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LARGE-SCALE DUAL REGULARIZED TOTAL LEAST SQUARES*

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Dedicated to Lothar Reichel on the occasion of his 60th birthday

Abstract. The total least squares (TLS) method is a successful approach for linear problems when not only the right-hand side but also the system matrix is contaminated by some noise. For ill-posed TLS problems, regularization is necessary to stabilize the computed solution. In this paper we present a new approach for computing an approximate solution of the dual regularized large-scale total least squares problem. An iterative method is proposed which solves a convergent sequence of projected linear systems and thereby builds up a highly suitable search space. The focus is on an efficient implementation with particular emphasis on the reuse of information.

Key words. total least squares, regularization, ill-posedness, generalized eigenproblem

AMS subject classifications. 65F15, 65F22, 65F30

1. Introduction.

Many problems in data estimation are governed by overdetermined linear systems

$$Ax \approx b, \qquad A \in \mathbb{R}^{m\times n},\ b \in \mathbb{R}^m, m \geq n. \tag{1.1}$$

In the classical least squares approach, the system matrix A is assumed to be free of error, and all errors are confined to the observation vector b. However, in engineering application this assumption is often unrealistic. For example, if not only the right-hand side b but A as well are obtained by measurements, then both are contaminated by some noise.

An appropriate approach to this problem is the total least squares (TLS) method, which determines perturbations $\Delta A \in \mathbb{R}^{m\times n}$ to the coefficient matrix and $\Delta b \in \mathbb{R}^m$ to the vector b such that

$$\|[\Delta A, \Delta b]\|_F^2 = \min! \quad \text{subject to } (A + \Delta A)x = b + \Delta b, \tag{1.2}$$

where $\|\cdot\|_F$ denotes the Frobenius norm of a matrix. An overview on total least squares methods and a comprehensive list of references is contained in [25, 30, 31].

The TLS problem (1.2) can be analyzed in terms of the singular value decomposition (SVD) of the augmented matrix $[A, b] = U\Sigma V^T$; cf. [8, 31]. A TLS solution exists if and only if the right singular subspace $\mathcal{V}_{min}$ corresponding to σ_{n+1} contains at least one vector with a nonzero last component. It is unique if $\sigma'_n > \sigma_{n+1}$ where σ'_n denotes the smallest singular value of A, and then it is given by

$$x_{TLS} = -\frac{1}{V(n+1, n+1)} V(1:n, n+1).$$

When solving practical problems, they are usually ill-conditioned, for example the discretization of ill-posed problems such as Fredholm integral equations of the first kind; cf. [4, 9]. Then least squares or total least squares methods for solving (1.1) often yield physically meaningless solutions, and regularization is necessary to stabilize the computed solution.

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To regularize problem (1.2), Fierro, Golub, Hansen, and O'Leary [5] suggested to filter its solution by truncating the small singular values of the TLS matrix $[A, b]$, and they proposed an iterative algorithm based on Lanczos bidiagonalization for computing approximate truncated TLS solutions.

Another well-established approach is to add a quadratic constraint to the problem (1.2) yielding the regularized total least squares (RTLS) problem

$$\|[\Delta A, \Delta b]\|_F^2 = \min! \quad \text{subject to } (A + \Delta A)x = b + \Delta b, \ \|Lx\| \le \delta, \tag{1.3}$$

where $\|\cdot\|$ denotes the Euclidean norm, $\delta > 0$ is the quadratic constraint regularization parameter, and the regularization matrix $L \in \mathbb{R}^{p\times n}$, $p \le n$ defines a (semi-)norm on the solution space, by which the size of the solution is bounded or a certain degree of smoothness can be imposed. Typically, it holds that $\delta < \|Lx_{TLS}\|$ or even $\delta \ll \|Lx_{TLS}\|$, which indicates an active constraint. Stabilization of total least squares problems by introducing a quadratic constraint was extensively studied in [2, 7, 12, 14, 15, 16, 17, 19, 24, 26, 27, 28].

If the regularization matrix L is nonsingular, then the solution x_{RTLS} of the problem (1.3) is attained. For the more general case of a singular L, its existence is guaranteed if

$$\sigma_{min}([AF, b]) < \sigma_{min}(AF), \tag{1.4}$$

where $F \in \mathbb{R}^{n\times k}$ is a matrix the columns of which form an orthonormal basis of the nullspace of L; cf. [1].

Assuming inequality (1.4), it is possible to rewrite problem (1.3) into the more tractable form

$$\frac{\|Ax - b\|^2}{1 + \|x\|^2} = \min! \quad \text{subject to} \quad \|Lx\| \le \delta. \tag{1.5}$$

Related to the RTLS problem is the approach of the dual RTLS that has been introduced and investigated in [22, 24, 29]. The dual RTLS (DRTLS) problem is given by

$$\|Lx\| = \min! \quad \text{subject to} \quad (A + \Delta A)x = b + \Delta b, \ \|\Delta b\| \le h_b, \ \|\Delta A\|_F \le h_A, \tag{1.6}$$

where suitable bounds for the noise levels h_b and h_A are assumed to be known. It was shown in [24] that in case the two constraints $\|\Delta b\| \le h_b$ and $\|\Delta A\|_F \le h_A$ are active, the DRTLS problem (1.6) can be reformulated into

$$\|Lx\| = \min! \quad \text{subject to} \quad \|Ax - b\| = h_b + h_A\|x\|. \tag{1.7}$$

Note that due to the two constraint parameters, h_b and h_A, the solution set of the dual RTLS problem (when varying h_b and h_A) is larger than that one of the RTLS problem with only one constraint parameter δ. For every RTLS problem, there exists a corresponding dual RTLS problem with an identical solution, but this does not hold vice versa.

In this paper we propose an iterative projection method which combines orthogonal projections to a sequence of generalized Krylov subspaces of increasing dimensions and a one-dimensional root-finding method for the iterative solution of the first order optimality conditions of (1.6). Taking advantage of the eigenvalue decomposition of the projected problem, the root-finding can be performed efficiently such that the essential costs of an iteration step are two matrix-vector products. Since usually a very small number of iteration steps is required for convergence, the computational complexity of our method is essentially of the order of a matrix-vector product with the matrix A.

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The paper is organized as follows. In Section 2, basic properties of the dual RTLS problem are summarized, the connection to the RTLS problem is presented, and two methods for solving small-sized problems are investigated. For solving large-scale problems, different approaches based on orthogonal projection are proposed in Section 3. The focus is on the reuse of information when building up well-suited search spaces. Section 4 contains numerical examples demonstrating the efficiency of the presented methods. Concluding remarks can be found in Section 5.

2. Dual regularized total least squares. In Section 2.1, important basic properties of the dual RTLS problem are summarized and connections to related problems are regarded, especially the connection to the RTLS problem (1.3). In Section 2.2, existing methods for solving small-sized dual RTLS problems (1.6) are reviewed, difficulties are discussed, and a refined method is proposed.

2.1. Dual RTLS basics. Literature about dual regularized total least squares (DRTLS) problems is limited, and they are by far less intensely studied than the RTLS problem (1.3). The origin of the DRTLS probably goes back to Golub, who analyzed in [6] the dual regularized least squares problem

$$\|x\| = \min! \quad \text{subject to} \quad \|Ax - b\| = h_b \tag{2.1}$$

assuming an active constraint, i.e., $h_b < \|Ax_{LS} - b\|$ with $x_{LS} = A^{\dagger}b$ being the least squares solution. His results are also valid for the non-standard case $L \neq I$

$$\|Lx\| = \min! \quad \text{subject to} \quad \|Ax - b\| = h_b. \tag{2.2}$$

In [6], an approach with a quadratic eigenvalue problem is presented from which the solution of (2.1) can be obtained. The dual regularized least squares problem (2.2) is exactly the dual RTLS problem with $h_A = 0$, i.e., with no error in the system matrix A. In the following we review some facts about the dual RTLS problem.

THEOREM 2.1 ([23]). *If the two constraints $\|\Delta b\| \leq h_b$ and $\|\Delta A\| \leq h_A$ of the dual RTLS problem (1.6) are active, then its solution $x = x_{DRTLS}$ satisfies the equation*

$$(A^T A + \alpha L^T L + \beta I)x = A^T b \tag{2.3}$$

with the parameters α, β solving

$$\|Ax(\alpha,\beta) - b\| = h_b + h_A\|x(\alpha,\beta)\|, \quad \beta = -\frac{h_A(h_b + h_A\|x(\alpha,\beta)\|)}{\|x(\alpha,\beta)\|}, \tag{2.4}$$

where $x(\alpha,\beta)$ is the solution of (2.3) for fixed α and β.

In this paper we throughout assume active inequality constraints of the dual RTLS problem, and we mainly focus on the first order necessary conditions (2.3) and (2.4).

REMARK 2.2. In [21], a related problem is considered, i.e., the generalized discrepancy principle for Tikhonov regularization. The corresponding problem reads:

$$\|Ax(\alpha) - b\|^2 + \alpha\|Lx(\alpha)\|^2 = \min!$$

with the value of α chosen such that

$$\|Ax(\alpha) - b\| = h_b + h_A\|x(\alpha)\|.$$

Note that this problem is much easier than the dual RTLS problem. A globally convergent algorithm can be found in [21].

