)}{\|(GG^T)^{-1/2}x\|_2}.$$

If G is chosen by (5.3), then we obtain from Theorem 5.3 that the dual RTLS solution of the problem (5.2) can be characterized as follows.

Corollary 5.4. *Let G be chosen by (5.3). If the two constraints $\|y - y_\delta\|_2 \le \delta$ and $\|(A - A_h)G\|_F \le h$ of the dual RTLS problem (5.2) are active, then the dual RTLS solution satisfies the equations*

$$(A_h^T A_h + \alpha B^T B)x = A_h^T y_\delta \quad \text{and} \quad \|A_h x - y_\delta\|_2 = \delta + h\|Bx\|_2. \tag{5.10}$$

6. Error bounds in the standard form case B = I

To the best of our knowledge, so far in the literature there are no error bounds characterizing the accuracy of the approximations $\hat{x}$ of the both problems (1.7) and (1.8). Our aim in this section is to prove order optimal error bounds in the special case $B = I$ under the classical source condition

$$x^\dagger = A_0^* v \quad \text{with} \quad v \in Y. \tag{6.1}$$

6.1. Error bounds for RTLS.

Theorem 6.1. *Assume that the exact solution $x^\dagger$ of the problem (1.1) satisfies the source condition (6.1) and the side condition $\|x^\dagger\| = R$. Let in addition $\hat{x}$ be the RTLS solution of the problem (1.7), then*

$$\|\hat{x} - x^\dagger\| \le (2 + 2\sqrt{2})^{1/2} \|v\|^{1/2} \max\{1, R^{1/2}\} \sqrt{\delta + h}\,. \tag{6.2}$$

Proof. Since both $(x^\dagger, y_0, A_0)$ and $(\hat{x}, \hat{y}, \hat{A})$ satisfy the two side conditions $Ax = y$ and $\|x\| \le R$ of the RTLS problem (1.7), we obtain from (1.7) and (1.2), (1.3) that

$$\|\hat{A} - A_h\|^2 + \|\hat{y} - y_\delta\|^2 \le \|A_0 - A_h\|^2 + \|y_0 - y_\delta\|^2 \le h^2 + \delta^2. \tag{6.3}$$

Next, since $\|\hat{x}\| \le R$ and $\|x^\dagger\| = R$ we have $\|\hat{x}\|^2 \le \|x^\dagger\|^2$, or equivalently,

$$\|\hat{x} - x^\dagger\|^2 \le 2(x^\dagger, x^\dagger - \hat{x}).$$

Due to (6.1) and the Cauchy-Schwarz inequality we obtain

$$\|\hat{x} - x^\dagger\|^2 \le 2(A_0^* v, x^\dagger - \hat{x}) \le 2\|v\|\, \|A_0 x^\dagger - A_0 \hat{x}\|. \tag{6.4}$$

By triangle inequality we have

$$\begin{aligned} \|A_0 x^\dagger - A_0 \hat{x}\| &\le \|A_0 x^\dagger - \hat{y}\| + \|\hat{y} - A_0 \hat{x}\| \\ &\le \|A_0 x^\dagger - y_\delta\| + \|\hat{y} - y_\delta\| + \|\hat{y} - A_h \hat{x}\| + \|A_0 \hat{x} - A_h \hat{x}\|. \end{aligned} \tag{6.5}$$

For estimating the sum of the first and fourth summand in the bracket of (6.5) we use the identity $A_0 x^\dagger = y_0$, apply (1.2), (1.3) and obtain

$$\|A_0 x^\dagger - y_\delta\| + \|A_0 \hat{x} - A_h \hat{x}\| \le \delta + h\|\hat{x}\| \le \max\{1, \|\hat{x}\|\}(\delta + h). \tag{6.6}$$

For estimating the sum of the second and third summand in the bracket of (6.5) we use the identity $\hat{y} = \hat{A}\hat{x}$, apply the inequality $a + b \le \sqrt{2}\sqrt{a^2 + b^2}$, the estimate (6.3) and the inequality $\sqrt{a^2 + b^2} \le a + b$ to obtain

$$\begin{aligned} \|\hat{y} - y_\delta\| + \|\hat{y} - A_h \hat{x}\| &\le \|\hat{y} - y_\delta\| + \|\hat{A} - A_h\|\, \|\hat{x}\| \\ &\le \max\{1, \|\hat{x}\|\} \left(\|\hat{y} - y_\delta\| + \|\hat{A} - A_h\| \right) \\ &\le \max\{1, \|\hat{x}\|\} \sqrt{2} \sqrt{\|\hat{y} - y_\delta\|^2 + \|\hat{A} - A_h\|^2} \\ &\le \max\{1, \|\hat{x}\|\} \sqrt{2} \sqrt{\delta^2 + h^2} \\ &\le \max\{1, \|\hat{x}\|\} \sqrt{2}\, (\delta + h)\,. \end{aligned} \tag{6.7}$$