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By comparing the solution of the RTLS problem (1.3) and of the dual RTLS problem (1.6) assuming active constraints in either case, some basic differences of the two problems can be revealed: using the RTLS solution x_{RTLS}, the corresponding corrections of the system matrix and the right-hand side are given by

$$\Delta A_{RTLS} = \frac{(b - Ax_{RTLS})x_{RTLS}^T}{1 + \|x_{RTLS}\|^2}\,,$$
$$\Delta b_{RTLS} = \frac{Ax_{RTLS} - b}{1 + \|x_{RTLS}\|^2}\,,$$

whereas the corrections for the dual RTLS problem are given by

$$\Delta A_{DRTLS} = h_A \frac{(b - Ax_{DRTLS})x_{DRTLS}^T}{\|(b - Ax_{DRTLS})x_{DRTLS}^T\|_F}\,,\qquad \Delta b_{DRTLS} = h_b \frac{Ax_{DRTLS} - b}{\|Ax_{DRTLS} - b\|}\,, \tag{2.5}$$

with x_{DRTLS} as the dual RTLS solution. Notice, that the corrections for the system matrices of the two problems are always of rank one. A sufficient condition for identical corrections is given by $x_{DRTLS} = x_{RTLS}$ and

$$h_A = \frac{\|x_{RTLS}\|\|b - Ax_{RTLS}\|}{1 + \|x_{RTLS}\|^2} \quad \text{and} \quad h_b = \frac{\|Ax_{RTLS} - b\|}{1 + \|x_{RTLS}\|^2}. \tag{2.6}$$

In this case the value for β in (2.4) can also be expressed as

$$\beta = -\frac{h_A(h_b + h_A\|x_{RTLS}\|)}{\|x_{RTLS}\|} = -\frac{\|Ax_{RTLS} - b\|^2}{1 + \|x_{RTLS}\|^2}.$$

By the first order conditions, the solution x_{RTLS} of problem (1.3) is a solution of the problem

$$(A^TA + \lambda_I I_n + \lambda_L L^TL)x = A^Tb,$$

where the parameters λ_I and λ_L are given by

$$\lambda_I = -\frac{\|Ax - b\|^2}{1 + \|x\|^2}, \quad \lambda_L = \frac{1}{\delta^2}\left(b^T(b - Ax) - \frac{\|Ax - b\|^2}{1 + \|x\|^2}\right).$$

Identical solutions for the RTLS and the dual RTLS problem can be constructed by using the solution x_{RTLS} of the RTLS problem to determine values for the corrections h_A and h_b as stated in (2.6). This does not hold the other way round, i.e., with the solution x_{DRTLS} of a dual RTLS problem at hand, it is in general not possible to construct a corresponding RTLS problem since the parameter δ cannot be adjusted such that the two parameters of the dual RTLS problem are matched.

2.2. Solving the Dual RTLS problems. Although the formulation (1.7) of the dual RTLS problem looks tractable, this is generally not the case. In [24] suitable algorithms are proposed for special cases of the DRTLS problem, i.e., when $h_A = 0$, $h_b = 0$, or $L = I$, where the DRTLS problem degenerates to an easier problem. In [29] an algorithm for the general case dual RTLS problem formulation, (2.3) and (2.4), is suggested. This idea has been worked out as a special two-parameter fixed-point iteration in [22, 23], where a couple

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of numerical examples can be found. Note that these methods for solving the dual RTLS problem require the solution of a sequence of linear systems of equations, which means that complexity and effort are much higher compared to existing algorithms for solving the related RTLS problem (1.3); cf. [12, 14, 15, 16, 17, 19]. In the following, inconsistencies of the two DRTLS methods are investigated, and a refined method is worked out.

Let us review the DRTLS algorithm from [29] for computing the dual RTLS solution; it will serve as the basis for the methods developed later in this paper.

Algorithm 1 Dual Regularized Total Least Squares Basis Method.

Require: $\varepsilon > 0, A, b, L, h_A, h_b$
1: Choose a starting value $\beta_0 = -h_A^2$
2: **for** $i = 0, 1, \dots$ until convergence **do**
3: Find pair (x_i, α_i) that solves

$$(A^T A + \beta_i I + \alpha_i L^T L)x_i = A^T b, \text{ s.t. } \|Ax_i - b\| = h_b + h_A\|x_i\| \tag{2.7}$$

4: Compute $\beta_{i+1} = -\dfrac{h_A(h_b + h_A\|x_i\|)}{\|x_i\|}$
5: Stop if $|\beta_{i+1} - \beta_i| < \varepsilon$
6: **end for**
7: Determine an approximate dual RTLS solution $x_{DRTLS} = x_i$

The pseudo-code of Algorithm 1 (directly taken from [29]) is not very precise since the solution of (2.7) is nonunique in general and a suitable pair has to be selected. Note that the motivation for Algorithm 1 in [29] is given by the analogy to a similar looking fixed point algorithm for the RTLS problem (1.5) with an efficient implementation to be found in [12, 14, 15, 16, 17].

The method proposed in [22] is based on a model function approach for solving the minimization problem

$$\|Ax(\alpha, \beta) - b\|^2 + \alpha\|Lx(\alpha, \beta)\|^2 + \beta\|x(\alpha, \beta)\|^2 = \min! \tag{2.8}$$

subject to the constraints

$$\|Ax(\alpha, \beta) - b\| = h_b + h_A\|x(\alpha, \beta)\| \quad \text{and} \quad \beta = -h_A^2 - \frac{h_A h_b}{\|x(\alpha, \beta)\|}. \tag{2.9}$$

The corresponding method for solving (2.8) with (2.9) is given below as Algorithm 2; cf. [22]. This approach is shown to work fine for a couple of numerical examples (cf. [22, 23]), but a proof of global convergence is only given for special cases, e.g., for $h_A = 0$. In [20], details about the model function approach for the more general problem of multi-parameter regularization can be found.

The following example shows that Algorithm 2 does not necessarily converge to a solution of the dual RTLS problem (1.6).

EXAMPLE 2.3. Consider the undisturbed problem

$$A_{true} = \begin{bmatrix} 0.5 & -0.5 \\ 1 & 1 \\ 1 & -1 \end{bmatrix}, \; b_{true} = \begin{bmatrix} 0.5 \\ 1 \\ 1 \end{bmatrix} \text{ with solution } x_{true} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

which is nicely scaled since the norm of b_{true} is equal to the norm of a column of A_{true}, and

Algorithm 2 DRTLS Model Function Approach.

Require: $\varepsilon > 0, A, b, L, h_A, h_b$

Choose starting values $\alpha_0 \geq \alpha^*$, $\beta_0 = -h_A^2$
for $i = 0, 1, \dots$ until convergence **do**
  Solve $(A^TA + \beta_i I + \alpha_i L^T L)x_i = A^T b$
  Compute $F_1 = \|Ax_i - b\|^2 + \alpha_i \|Lx_i\|^2 + \beta_i \|x_i\|^2$,
    $F_2 = \|Lx_i\|^2$, $F_3 = \|x_i\|^2$, $D = -(\|b\|^2 - F_1 - \alpha_i F_2)^2 / F_3$,
    $T = (\|b\|^2 - F_1 - \alpha_i F_2)/F_3 - \beta_i$
  Update $\beta_{i+1} = -\dfrac{h_A(h_b + h_A\|x_i\|)}{\|x_i\|}$ and compute
    $N = \|b\|^2 - h_b^2 - \dfrac{2h_A h_b \sqrt{-D}}{T + \beta_{i+1}} + \dfrac{D(T + 2\beta_{i+1} + h_A^2)}{(T + \beta_{i+1})^2}$
  Update $\alpha_{i+1} = 2\alpha_i^2 F_2 / N$
  Stop if $|\alpha_{i+1} - \alpha_i| + |\beta_{i+1} - \beta_i| < \varepsilon$
end for
Solve $(A^TA + \beta_{i+1} I + \alpha_{i+1} L^T L)x_{DRTLS} = A^T b$ for the dual RTLS solution

thus $\sqrt{2}\|b_{true}\| = \|A_{true}\|_F$. Assume the following noise:

$$A_{noise} = \begin{bmatrix} -1/\sqrt{2} & 0 \\ 0 & 0 \\ \sqrt{0.14} & 0 \end{bmatrix}, \; b_{noise} = \begin{bmatrix} 0.4 \\ 0 \\ -0.4 \end{bmatrix}$$

with $\sqrt{2}\|b_{noise}\| = \|A_{noise}\|_F$. Thus, the system matrix and the right-hand side are given by $A = A_{true} + A_{noise}$ and $b = b_{true} + b_{noise}$. The constraints h_A, h_b, and the regularization matrix L are chosen as

$$h_A = \|A_{noise}\|_F = 0.8, \quad h_b = \|b_{noise}\| = 0.8/\sqrt{2}, \quad L = \begin{bmatrix} 2 & 0 \\ 1 & 1 \end{bmatrix}.$$

When applying Algorithm 2 to this example with $\alpha_0 = 100 > \alpha^*$ and $\varepsilon = 10^{-8}$, the following fixed point is reached after 19 iterations

$$x^* = (0.9300, 0.1781)^T \text{ with } \alpha^* = 0, \; \beta^* = -1.1179, \; \|Lx^*\| = 2.1650.$$

The initial value $\alpha_0 = 100$ seems to be unnecessarily far away from the limit α^*. Note that for an initial value of $\alpha_0 = 2 > \alpha^*$, the same fixed point is reached after 28 iterations. Then the constraint condition (2.9) is not satisfied, $\|Ax^* - b\| - (h_b + h_A\|x^*\|) = -0.0356 \neq 0$, and therefore this fixed point is not the solution of the dual RTLS problem.

The solution of this example is given by

$$x_{DRTLS} = (0.7353, 0.0597)^T \text{ with } \alpha_{DRTLS} = 0.1125, \; \beta_{DRTLS} = -1.2534,$$

with $\|Lx_{DRTLS}\| = 1.6718 < \|Lx^*\|$ and $\|Ax_{DRTLS} - b\| - (h_b + h_A\|x_{DRTLS}\|) = 0$. Note that for an initial value of $\alpha_0 = 1$, this solution is reached after 65 iterations.

Example 2.3 shows that Algorithm 2 is not guaranteed to converge to the dual RTLS solution. Hence, in the following we will focus on Algorithm 1. The main difficulty of Algorithm 1 is the constraint condition in (2.7), i.e., $\|Ax - b\| = h_b + h_A\|x\|$. The task to find a pair (x, α) for a given value of β such that

$$(A^TA + \beta I + \alpha L^T L)x = A^T b, \text{ s.t. } \|Ax - b\| = h_b + h_A\|x\|$$

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can have a unique solution, more than one solution, or no solution. In the following we try to shed some light on this problem.

Let us introduce the function

$$g(\alpha;\beta) := \|Ax(\alpha)-b\| - h_b - h_A\|x(\alpha)\| \quad \text{with} \quad x(\alpha) = (A^TA+\beta I+\alpha L^TL)^{-1}A^Tb$$

for a given fixed value of β. In analogy to the solution of RTLS problems, we are looking for the rightmost non-negative root of g, i.e., the largest $\alpha \geq 0$; cf. [12, 14, 16, 28]. A suitable tool for the investigation of g is the generalized eigenvalue problem (GEVP) of the matrix pair $(A^TA+\beta I, L^TL)$. It is assumed that the regularization matrix L has full rank n, hence the GEVP is definite. Otherwise, a spectral decomposition of L^TL could be employed to reduce the GEVP to the range of L; this case is not worked out here.

LEMMA 2.4. *Let* $[V, D] = \texttt{eig}(A^TA+\beta I, L^TL)$ *be the spectral decomposition of the matrix pencil* $(A^TA+\beta I, L^TL)$ *with* $V^T(A^TA+\beta I)V = D =: diag\{d_1,\dots d_n\}$ *and* $V^TL^TLV = I$*, and let* $c := V^TA^Tb$*.*
Then $g(\cdot) := g(\cdot;\beta) : \mathbb{R}_+ \to \mathbb{R}$ *has the following properties:*

(i) *g is a rational function, the only poles of which are the negative eigenvalues* d_k *with* $c_k \neq 0$*.*
(ii) $\lim_{\alpha\to\infty} g(\alpha) = \|b\| - h_b$*.*
(iii) *Let* d_k *be a simple negative eigenvalue with* $c_k \neq 0$ *and let* v_k *be a corresponding eigenvector. If* $\|Av_k\| < h_A\|v_k\|$*, then* $\lim_{\alpha\to -d_k} = -\infty$*, and if* $\|Av_k\| > h_A\|v_k\|$*, then* $\lim_{\alpha\to -d_k} = \infty$*.*

Proof. The spectral decomposition of $(A^TA+\beta I, L^TL)$ yields

$$A^TA+\beta I+\alpha L^TL = V^{-T}(D+\alpha I)V^{-1}.$$

Hence,

$$\begin{aligned} x(\alpha) &= (A^TA+\beta I+\alpha L^TL)^{-1}A^Tb = V(D+\alpha I)^{-1}V^TA^Tb \\ &= V\,\text{diag}\left\{\frac{1}{d_i+\alpha}\right\}c \end{aligned} \tag{2.10}$$

with $c = V^TA^Tb$, which immediately yields statement (i) and $\lim_{\alpha\to\infty} x(\alpha) = 0$, from which we get (ii).

If d_k is a simple eigenvalue with $c_k \neq 0$ and v_k a corresponding eigenvector, then

$$\lim_{\alpha\to -d_k}\left(\frac{d_k+\alpha}{c_k}x(\alpha) - v_k\right) = 0,$$

and therefore

$$g(\alpha) \approx f(\alpha)(\|Av_k\| - h_A\|v_k\|) \quad \text{with } f(\alpha) = |c_k/(d_k+\alpha)|$$

holds for $\alpha \neq -d_k$ sufficiently close to $-d_k$, which proves statement (iii). □

From Lemma 2.4 we obtain the following results about the roots of g. We assume that $\|b\| - h_b > 0$, which applies for reasonably posed problems. If $g(0) < 0$, then it follows (independently of the presence of poles) from (i) and (iii) that g has at least one positive root, and if $g(0) > 0$ and a simple negative eigenvalue d_k exists with non-vanishing c_k and $\|Av_k\| < h_A\|v_k\|$, then the function g has at least two positive roots. Otherwise, it may happen that g is positive on $\mathbb{R}_+$ and has no root in $\mathbb{R}_+$.

Since the function $g(\alpha;\beta)$ is not guaranteed to have a root, it appears suitable to replace the constraint condition in (2.7) by a corresponding minimization of

$$g(\alpha;\beta) := \|Ax-b\| - h_b - h_A\|x\| \quad \text{in } \mathbb{R}_+,$$

Algorithm 3 Dual Regularized Total Least Squares Method.

Require: $\varepsilon > 0, A, b, L, h_A, h_b$
1: Choose a starting value $\beta_0 = -h_A^2$
2: **for** $i = 0, 1, \dots$ until convergence **do**
3: Find pair (x_i, α_i) for the rightmost $\alpha_i \geq 0$ that solves

$$(A^TA + \beta_i I + \alpha_i L^TL)x_i = A^Tb, \text{ s.t. } \min! = |g(\alpha_i; \beta_i)| \tag{2.11}$$

4: Compute $\beta_{i+1} = -\dfrac{h_A(h_b + h_A\|x_i\|)}{\|x_i\|}$
5: Stop if $|\beta_{i+1} - \beta_i| < \varepsilon$
6: **end for**
7: Determine an approximate dual RTLS solution $x_{DRTLS} = x_i$

yielding the revised Algorithm 3.

REMARK 2.5. If a simple negative leftmost eigenvalue d_n exists with non-vanishing component c_n and $\|Av_n\| < h_A\|v_n\|$, then it is sufficient to restrict the root-finding of $g(\alpha)$ to the interval $(-d_n, \infty)$, which contains the rightmost root of g.

REMARK 2.6. A note on the idea to extend the domain of the function $g(\alpha)$ to negative values of α, i.e., to eventually keep the root-finding instead of the minimization constraint in equation (2.11). Unfortunately, it is of no principle remedy to allow negative values of α. The limit of g for $\alpha \to -\infty$ is identical to that for $\alpha \to \infty$, i.e., $g(\alpha)|_{\alpha\to-\infty} = \|b\| - h_b > 0$. Hence, it may happen that after extending the function $g(\alpha)$ to $\mathbb{R} \to \mathbb{R}$, only poles are present with $\|Av_i\| > h_A\|v_i\|, i = 1, \dots, n$ and thus still no root of g may exist. Notice that α should be positive at the dual RTLS solution in case of active constraints.

REMARK 2.7. Note that the quantity $\|Lx\|$ which is to be minimized in the dual RTLS problem is not necessarily monotonic. Non-monotonic behavior may occur for the iterations of Algorithm 3, i.e., for $\|Lx_i\|, i = 0, 1, \dots$, as well as for the function $\|Lx(\alpha)\|$ within an iteration with a fixed value of β and $x(\alpha) = (A^TA + \beta I + \alpha L^TL)^{-1}A^Tb$. This is in contrast to the quantity $f(x)$ for RTLS problems; cf. [14, 16].

Let us apply Algorithm 3 to Example 2.3. The function $g(\alpha; \beta_0)$ is shown in Figure 2.1 for the starting value of $\beta_0 = -h_A^2 = -0.64$. For the limit as $\alpha \to \infty$, it holds that $g(\alpha)|_{\alpha\to\infty} = \|b\| - h_b = 0.9074$, and for $\alpha \to 0$ we have $g(0) = 0.0017$. The eigenvalues of the matrix $(A^TA + \beta_0 I)$ are positive and so are the eigenvalues of the matrix pair $(A^TA + \beta_0 I, L^TL)$. Hence, no poles exist for positive values of α. Furthermore, in this example no positive root exists. There do exist negative roots, i.e., the rightmost negative root is located at $\alpha = -0.0024$, but this is not considered any further; cf. Remark 2.6. Thus, in the first iteration of Algorithm 3, the pair $(x_0, \alpha_0) = ([0.7257, 0.0909]^T, 0)$ is selected as the minimizer of $|g(\alpha; -h_A^2)|$ for all non-negative values of α. In the following iterations, the function $g(\alpha, \beta_i), i = 1, \dots$ always has a unique positive root. Machine precision 2^{-52} is reached after 5 iterations of Algorithm 3. The method of choice to find the rightmost root or to find the minimizer of $|g(\alpha)|$, respectively, is discussed in Section 3. Up to now, any one-dimensional minimization method suffices to solve an iteration of a small-sized dual regularized total least squares problem.