Combining (6.5), (6.6), (6.7) we have

$$\|A_0 \hat{x} - A_0 x^\dagger\| \le \max\{1, \|\hat{x}\|\}(1 + \sqrt{2})(\delta + h). \tag{6.8}$$

Since $\|\hat{x}\| \le \|x^\dagger\| = R$, this estimate and (6.4) provide (6.2). □

6.2. **Error bounds for dual RTLS.**

Theorem 6.2. *Assume that the exact solution $x^\dagger$ of the problem (1.1) satisfies the source condition (6.1) and let $\hat{x}$ be the dual RTLS solution of the problem (1.8). Then,*

$$\|\hat{x} - x^\dagger\| \le 2\|v\|^{1/2}\sqrt{\delta + h\|x^\dagger\|}. \tag{6.9}$$

Proof. Since both $(x^\dagger, y_0, A_0)$ and $(\hat{x}, \hat{y}, \hat{A})$ satisfy the three side conditions $Ax = y$, $\|y - y_\delta\| \le \delta$ and $\|A - A_h\| \le h$ of the dual RTLS problem (1.8), and since $\hat{x}$ is the solution of (1.8) we have

$$\|\hat{x}\|^2 \le \|x^\dagger\|^2, \tag{6.10}$$

or equivalently, $\|\hat{x} - x^\dagger\|^2 \le 2(x^\dagger, x^\dagger - \hat{x})$. Using (6.1) and the Cauchy-Schwarz inequality we obtain

$$\|\hat{x} - x^\dagger\|^2 \le 2(A_0^* v, x^\dagger - \hat{x}) \le 2\|v\|\,\|A_0 x^\dagger - A_0\hat{x}\|. \tag{6.11}$$

From (1.2) we have $\|y_0 - y_\delta\| \le \delta$, and from (1.8) we have $\|\hat{y} - y_\delta\| \le \delta$. Consequently, by triangle inequality and the identity $A_0 x^\dagger = y_0$ we have

$$\|A_0 x^\dagger - \hat{y}\| \le \|y_0 - y_\delta\| + \|\hat{y} - y_\delta\| \le 2\delta. \tag{6.12}$$

From (1.3) we have $\|A_0 - A_h\| \le h$ and from (1.8) we have $\|\hat{A} - A_h\| \le h$. Hence, by triangle inequality, the identity $\hat{y} = \hat{A}\hat{x}$ and estimate (6.10) we have

$$\|\hat{y} - A_0\hat{x}\| \le \left(\|\hat{A} - A_h\| + \|A_0 - A_h\|\right)\|\hat{x}\| \le 2h\|\hat{x}\| \le 2h\|x^\dagger\|. \tag{6.13}$$

We apply again the triangle inequality together with (6.12), (6.13) and obtain

$$\|A_0 x^\dagger - A_0\hat{x}\| \le \|A_0 x^\dagger - \hat{y}\| + \|\hat{y} - A_0\hat{x}\| \le 2\delta + 2h\|x^\dagger\|. \tag{6.14}$$

From this estimate and (6.11) we obtain (6.9). □

7. Error bounds for B ≠ I

In this section our aim is to provide order optimal error bounds in the general case $B \ne I$. These error bounds are not restricted to finite dimensional spaces X and Y but are also valid for infinite dimensional Hilbert spaces. For error bounds in the special case $h = 0$ see [2, 4, 13, 16, 17].

7.1. **Smoothness assumptions.** We formulate our smoothness assumptions in terms of some densely defined unbounded selfadjoint strictly positive operator $B : X \to X$. We introduce a *Hilbert scale* $(X_r)_{r\in\mathbb{R}}$ induced by the operator B, which is the completion of $\cap_{k=0}^{\infty}\mathcal{D}(B^k)$ with respect to the Hilbert space norm $\|x\|_r = \|B^r x\|$, $r \in \mathbb{R}$.