REMARK 2.8. Another interesting approach for obtaining an approximation of the dual RTLS solution is to treat the constraints $h_A = \|\Delta A\|_F$ and $h_b = \|\Delta b\|$ separately. In the first stage, the value h_A can be used to make the system matrix A better conditioned, e.g., by a shifted SVD, truncated SVD, shifted normal equations, or most promising for large-scale problems by a truncated bidiagonalization of A. In the second stage, the resulting problem

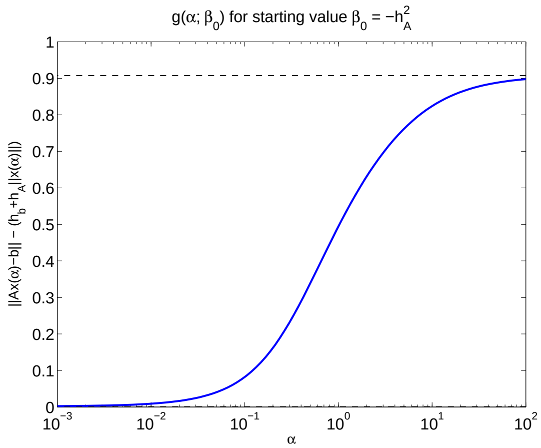

FIGURE 2.1. *Initial function* $g(\alpha;\beta_0)$ *for Example 2.3.*

has to be solved, i.e., a Tikhonov least squares problem using h_b as discrepancy principle. This means that with the corrected matrix $\hat{A} = A + \Delta\hat{A}$, the following problem has to be solved

$$\|Lx\| = \min! \quad \text{subject to} \quad \|\hat{A}x - b\| = h_b.$$

The first order optimality conditions can be obtained from the derivative of the Lagrangian

$$\mathcal{L}(x,\mu) = \|Lx\|^2 + \mu(\|\hat{A}x - b\|^2 - h_b^2).$$

Setting the derivative equal to zero yields

$$(\hat{A}^T\hat{A} + \mu^{-1}L^TL)x = \hat{A}^Tb \quad \text{subject to} \quad \|\hat{A}x - b\| = \|\Delta\hat{b}\| = h_b,$$

which is just the problem of determining the correct value μ for the Tikhonov least squares problem such that the discrepancy principle holds with equality. Hence, a function

$$f(\mu) = \|\hat{A}x_\mu - b\|^2 - h_b^2 \quad \text{with} \quad x_\mu := (\hat{A}^T\hat{A} + \mu^{-1}L^TL)^{-1}\hat{A}^Tb$$

can be introduced, where its root $\bar{\mu}$ determines the solution $x_{\bar{\mu}}$; cf. [13]. A root exists if

$$\|\mathcal{P}_{\mathcal{N}(\hat{A}^T)}b\| = \|\hat{A}x_{LS} - b\| < h_b < \|b\| \quad \text{with} \quad x_{LS} = \hat{A}^\dagger b.$$

Note, that this condition here does not hold automatically, which may lead to difficulties. Another weak point of this approach is that none of the proposed variants in the first stage uses corrections $\Delta\hat{A}$ of small rank although the solution dual RTLS correction matrix is of rank one; see equation (2.5).

3. Solving large DRTLS problems. When solving large-scale problems, it is prohibitive to solve a large number of huge linear systems. A natural approach would be to project the linear system in equation (2.11) in line 3 of Algorithm 3 onto search spaces of much smaller dimensions and then only to work with the projected problems. In this paper we propose an iterative projection method that computes an approximate solution of (2.11) in a generalized Krylov subspace $\mathcal{V}$, which is then used to solve the corresponding restricted minimization problem $\min! = |g_V(\alpha_i;\beta_i)|$ with $g_V(\alpha;\beta) := \|AVy - b\| - h_b - h_A\|Vy\|$ and

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where the columns of V form an orthonormal basis of $\mathcal{V}$. For the use of generalized Krylov subspaces in related problems, see [13, 18]. The minimization of $|g_V(\alpha;\beta)|$ is in almost all practical cases equal to the determination of the rightmost root of $g_V(\alpha;\beta)$. Therefore in the following, only root-finding methods are considered for solving the minimization constraint. The root can be computed, e.g., by bracketing algorithms that enclose the rightmost root, and it turned out to be beneficial to use rational inverse interpolation; see [15, 17]. Having determined the root α_i for a value of β_i, a new value β_{i+1} is calculated. These inner iterations are carried out until the projected dual RTLS problem is solved. Only then is the search space $\mathcal{V}$ expanded by the residual of the original linear system (2.11). After expansion, a new projected DRTLS problem has to be solved, i.e., zero-finding and updating of β is repeated until convergence. The outer subspace enlargement iterations are performed until α, β, or $x(\beta) = Vy(\beta)$ satisfy a stopping criterion. Since the expansion direction depends on the parameter α, the search space $\mathcal{V}$ is not a Krylov subspace. Numerical examples illustrate that the stopping criterion typically is satisfied for search spaces $\mathcal{V}$ of fairly small dimension.

The cost of enlarging the dimension of the search space by one is of the order of $\mathcal{O}(mn)$ arithmetic floating point operations and so is the multiplication of a vector by the matrix $(A^TA + \beta I + \alpha L^TL)$. This cost is higher than the determination of the dual RTLS solution of a projected problem. We therefore solve the complete projected DRTLS problem after each increase of $\dim(\mathcal{V})$ by one. The resulting method is given in Algorithm 4.

Algorithm 4 Generalized Krylov Subspace Dual RTLS Method.

Require: $\varepsilon > 0, A, b, L, h_A, h_b$ and initial basis V_0, $V_0^TV_0 = I$

1: Choose a starting value $\beta_0^0 = -h_A^2$
2: **for** $j = 0, 1, \dots$ until convergence **do**
3: **for** $i = 0, 1, \dots$ until convergence **do**
4: Find pair $(y(\beta_i^j), \alpha_i^j)$ for rightmost $\alpha_i^j \geq 0$ that solves

$$V_j^T(A^TA + \beta_i^j I + \alpha_i^j L^TL)V_j y(\beta_i^j) = V_j^T A^T b, \text{ s.t. } \min! = |g_{V_j}(\alpha_i^j;\beta_i^j)| \tag{3.1}$$

5: Compute $\beta_{i+1}^j = -\dfrac{h_A(h_b + h_A\|y(\beta_i^j)\|)}{\|y(\beta_i^j)\|}$
6: Stop if $|\beta_{i+1}^j - \beta_i^j|/|\beta_i^j| < \varepsilon$
7: **end for**
8: Compute $r^j = (A^TA + \beta_i^j I + \alpha_i^j L^TL)V_j y(\beta_i^j) - A^Tb$
9: Compute $\hat{r}^j = M^{-1}r^j$ (where M is a preconditioner)
10: Orthogonalize $\tilde{r}^j = (I - V_jV_j^T)\hat{r}^j$
11: Normalize $v_{\text{new}} = \tilde{r}^j/\|\tilde{r}^j\|$
12: Enlarge search space $V_{j+1} = [V_j, v_{\text{new}}]$
13: **end for**
14: Determine an approximate dual RTLS solution $x_{DRTLS} = V_j y(\beta_i^j)$

Algorithm 4 iteratively adjusts the parameters α and β and builds up a search space simultaneously. Generally, "convergence" is achieved already for search spaces of fairly small dimension; see Section 4. Most of the computational work is done in line 8 for computing the residual since solving the projected dual RTLS problem in lines 3–7 is comparably inexpensive.

We can use several convergence criteria in line 2:

- Stagnation of the sequence $\{\beta^j\}$: the relative change of two consecutive values β^j at the solution of the corresponding dual RTLS problems is small, i.e., $|\beta^{j+1} - \beta^j|/|\beta^j|$ is smaller than a given tolerance.

- Stagnation of the sequence $\{\alpha^j\}$: the relative change of two consecutive values α^j at the solution of the corresponding dual RTLS problems is small, i.e., $|\alpha^{j+1} - \alpha^j|/|\alpha^j|$ is smaller than a given tolerance.
- The relative change of two consecutive Ritz vectors $x(\beta^j) = V_j y(\beta^j)$ at the solution of a projected DRTLS problems is small, i.e., $\|x(\beta^{j+1}) - x(\beta^j)\|/\|x(\beta^j)\|$ is smaller than a given tolerance.
- The absolute values of the last s elements of the vector $y(\beta^j)$ at the solution of a projected DRTLS problem are several orders of magnitude smaller than the first t elements, i.e., a recent increase of the search space does not affect the computed solution significantly.
- The residual r^j from line 8 is sufficiently small, i.e., $\|r^j\|/\|A^T b\|$ is smaller than a given tolerance.

We now discuss how to efficiently determine an approximate solution of the large-scale dual RTLS problem (1.6) with Algorithm 4. For large-scale problems, matrix valued operations are prohibitive, thus our aim is to carry out the algorithm with a computational complexity of $\mathcal{O}(mn)$, i.e., of the order of a matrix-vector product (MatVec) with a (general) dense matrix $A \in \mathbb{R}^{m \times n}$.

- The algorithm can be used with or without preconditioner. If no preconditioner is to be used, then $M = I$ and line 9 can be neglected. When a preconditioner is used, it is suggested to choose $M = L^T L$ if $M > 0$ and L is sparse, and otherwise to employ a positive definite sparse approximation $M \approx L^T L$. For solving systems with M, a Cholesky decomposition has to be computed once. The cost of this decomposition is less than $\mathcal{O}(mn)$, which includes the solution of the subsequent system with the matrix M.
- A suitable starting basis V_0 is an orthonormal basis of small dimension (e.g. $\ell = 5$) of the Krylov space $\mathcal{K}_\ell\left(M^{-1}A^T A, M^{-1}A^T b\right)$.
- The main computational cost of Algorithm 4 consists in building up the search space $\mathcal{V}_j$ of dimension $\ell + j$ with $\mathcal{V}_j := span\{V_j\}$. If we assume A to be unstructured and L to be sparse, the costs for determining V_j are roughly $2(\ell + j) - 1$ matrix-vector multiplications with A, i.e., one MatVec for $A^T b$ and $\ell + j - 1$ MatVecs with A and A^T, respectively. If L is dense, the costs roughly double.
- An outer iteration is started with the previously determined value of β from the last iteration, i.e., $\beta_0^{j+1} := \beta_i^j, j = 0, 1, \ldots$.
- When the matrices $V_j, AV_j, A^T AV_j, L^T LV_j$ are stored and one column is appended at each iteration, no additional MatVecs have to be performed.
- With $y = (V_j^T (A^T A + \beta_i^j I + \alpha L^T L) V_j)^{-1} V_j^T A^T b$ and the matrix $V_j \in \mathbb{R}^{n \times (\ell + j)}$ having orthonormal columns, we get $g_{V_j}(\alpha; \beta_i) = \|AV_j y - b\| - h_b - h_A \|y\|$.
- Instead of solving the projected linear system (3.1) several times, it is sufficient to solve the eigenproblem of the projected pencil $(V_j^T (A^T A + \beta_i^j I) V_j, V_j^T L^T L V_j)$ once for every β_i^j, which then can be used to obtain an analytic expression for $y(\alpha) = (V_j^T (A^T A + \beta_i^j I + \alpha L^T L) V_j)^{-1} V_j^T A^T b$; cf. equations (2.10) and (3.2). This enables efficient root-finding algorithms for $|g_{V_j}(\alpha_i^j; \beta_i^j)|$.
- With the vector $y^j = y(\beta_i^j)$, the residual in line 8 can be written as

$$r^j = A^T AV_j y^j + \alpha_i^j L^T LV_j y^j + \beta_i^j x(\beta_i^j) - A^T b.$$

Note that in exact arithmetic the direction $\bar{r} = A^T AV_j y^j + \alpha_i^j L^T LV_j y^j + \beta_i^j x(\beta_i^j)$ leads to the same new expansion of v_{new}.