Assumption A1. There exist positive constants m and a such that

$$m\|B^{-a}x\| \le \|A_0 x\| \qquad \text{for all } x \in X.$$

Assumption A2. For some positive constants E and p we assume the *solution smoothness* $x^\dagger = B^{-p}v$ with $v \in X$ and $\|v\| \le E$. That is,

$$x^\dagger \in M_{p,E} = \left\{ x \in X \,\middle|\, \|x\|_p \le E \right\}.$$

Assumption A1, which we will call *link condition* characterizes the smoothing properties of the operator A_0 relative to the operator B^{-1}. Assumption A2 characterizes the smoothness of the unknown solution $x^\dagger$ in the scale $(X_r)_{r\in\mathbb{R}}$. By using A2 we can study different smoothness situations for $x^\dagger$.

7.2. **RTLS.** For deriving error bounds under the assumptions A1 and A2 we will use the argument from the Section 6 combined with the interpolation inequality

$$\|x\|_r \le \|x\|_{-a}^{(s-r)/(s+a)} \|x\|_s^{(a+r)/(s+a)}, \tag{7.1}$$

that holds true for any $r \in [-a, s]$, $a + s \ne 0$, see [9].

Theorem 7.1. *Assume the link condition A1, the smoothness condition A2 with $1 \le p \le 2 + a$, and that the exact solution $x^\dagger$ of the problem (1.1) satisfies the side condition $\|Bx^\dagger\| = R$. Let in addition $\hat{x}$ be the RTLS solution of the problem (1.7), then*

$$\begin{aligned}\|\hat{x} - x^\dagger\| &\le (2E)^{\frac{a}{p+a}} \left(\frac{\max\{1, \|\hat{x}\|\}(1+\sqrt{2})}{m} (\delta + h) \right)^{\frac{p}{p+a}} \\ &= O\left((\delta + h)^{\frac{p}{p+a}} \right).\end{aligned} \tag{7.2}$$

Proof. Since $\|B\hat{x}\| \le R$ and $\|Bx^\dagger\| = R$ we have $\|B\hat{x}\|^2 \le \|Bx^\dagger\|^2$. Consequently, due to Assumption A2,

$$\begin{aligned}\|\hat{x} - x^\dagger\|_1^2 &= (B\hat{x}, B\hat{x}) - 2(B\hat{x}, Bx^\dagger) + (Bx^\dagger, Bx^\dagger) \\ &\le 2(Bx^\dagger, Bx^\dagger) - 2(B\hat{x}, Bx^\dagger) \\ &= 2(B^{2-p}(x^\dagger - \hat{x}), B^p x^\dagger) \\ &\le 2E\|\hat{x} - x^\dagger\|_{2-p}.\end{aligned} \tag{7.3}$$

For estimating $\|\hat{x} - x^\dagger\|_{2-p}$ we use the interpolation inequality (7.1) with $r = 2-p$, $s = 1$, and obtain from (7.3) the estimate

$$\|\hat{x} - x^\dagger\|_1^2 \le 2E \|\hat{x} - x^\dagger\|_{-a}^{(p-1)/(a+1)} \|\hat{x} - x^\dagger\|_1^{(a+2-p)/(a+1)}. \tag{7.4}$$

Rearranging terms in (7.4) gives

$$\|\hat{x} - x^\dagger\|_1 \le (2E)^{(a+1)/(a+p)} \|\hat{x} - x^\dagger\|_{-a}^{(p-1)/(a+p)}. \tag{7.5}$$

From Assumption A1 and estimate (6.8) of the Theorem 6.1 we obtain

$$\|\hat{x} - x^\dagger\|_{-a} \le \frac{\|A_0\hat{x} - A_0 x^\dagger\|}{m} \le \frac{\max\{1, \|\hat{x}\|\}(1+\sqrt{2})(\delta + h)}{m}. \tag{7.6}$$

This estimate and (7.5) provide

$$\|\hat{x} - x^\dagger\|_1 \le (2E)^{(a+1)/(a+p)} \left(\frac{\max\{1, \|\hat{x}\|\}(1+\sqrt{2})(\delta + h)}{m} \right)^{(p-1)/(a+p)}. \tag{7.7}$$

Now the desired estimate (7.2) follows from (7.6), (7.7) and the interpolation inequality (7.1) with $r = 0$ and $s = 1$. □

7.3. **Dual RTLS.** For deriving error bounds under the smoothness assumptions A1 and A2 we will proceed as in the Subsection 7.2.