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- For a moderate number of outer iterations $j \ll n$, the overall cost of Algorithm 4 is of the order $\mathcal{O}(mn)$.

The expansion direction of the search space in iteration j depends on the current values of α_i^j, β_i^j; see line 8. Since both parameters are not constant throughout the algorithm, the search space is not a Krylov space but a generalized Krylov space; cf. [13, 18].

A few words concerning the preconditioner. Most examples in Section 4 show that Algorithm 4 gives reasonable approximations to the solution x_{DRTLS} also without preconditioner but that it is not possible to obtain a high accuracy with a moderate size of the search space. In [18] the preconditioner $M = L^T L$ or an approximation $M \approx L^T L$ has been successfully applied for solving the related Tikhonov RTLS problem, and in [15, 17] a similar preconditioner has been employed for solving the eigenproblem occurring in the RTLSEVP method of [26]. For Algorithm 4 with preconditioner, convergence is typically achieved after a fairly small number of iterations.

3.1. Zero-finding methods. For practical problems, the minimization constraint condition in (3.1) almost always reduces to the determination of the rightmost root of $g_{V_j}(\alpha; \beta_i^j)$. Thus, in this paper we focus on the use of efficient zero-finders, which only use a cheap evaluation of the constraint condition for a given pair $(y(\beta_i^j), \alpha)$. As introduced in Section 2.2, it is beneficial for the investigation of $g_{V_j}(\alpha; \beta_i^j)$ to compute the corresponding eigendecomposition of the projected problem. It is assumed that the projected regularization matrix $V_j^T L^T L V_j$ is of full rank, which directly follows from the full rank assumption of $L^T L$, but this may even hold for singular $L^T L$. An explicit expression for $y(\alpha)$ can be derived analogously to the expression for $x(\alpha)$ in equation (2.10). With the decomposition $[W, D] = \texttt{eig}(V_j^T A^T A V_j + \beta_i^j I, V_j^T L^T L V_j) = \texttt{eig}(V_j^T (A^T A + \beta_i^j I, L^T L) V_j)$ of the projected problem, the following relations for the eigenvector matrix W and the corresponding eigenvalue matrix D hold. With $W^T V_j^T L^T L V_j W = I$ and $W^T V_j^T (A^T A + \beta_i^j I) V_j W = D$, the matrix $V_j^T (A^T A + \beta_i^j I + \alpha L^T L) V_j$ can be expressed as $W^{-T}(D + \alpha I) W^{-1}$. Hence,

$$
\begin{aligned}
y(\alpha; \beta_i^j) &= \left(V_j^T (A^T A + \beta_i^j I + \alpha L^T L) V_j \right)^{-1} V_j^T A^T b \\
&= W (D + \alpha I)^{-1} W^T V_j^T A^T b = W \operatorname{diag}\left\{ \frac{1}{d_i + \alpha} \right\} c
\end{aligned}
\tag{3.2}
$$

with $c = W^T V_j^T A^T b$ and $V \in \mathbb{R}^{n \times (\ell + j)}$. For the function $g_{V_j}(\alpha; \beta_i^j)$, the characterization regarding poles and zeros as stated in Section 2.2 for $g(\alpha; \beta)$ holds accordingly. So, after determining the eigenvalue decomposition in an inner iteration for an updated value of β_i^j, all evaluations of the constraint condition are then available at almost no cost.

We are in a position to discuss the design of efficient zero-finders. Newton's method is an obvious candidate. This method works well if a fairly accurate initial approximation of the rightmost zero is known. However, if our initial approximation is larger than and not very close to the desired zero, then the first Newton step is likely to give a worse approximation of the zero than the initial approximation; see Figure 4.1 for a typical plot of $g(\alpha)$. The function g is flat for large values of $\alpha > 0$ and may contain several poles.

Let us review some facts about poles and zeros of $g_V(\alpha) := g_{V_j}(\alpha; \beta_i^j)$ that can be exploited for zero-finding methods; cf. also Lemma 2.4. The limit as $\alpha \to \infty$ is given by $g_V(\alpha)|_{\alpha \to \infty} = \|b\| - h_b$, which is equal to the limit of the original function $g(\alpha)$ and should be positive for a reasonably posed problem where the correction of b is assumed to be smaller than the norm of the right-hand side itself. Assuming simple eigenvalues and the ordering $d_1 > \cdots > d_{m-1} > 0 > d_m > \cdots > d_{\ell+j}$, the shape of g_V can be characterized as follows

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- If no negative eigenvalue occurs, $g_V(\alpha)$ has no poles for $\alpha > 0$ and nothing can be exploited.
- For every negative eigenvalue $d_k, k = m, \dots, \ell + j$, with w_k the corresponding eigenvector, the expression $\|AV_j w_k\| - h_A\|w_k\|$ can be evaluated, i.e., the kth column of the eigenvector matrix $W \in \mathbb{R}^{(\ell+j)\times(\ell+j)}$. If $c_k \neq 0$ with c_k the kth component of the vector $c = W^T V_j^T A^T b$ and if $\|AV_j w_k\| - h_A\|w_k\| > 0$, then the function $g_V(\alpha)$ has a pole at $\alpha = -d_k$ with $\lim_{\alpha\to -d_k} g_V(\alpha) = +\infty$. If $\|AV_j w_k\| - h_A\|w_k\| < 0$ with $c_k \neq 0$, then $g_V(\alpha)$ has a pole at $\alpha = -d_k$ with $\lim_{\alpha\to -d_k} g_V(\alpha) = -\infty$.
- The most frequent case in practical problems is the occurrence of a negative smallest eigenvalue $d_{\ell+j} < 0$ with a non-vanishing component $c_{\ell+j}$ such that $\|AV_j w_{\ell+j}\| < h_A\|w_{\ell+j}\|$. Then it is sufficient to restrict the root-finding to the interval $(-d_{\ell+j}, \infty)$ which contains the rightmost root. This information can directly be exploited in a bracketing zero-finding algorithm.
- Otherwise, the smallest negative eigenvalue corresponding to the rightmost pole of $g_V(\alpha)$ with $\lim_{\alpha\to -d_k} g_V(\alpha) = -\infty$ is determined, i.e., the smallest eigenvalue $d_k, k = m, \dots, \ell + j$ for which $c_k \neq 0$ and $\|AV_j w_k\| < h_A\|w_k\|$. This rightmost pole is then used as a lower bound for a bracketing zero-finder, i.e., the interval is restricted to $(-d_k, \infty)$.

In this paper two suitable bracketing zero-finding methods are suggested. As a standard bracketing algorithm for determining the root in the interval $(-d_{\ell+j}, \infty)$, $(-d_k, \infty)$, or $[0, \infty)$, the King method is chosen; cf. [11]. The King method is an improved version of the Pegasus method, such that after each secant step, a modified step has to follow.

In a second bracketing zero-finder, a suitable model function for g_V is used; cf. also [13, 15, 17]. Since the behavior at the rightmost root is not influenced much by the rightmost pole but much more by the asymptotic behavior of g_V as $\alpha \to \infty$, it is reasonable to incorporate this knowledge. Thus, we derive a zero-finder based on rational inverse interpolation, which takes this behavior into account. Consider the model function for the inverse of $g_V(\alpha)$,

$$g_V^{-1} \approx h(g) = \frac{p(g)}{g - g_\infty} \quad \text{with a polynomial} \quad p(g) = \sum_{i=0}^{k-1} a_i g^i, \tag{3.3}$$

where $g_\infty = \|b\| - h_b$ independently of the search space $\mathcal{V}$. The degree of the polynomial can be chosen depending on the information of g_V that is to be used in each step. We propose to use three function values, i.e., $k = 3$. This choice yields a small linear systems of equations with a $k \times k$ matrix that have to be solved in each step.

Let us consider the use of three pairs $\{\alpha^i, g_V(\alpha^i)\}$, $i = 1, 2, 3$; see also [15]. Assume that the following inequalities are satisfied,

$$\alpha^1 < \alpha^2 < \alpha^3 \quad \text{and} \quad g_V(\alpha^1) < 0 < g_V(\alpha^3). \tag{3.4}$$

Otherwise we renumber the values α^i so that (3.4) holds.

If g_V is strictly monotonically increasing in $[\alpha^1, \alpha^3]$, then (3.3) is a rational interpolant of $g_V^{-1} : [g_V(\alpha^1), g_V(\alpha^3)] \to \mathbb{R}$. Our next iterate is $\alpha_{\text{new}} = h(0)$, where the polynomial $p(g)$ is of degree 2. The coefficients a_0, a_1, a_2 are computed by solving the equations $h(g_V(\alpha^i)) = \alpha^i$, $i = 1, 2, 3$, which we formulate as a linear system of equations with a 3×3 matrix. In exact arithmetic, $\alpha_{\text{new}} \in (\alpha^1, \alpha^3)$, and we replace α^1 or α^3 by α_{new} so that the new triplet satisfies (3.4).

Due to round-off errors or possible non monotonic behavior of g, the computed value α_{new} might not be contained in the interval (α^1, α^3). In this case we carry out a bisection step, so that the interval is guaranteed to still contain the zero. If we have two positive values $g_V(\alpha^i)$, then we let $\alpha^3 = (\alpha^1 + \alpha^2)/2$; in the case of two negative values $g_V(\alpha^i)$, we let $\alpha^1 = (\alpha^2 + \alpha^3)/2$.

4. Numerical examples. To evaluate the performance of Algorithm 4, we use large-dimensional test examples from Hansen's *Regularization Tools*; cf. [10]. Most of the problems in this package are discretizations of Fredholm integral equations of the first kind, which are typically very ill-conditioned.

The MATLAB routines `baart`, `shaw`, `deriv2`(1), `deriv2`(2), `deriv2`(3), `ilaplace`(2), `ilaplace`(3), `heat`$(\kappa = 1)$, `heat`$(\kappa = 5)$, `phillips`, and `blur` provide square matrices $A_{true} \in \mathbb{R}^{n \times n}$, right-hand sides b_{true}, and true solutions x_{true}, with $A_{true} x_{true} = b_{true}$. In all cases, the matrices A_{true} and $[A_{true}, b_{true}]$ are ill-conditioned. The parameter κ for problem `heat` controls the degree of ill-posedness of the kernel: $\kappa = 1$ yields a severely ill-conditioned and $\kappa = 5$ a mildly ill-conditioned problem. The number in brackets for `deriv2` and `ilaplace` specifies the shape of the true solution, e.g., for `deriv2`, the '2' corresponds to a true continuous solution which is exponential while '3' corresponds to a piecewise linear one. The right-hand side is modified correspondingly.

To construct a suitable dual RTLS problem, the norm of the right hand side b_{true} is scaled such that $\sqrt{n}\|b_{true}\| = \|A_{true}\|_F$, and x_{true} is then scaled by the same factor.

The noise added to the problem is put in relation to the norm of A_{true} and b_{true}, respectively. Adding a white noise vector $e \in \mathbb{R}^n$ to b_{true} and a matrix $E \in \mathbb{R}^{n \times n}$ to A_{true} yields the error-contaminated problem $\bar{A}x \approx \bar{b}$ with $\bar{b} = b_{true} + e$ and $\bar{A} = A_{true} + E$. We refer to the quotient

$$\sigma := \frac{\|[E, e]\|_F}{\|[A_{true}, b_{true}]\|_F} = \frac{\|E\|_F}{\|A_{true}\|_F} = \frac{\|e\|}{\|b_{true}\|}$$

as the *noise level*. In the examples, we consider the noise levels $\sigma = 10^{-2}$ and $\sigma = 10^{-3}$.

To adapt the problem to an overdetermined linear system of equations, we stack two error-contaminated matrices and right-hand sides (with different noise realizations), i.e.,

$$A = \begin{bmatrix} \bar{A}_1 \\ \bar{A}_2 \end{bmatrix}, \qquad b = \begin{bmatrix} \bar{b}_1 \\ \bar{b}_2 \end{bmatrix},$$

with the resulting matrix $A \in \mathbb{R}^{2n \times n}$ and $b \in \mathbb{R}^{2n}$. Stacked problems of this kind arise when two measurements of the system matrix and right-hand side are available, which is, e.g., the case for some types of magnetic resonance imaging problems.

Suitable values of constraint parameters are given by $h_A = \gamma\|E\|_F$ and $h_b = \gamma\|e\|$ with $\gamma \in [0.8, 1.2]$.

For the small-scale example, the model function approach of Algorithm 2 as well as the refined Algorithm 3 and the iterative projection Algorithm 4 are applied using the two proposed zero-finders.

For several large-scale examples, two methods for solving the related RTLS problem are evaluated additionally for further comparison. The implementation of the RTLSQEP method is described in [14, 16, 17], and details of the RTLSEVP implementation can be found in [15, 17]. For both algorithms, the value of the quadratic constraint δ in (1.3) is set to $\delta = \gamma\|Lx_{true}\|$. Please note that the dual RTLS problem and the RTLS problem have different solutions; cf. Section 2.1.

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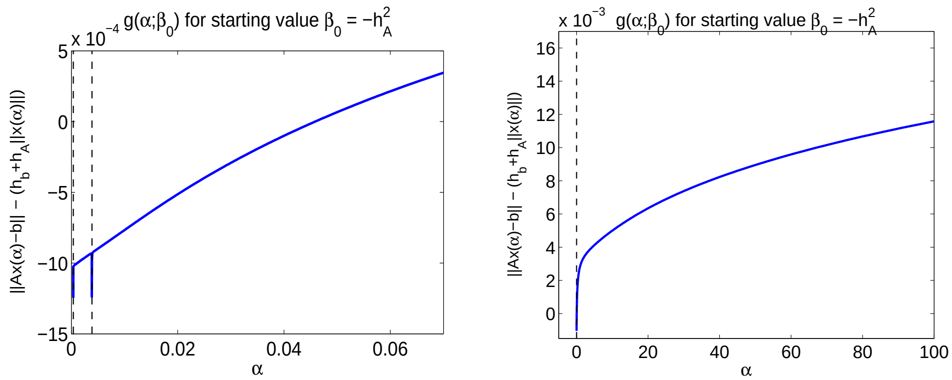

(a) $g(\alpha;\beta_0)$ with two poles indicated by dashed lines. (b) Zoom out of left subfigure.

FIGURE 4.1. *Initial function $g(\alpha)$ for a small-size example.*

The regularization matrix L is chosen as an approximation of the scaled discrete first order derivative operator in one space dimension,

$$L = \begin{bmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \end{bmatrix} \in \mathbb{R}^{(n-1)\times n}. \tag{4.1}$$

In all one-dimensional examples, we use the following invertible approximation of L

$$\widetilde{L} = \begin{bmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \\ & & & \varepsilon \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

This nonsingular approximation to L was introduced and studied in [3], where it was found that the performance of such a preconditioner is not very sensitive to the value of ε. In all computed examples we let $\varepsilon = 0.1$.

The numerical tests are carried out on an Intel Core 2 Duo T7200 computer with 2.3 GHz and 2GB RAM under MATLAB R2009a (actually our numerical examples require less than 0.5 GB RAM).

In Section 4.1, the problem `heat`$(\kappa{=}1)$ of small size is investigated in some detail. The projection Algorithm 4 is compared to the full DRTLS method described in Algorithm 3 and to the model function approach, Algorithm 2. Several examples from *Regularization Tools* of dimension 4000×2000 are considered in Section 4.2. A large two-dimensional problem with a system matrix of dimension 38809×38809 is investigated in Section 4.3.

4.1. Small-scale problems. In this section we investigate the convergence behavior of Algorithm 4. The convergence history of the relative approximation error norm is compared to Algorithm 2 and to the full DRTLS Algorithm 3. The system matrix $A \in \mathbb{R}^{400\times 200}$ is obtained by using `heat`$(\kappa = 1)$, adding noise of the level $\sigma = 10^{-2}$, and stacking two perturbed matrices and right hand sides as described above. The initial value for β is given by $\beta_0 = -h_A^2 = -3.8757 \cdot 10^{-5}$ and the corresponding initial function $g(\alpha;\beta_0)$ is displayed in Figure 4.1.

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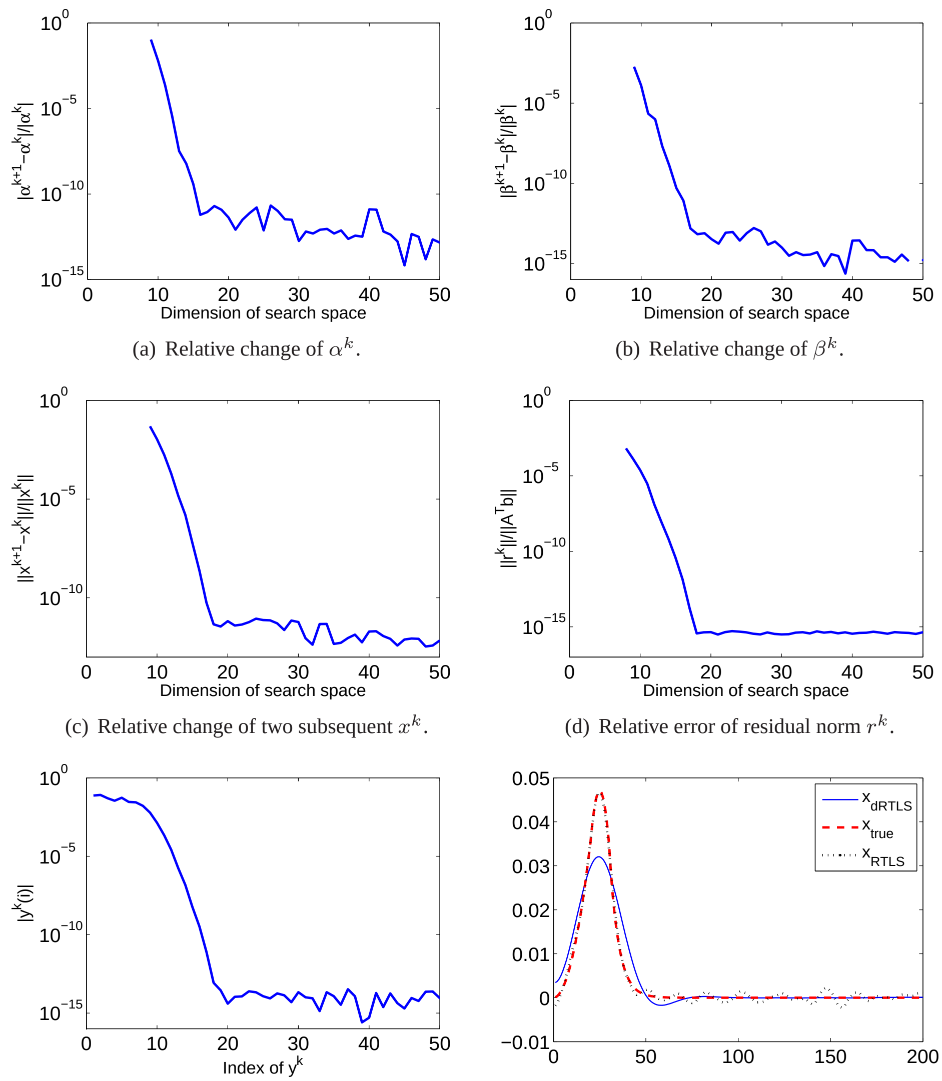

(a) Relative change of α^k.