Theorem 7.2. *Assume the link condition A1 and the smoothness condition A2 with $1 \le p \le 2 + a$, and let $\hat{x}$ be the dual RTLS solution of problem (1.8). Then,*

$$\|\hat{x} - x^\dagger\| \le 2E^{\frac{a}{p+a}} \left(\frac{\delta + h\|x^\dagger\|}{m} \right)^{\frac{p}{p+a}} = O\left((\delta + h)^{\frac{p}{p+a}} \right) . \tag{7.8}$$

Proof. Since both $(x^\dagger, y_0, A_0)$ and $(\hat{x}, \hat{y}, \hat{A})$ satisfy the three side conditions $Ax = y$, $\|y - y_\delta\| \le \delta$ and $\|A - A_h\| \le h$, since $\hat{x}$ is the solution of (1.8) we have $\|B\hat{x}\|^2 \le \|Bx^\dagger\|^2$. It gives us

$$\|\hat{x} - x^\dagger\|_1^2 \le 2E\|\hat{x} - x^\dagger\|_{2-p}. \tag{7.9}$$

From Assumption A1 and the estimate (6.14) of the Theorem 6.2 we obtain

$$\|\hat{x} - x^\dagger\|_{-a} \le \frac{\|A_0\hat{x} - A_0x^\dagger\|}{m} \le \frac{2\delta + 2h\|x^\dagger\|}{m}. \tag{7.10}$$

Now the desired estimate (7.8) can be proven as in the Subsection 7.2, where instead of (7.6) the estimate (7.10) has to be used. □

Let us give some comments. First, we have to mention that Theorem 7.1 requires the assumption $\|Bx^\dagger\| = R$ which means that we have to know the exact magnitude of $\|Bx^\dagger\|$. We do not know if error bounds (7.2) are valid if $\|Bx^\dagger\|$ is not exactly known. Second, we note that both Theorems 7.1 and 7.2 require the assumption $p \ge 1$, that is, the unknown solution has more smoothness than it is introduced into the problems (1.7) and (1.8). There arises the question whether the error bounds of the Theorems 7.1 and 7.2 are valid in the case $p < 1$. We will answer this question in a forthcoming paper and expect that this will be true under the two-sided link condition $m\|B^{-a}x\| \le \|A_0x\| \le M\|B^{-a}x\|$ instead of A1. Third, we mention that the power-type link condition A1 does not allow a study of severely ill-posed problems (1.1) where the operator A_0 is infinitely smoothing and B is finitely smoothing. In such situations the link condition A1 has to be generalized, see [2, 11, 13, 17] for results in the special case $h = 0$. The extension of our error analysis to this more general setup will also be subject of a forthcoming paper.

8. **Numerical experiments**

In the standard form case $B = I$ both RTLS and dual RTLS lead to solving an equation of the form (2.6). The same equation appears in the standard Tikhonov regularization, when data as well as an operator are noisy. So, all these methods differ only in the choice of the regularization parameter α. In the RTLS this choice can be made without a knowledge of the noise levels (h, δ). For the standard Tikhonov regularization such noise level free parameter choice strategies are also possible. Presummably, the most ancient of them is the one termed quasi-optimality. It was proposed in 1965 by Tikhonov and Glasko [19], who suggested to choose from a geometric sequence

$$\Gamma_N^p = \{\alpha_i : \alpha_i = \alpha_0 p^i, \quad i = 1, 2, \ldots, N\}, \quad p > 1,$$

such $\alpha = \alpha_m$ for which the quantity

$$v(\alpha_i) = \|x_{\alpha_i}^{\delta,h} - x_{\alpha_{i-1}}^{\delta,h}\|$$

has the minimum value $v(\alpha_m)$ in the chosen set Γ_N^p. For lack of a knowledge of noise levels, within the framework of quasi-optimality one needs to try a sufficiently large number N of regularization parameter α_i. It means that an equation of the form (2.6) should be solved many times with different α_i.

On the other hand, in RTLS one usually needs to solve only a few such equations prior the Algorithm 1 arrives at the stage 6.

But unlike quasi-optimality, RTLS requires a reliable bound R for the norm $\|x^\dagger\|$ of the unknown solution, and as it will be seen from our numerical experiments below, RTLS is sometimes too sensitive to a misspecification in the value of R.