(b) Relative change of β^k.

(c) Relative change of two subsequent x^k.

(d) Relative error of residual norm r^k.

(e) Absolute values of y^k over the index.

(f) Exact and reconstructed solutions.

FIGURE 4.2. *Convergence histories for* `heat`(1), *size* 400×200.

The function $g(\alpha; \beta_0)$ has 182 poles for $\alpha > 0$ with the rightmost pole located at the value $\alpha = -d_{200} = 0.0039$ and the second rightmost pole at $-d_{199} = 0.00038$ as indicated by the dashed lines in Figure 4.1. For these poles $\lim_{\alpha \to -d_k} g(\alpha) = -\infty$ holds since $\|Av_k\| - h_A\|v_k\| < 0$, for $k = n-1, n$. In the left subplot, it can be observed that the occurrence of the poles does not influence the behavior at the zero $\alpha_0 = 0.0459$. In the right subplot, the behavior for large values of α is displayed. The limit value is given by $g(\alpha; \beta_0)|_{\alpha \to \infty} = g_\infty = 0.0435$.

Figure 4.2 displays the convergence history of the Generalized Krylov Subspace Dual Regularized Total Least Squares Method (GKS-DRTLS) using the preconditioner $M = \widetilde{L}^T \widetilde{L}$ for different convergence measures.

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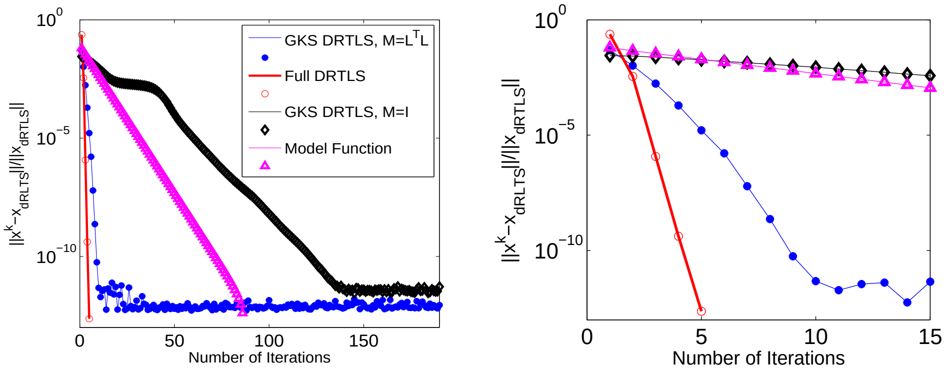

(a) Relative error of x^k (b) Zoom in of left subfigure

FIGURE 4.3. *Convergence history of approximations* x^k *for* heat(1)*, size* 400×200.

The size of the initial search space is equal to 8. Since no stopping criterion for the outer iterations is applied, Algorithm 4 actually runs until $\dim(\mathcal{V}) = 200$. Since all quantities shown in Figure 4.2(a)–(d) quickly converge, only the first part of each convergence history is shown. It can be observed that not all quantities converge to machine precision which is due to the convergence criteria used within an inner iteration. Note that for each subspace enlargement in the outer iteration, a DRTLS problem of the dimension of the current search space has to be solved. For the solution of these projected DRTLS problems, a zero-finder is applied, which in the following is referred to as inner iterations. For the computed example heat(1), the convergence criteria have been chosen as 10^{-12} for the relative error of $\{\beta^k\}$ in the inner iterations, and also 10^{-12} for the relative error of $\{\alpha^k\}$ and for the absolute value of $g_{V_j}(\alpha^k;\beta_i^j)$ within the zero-finder. In the upper left subplot of Figure 4.2, the convergence history of $\{\alpha^k\}$ is shown. In every outer iteration, the dimension of the search space is increased by one. Convergence is achieved within 12 iterations corresponding to a search space of dimension 20. In Figure 4.2(b) the relative change of $\{\beta^k\}$ is displayed logarithmically, roughly reaching machine precision after 12 iterations. The Figures 4.2(c) and (d) show the relative change of the GKS-DRTLS iterates $\{x^k\}$, i.e., the approximate solutions $V_j y(\beta_i^j)$ obtained from the projected DRTLS problems and the norm of the residual $\{r^k\}$, respectively. For a search space dimension of about 20, convergence is reached for these quantities, too. Note that convergence does not have to be monotonically decreasing. Figure 4.2(e) displays logarithmically the first 50 absolute values of the entries in the coefficient vector y^{200}. This stresses the quality of the first 20 columns of the basis V of the search space. The coefficients corresponding to basis vectors with a column number larger than 20 are basically zero, i.e., around machine precision. In Figure 4.2(f) the true solution together with the GKS-TTLS approximation x^{12} are shown. The relative error $\|x_{true} - x^{12}\|/\|x_{true}\|$ is approximately 30%. Note that identical solutions x_{DRTLS} are obtained with the GKS-DRTLS method without preconditioner, the full DRTLS method, and the model function approach. The RTLS solution x_{RTLS} has a relative error of $\|x_{true} - x_{RTLS}\|/\|x_{true}\| = 8\%$, but it has to be stressed that this corresponds to the solution of a different problem. Note that identical solutions x_{RTLS} are obtained by the RTLSEVP and the RTLSQEP method. The dual RTLS solution does not exactly match the peak of x_{true}, but on the other hand does not show the ripples from the RTLS solution. In Figure 4.3 the convergence history of the relative error norms of $\{x^k\}$ with respect to the solution x_{DRTLS} are displayed for Algorithm 4 with and without preconditioner, the model function Algorithm 2, and the full DRTLS Algorithm 3.

In the left subplot of Figure 4.3, the whole convergence history of the approximation error norms of both GKS-DRTLS iterates are shown, i.e., until $\dim(\mathcal{V}) = 200$ which corresponds to 192 outer iterations. As mentioned above, machine precision is not reached due to the applied convergence criteria for the inner iterations, i.e., it is reached a relative approximation error of 10^{-12}. Additionally the convergence history of Algorithms 2 and 3 to the same approximation level is shown. The right subplot is a close–up of the left one that only displays the first 15 iterations. While the full DRTLS method converges within 5 and the GKS-DRTLS method with preconditioner $M = \widetilde{L}^T\widetilde{L}$ in about 12 iterations to the required accuracy, the GKS-DRTLS method without preconditioner requires 140 iterations. This is a very typical behavior of the GKS-DRTLS method without preconditioner, i.e., it is in need of a rather large search space; here 140 vectors of $\mathbb{R}^{200}$ are needed. The model function approach was started with the initial value $\alpha_0 = 1.5\alpha^*$ with $\alpha^* = 0.04702$ as the value at the solution x_{DRTLS}. Despite the good initial value, the required number of iterations was 85, where in each iteration of Algorithm 2, a different large linear system of equations has to be solved. The main effort of one iteration of the full DRTLS method Algorithm 3 lies in computing a large eigendecomposition such that the zero-finding problem can then be carried out at negligible costs. Hence, the costs of the full DRTLS method are much less compared to the model function approach. Note that the costs for obtaining the approximation x^{12} of the GKS-DRTLS method with preconditioner are essentially only 39 MatVecs, i.e., 15 for building up the initial space and 24 for the resulting search space $\mathcal{V} \in \mathbb{R}^{200\times 20}$.

A few words concerning the zero-finders for the full DRTLS method and the GKS-DRTLS Algorithm 4. We start the bracketing zero-finders by first determining values α^k such that not all $g(\alpha^k;\beta_i)$ or $g_{V_j}(\alpha^k;\beta_i^j)$ are of the same sign. Such values can be determined by multiplying available values of the parameter α by 0.01 or 100 depending on the sign of $g(\alpha,\beta_i)$. After very few steps, this gives an interval that contains a root of $g(\alpha,\beta_i)$. For the King method, two values $\alpha^k, k = 1,2$, with $g(\alpha^1;\beta_i)g(\alpha^2;\beta_i) < 0$ are sufficient for initialization while for the rational inverse interpolation three pairs $(\alpha^k, g(\alpha^k;\beta_i)), k = 1,2,3$, have to be given with not all $g(\alpha^k;\beta_i), k = 1,2,3$, having the same sign. For Algorithm 3 the initial value for α is chosen as $\alpha^1 = -1.1d_{200} = 0.0043$ with d_{200} being the smallest eigenvalue of $(A^TA + \beta_0 I, \widetilde{L}^T\widetilde{L})$. This initial guess is located slightly right from the rightmost pole; see also Figure 4.1. For the GKS-DRTLS method Algorithm 4, no pole of $g_{V_0}(\alpha;\beta_0^0)$ for the initial search space $V_0 \in \mathbb{R}^{200\times 8}$ exists, thus the initial value was set to $\alpha^1 = 1$. Note that nevertheless $g_{V_0}(\alpha;\beta_0^0)$ does have a positive root. When, subsequently, the dimension of the search space is increased, the initial value for the parameter β_0^{j+1} is set equal to the last determined value β_i^j. The first value of the parameter α, i.e., α^1, used during initialization for the zero-finding problems $g_{V_j}(\alpha;\beta_i^j) = 0, i = 1,2,\ldots$, is set equal to the last calculated value α_i^{j-1}.