As to the dual RTLS, it is free from above mentioned drawback of RTLS, and still only a few calls of a solver for equations of the form (2.6) are necessary. At the same time, using dual RTLS one needs to know noise levels.

Following [3] to preform numerical experiments we use test problems from [5]. The first test is based on the function $shaw(n)$ in [5] which is a discretization of a Fredholem integral equation

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} k(s,t)f(t)dt = g(s), \quad s \in [-\frac{\pi}{2}, \frac{\pi}{2}],$$

where the kernel and the solution are given by

$$k(s,t) = (\cos(s) + \cos(t))^2 \left(\frac{\sin(u)}{u}\right)^2, \quad u = \pi(\sin(s) + \sin(t)),$$

$$f(t) = a_1 e^{-c_1(t-t_1)^2} + a_2 e^{-c_2(t-t_2)^2},$$

$$a_1 = 2, \quad a_2 = 1, \quad c_1 = 6, \quad c_2 = 2, \quad t_1 = 0.8, \quad t_2 = -0.5.$$

The kernel and the solution are discretized by simple collocation with $n = 30$ points to produce a matrix A and the vector $x^\dagger$. Then the discrete right-hand side is produced as $y_0 = Ax^\dagger$.

Following [3] the perturbed right-hand side is generated as

$$y_\delta = (A + \sigma\|E\|_F^{-1}E)x^\dagger + \sigma\|e\|_2^{-1}e,$$

where E and e are from a normal distribution with zero mean and unit standard deviation. In all experiments we take $\sigma = 0.1$. We present the results where data errors are in fact between 0.099217 and 0.122227.

To implement the quasi-optimality criterion we take $\alpha_0 = 10^{-3}$, $p = 1.1$, $N = 70$.

In Algorithm 1 solving RTLS problem in the standard form case we take $\varepsilon = 0.8$, $R = 8$. Making such a choice of R we, in fact, overestimate the norm of the exact

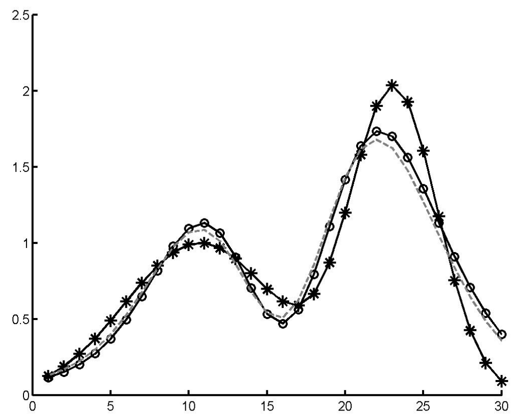

FIGURE 1. The graphs of the exact solution, and approximate solution given by Tikhonov method equipped with the quasi-optimality criterion are labelled respectively by ($\star$) and ($\circ$). The gray dash line is RTLS-solution.

solution $\|x^\dagger\|$. In the presented case the latter one is 5.64. Note also that $R = 8$ meets the condition (2.8), since in considered case $\|x^\dagger_{\delta,h}\| = 7.6705 \cdot 10^7$.

The Algorithm 1 terminates after 5 steps with $\alpha = 0.0683$ that corresponds to a relative error 0.1846. The quasi-optimality criterion suggests the choice of $\alpha = 0.0232$ (in the presented case the optimal choice is $\alpha = 0.0255$). It leads to a relative error 0.1753.

The graphs of corresponding approximate solutions are displayed in Fig.1 together with the exact one. In considered case the Algorithm 3 solving the dual RTLS problem terminates with $\alpha = 0.2208$ and gives a relative error 0.1589.

Thus, all considered methods produce reliable results, but both RTLS algorithms require essentially less computational efforts than the standard Tikhonov regularization equipped with the quasi-optimality criterion.

In the second test we use a discretization of the Fredholm equations

$$\int_0^\pi e^{s\cos t} f(t)dt = 2\frac{\sin s}{s}, \qquad s \in [0, \frac{\pi}{2}],$$

implemented in the function $baart(n)$ in [5]. The solution is given by $f(t) = \sin t$. We use $baart(n)$ with $n = 32$, that gives us a matrix A and the vector y_0. Noisy data are simulated in the same way as in our first test.

At first we implement the Algorithm 1 for RTLS with $R = 1.2$, which is a good approximation for the norm $\|x^\dagger\| = \|\sin(\cdot)\| = \frac{\sqrt{\pi}}{2}$. The algorithm terminates with $\alpha = 0.0016$ and gives a relative error 0.1846. The standard Tikhonov regularization equipped with quasi-optimality criterion gives a relative error 0.2402 for $\alpha = 0.0144$. Corresponding graphs are displayed in Fig.2.

To demonstrate an instability of RTLS-algorithm for this particular example we take $R = 2$, which is still not so far from the real value of $\|x^\dagger\|$. In Fig.3 one

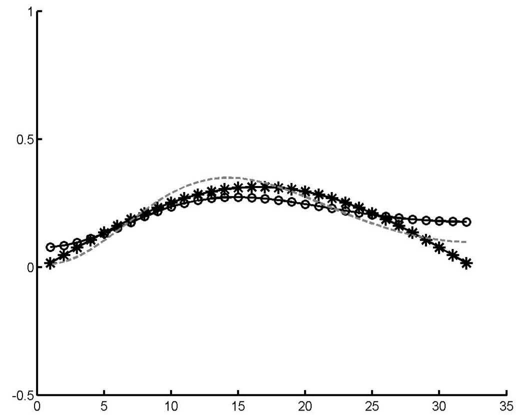

Figure 2. The results of the second experiment. The graphs are labelled as in Fig.1. In RTLS-algorithm $R = 1.2$.

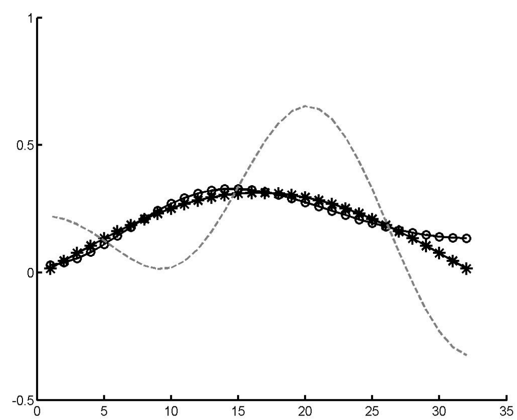

Figure 3. The results of the third test. The graphs are labelled as in Fig.1. In RTLS-algorithm $R = 2$. The relative error of the Tikhonov method equipped with the quasi-optimality criterion is 0.1565, $\alpha = 0.0010$. For RTLS $\alpha = 0.0004969$, and relative error is 0.9826.

can easily see a dramatic change in the behavior of RTLS-approximate solution. A relative error is now 0.9826, and it is obtained for $\alpha = 0.0004969$. In contrast to our first test, we can observe now a non-disarable sensitivity of RTLS-algorithm to a misspecification of a bound R for the norm $\|x^\dagger\|$. It can be explained by the fact that the kernel of the Fredholm equation is now an analytic function, that hints at a severely ill-posedness of considered problem, which was not the case in our first test.

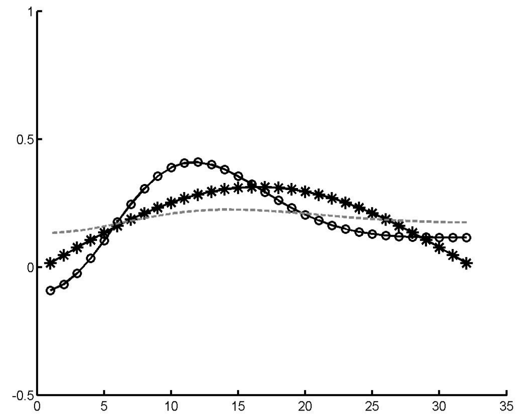

FIGURE 4. The gray dash line is a graph of an approximate solution given by dual RTLS-algorithm. Other lines are labelled as in Fig.1.

At the same time, dual RTLS realized by the Algorithm 3 demonstrates a stable behavior, as it can be seen from Fig.4. Of course, it requires a knowledge of a noise level, which is 0.102796 in considered case. The Algorithm 3 terminates after 4 steps with $\alpha = 0.0822$, and gives a relative error 0.3336.

From our numerical experiments one may make a conclusion that in case of known noise level dual RTLS can be suggested as a method of choice. Without knowledge of a noise level Tikhonov regularization equipped with the quasi-optimality criterion seems to be more reliable than RTLS.

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