Tables 4.1 and 4.2 show the number of outer and inner iterations as well as the iterations required for the zero-finder within one inner iteration for the full DRTLS method and the generalized Krylov subspace DRTLS method with and without preconditioner. In Table 4.1 the iterations required for Algorithm 3 are compared to the inner and outer iterations of Algorithm 4 when no preconditioner is applied, i.e., with $M = I$. The King method and the rational inverse interpolation zero-finder introduced in Section 3.1 are compared for solving all the inner iterations.

The first outer iteration of the GKS-DRTLS method is treated separately since it corresponds to solving the projected DRTLS with the starting basis V_0 where no information from previous iterations can be used as initial guess for the parameters α and β. Thus, this leads to a number of 5 or 6 inner iterations, i.e., updates of β_i^0, depending on the applied zero-finder. The iterations required by the zero-finder is 6 and 7, respectively, for determining the very

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TABLE 4.1
Number of iterations for Full and GKS-DRTLS with $M = I$.

Zero-finder	Alg.	Outer iters	Inner iters	1st it.	2nd it.	3rd it.	ith it.
Rat.-Inv.	GKS	1	6	6	2	1	0
Rat.-Inv.	GKS	2–60	3–4	1–2	0–1	0	0
Rat.-Inv.	GKS	>60	1–3	0–1	0	0	-
Rat.-Inv.	Full	-	6	6	2	1	0
King	GKS	1	5	7	3	3	0–1
King	GKS	2–60	3–4	2–3	1–3	0–1	0–1
King	GKS	>60	1–2	0–1	0	-	-
King	Full	-	5	7	3	3	0–1

first update of β_0^0, i.e., β_1^0. The effort for determining the subsequent values $\beta_i^0, i = 2, 3, \dots,$ drastically decreases, e.g., for the rational inverse interpolation zero-finder, determining β_2^0 requires 2 iterations and determining β_3^0 requires only 1 iteration of the zero-finder. Determining the zeros in the following 60 outer iterations only consists of 3–4 inner iterations each time. After more than 60 outer iterations have been carried out, i.e., the dimension of the search space satisfies $\dim(\mathcal{V}_j) \geq 68$, typically one or two inner iterations are sufficient for solving the projected DRTLS problem. Note that a '0' in Table 4.1 for the number of iterations of a zero-finder means that the corresponding initialization was sufficient to fulfill the convergence criteria. The King method and the rational inverse interpolation scheme perform similarly. The full DRTLS does not carry out any outer projection iterations and directly treats the full problem. So the meaning of inner iterations as updating the parameter β is identical for Algorithms 3 and 4.

In Table 4.2 the number of iterations required for the full DRTLS algorithm is compared to the GKS-DRTLS method when the preconditioner $M = \widetilde{L}^T\widetilde{L}$ is applied.

TABLE 4.2
Number of iterations for Full and GKS-DRTLS with $M = \widetilde{L}^T\widetilde{L}$.

Zero-finder	Alg.	Outer iters	Inner iters	1st it.	2nd it.	3rd it.	ith it.
Rat.-Inv.	GKS	1	5	6	2	1	0
Rat.-Inv.	GKS	2–8	2–5	0–3	0–1	0	0
Rat.-Inv.	GKS	>8	1	0	-	-	-
Rat.-Inv.	Full	-	6	6	2	1	0
King	GKS	1	5	6	3	2	0
King	GKS	2–8	3–4	1–4	0–3	0–1	0–1
King	GKS	>8	1	0	-	-	-
King	Full	-	5	7	3	3	0–1

Table 4.2 shows a similar behavior to that already observed in Table 4.1: the King method and rational inverse interpolation zero-finder perform comparably well, and the greater the inner iteration number is, the fewer the number of zero-finder iterations. In contrast to the method without preconditioner, here much fewer outer iterations are needed for convergence. Convergence of the GKS-DRTLS method corresponds to an almost instant solution of the

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zero-finder in only one inner iteration. Note that no convergence criterion for stopping the outer iterations has been applied.

4.2. Large-scale examples. In this section we compare the accuracy and performance of Algorithm 4 with and without preconditioner, the RTLSQEP method from [14, 16, 17], and the RTLSEVP method from [15, 17]. Various examples from Hansen's *Regularization Tools* are employed to demonstrate the efficiency of the proposed Generalized Krylov Subspace Dual RTLS method. All examples are of the size 4000×2000. With a value γ from the interval $[0.8, 1.2]$, the quadratic constraint of the RTLS problem is set to $\delta = \gamma\|\widetilde{L}x_{true}\|$, and the constraints for the dual RTLS are set to γh_A and γh_b, respectively. The stopping criterion for the RTLSQEP method is chosen as the relative change of two subsequent values of $f(x^k)$ being less than 10^{-6}. The initial space is $\mathcal{K}_7(\widetilde{L}^{-T}A^TA\widetilde{L}^{-1}, A^Tb)$. The RTLSEVP method also solves the quadratically constrained TLS problem (1.3). For all examples, it computes values of $\lambda_L = \alpha$ almost identical to the RTLSQEP method. The stopping criterion for the RTLSEVP method is chosen as the residual norm of the first order condition to be less than 10^{-8}, which has also been proposed in [15]. The starting search space is $\mathcal{K}_5([A, b]^T[A, b], [0, \dots, 0, 1]^T)$.

For the GKS-DRTLS method, the dimension of the initial search space is 6 for all examples unless stated differently and the following stopping criterion is applied: the relative change of subsequent approximations for α and β in two outer iterations has to be less than 10^{-10}. For the variant without preconditioner, an additional stopping criterion is applied: the dimension of the search space is not allowed to exceed 100, which corresponds to a maximum number of 94 iterations. For all examples, 10 different noise realizations are computed and the averaged results can be found in Tables 4.3 and 4.4.

In Table 4.3 several problems from *Regularization Tools* [10] are investigated with respect to under- and over-regularization for the noise level $\sigma = 10^{-2}$. For all problems in Table 4.3, the residual of the GKS-DRTLS method with preconditioner (denoted as 'DRTLS') converges to almost machine precision. The variant without preconditioner (denoted as 'DRTLSnp') is not very accurate, e.g., with residual norms between 0.01–10% while using the same convergence criterion. This deficiency is also highlighted in Figure 4.3. The accuracy of the RTLSQEP and RTLSEVP methods are somewhere in between, where in most examples the latter one yields more accurate approximations. In the fourth column, the relative error of the corresponding constraint condition is given: for Algorithm 4 this is

$$\frac{|g(\alpha^*;\beta^*)|}{h_b + h_A\|x_{DRTLS}\|} = \frac{|\|Ax_{DRTLS} - b\| - h_b - h_A\|x_{DRTLS}\||}{h_b + h_A\|x_{DRTLS}\|}$$

and for the RTLS methods this is $|(\|\widetilde{L}x_{RTLS} - \delta)|/\delta$. The constraint condition within the DRTLS methods is fulfilled with almost machine precision while for the used implementations of the RTLS methods this quantity varies with the underlying problem. The number of iterations for DRTLSnp is always equal to the maximum number of iterations, which is 94 in most cases. For `heat`(1) and `heat`(5), the dimension of the initial search space was increased to 8 and 10, respectively, to ensure that the function $g_{V_0}(\alpha;\beta_0^0)$ has a positive root. Note that this is not essential for Algorithm 4 if it is equipped with a minimizer for $|g_{V_j}(\alpha_i^j;\beta_i^j)|$ and not only a zero-finder. For these examples, the convergence criteria $|\alpha_i^{j+1} - \alpha_i^j|/\alpha_i^j| < 10^{-10}$ and $|\beta_i^{j+1} - \beta_i^j|/\beta_i^j| < 10^{-10}$ are never achieved by Algorithm 4 without preconditioner, but the variant with $M = \widetilde{L}^T\widetilde{L}$ always converged. The DRTLS and DRTLSnp algorithm increase the search space by one vector every iteration, whereas the RTLSQEP and RTLSEVP methods may add several new vectors in one iteration. More interesting is the number of overall matrix-vector multiplications (MatVecs). For the DRTLSnp

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TABLE 4.3
Problems from Regularization Tools, noise level $\sigma = 10^{-2}$.

Problem factor γ	Method	$\frac{\|r^j\|}{\|A^T b\|}$	Constr.	Iters	Mat-Vecs	CPU time	$\frac{\|x-x_{true}\|}{\|x_{true}\|}$ (small-scale)	$\|\widetilde{L}x\|$
`shaw`	DRTLS	1.4e-13	2.6e-13	3.0	17.0	0.32	3.4e-1 (4.6e-1)	6.0e-5
$\gamma = 1.2$	DRTLSnp	7.7e-02	1.0e-12	94.0	199.0	6.47	2.6e-1 (4.6e-1)	6.7e-5
	RTLSQEP	4.0e-07	3.8e-05	6.7	104.3	3.01	1.2e-1 (1.3e-1)	1.3e-4
	RTLSEVP	1.3e-12	1.1e-02	4.0	54.2	0.92	1.2e-1 (1.3e-1)	1.3e-4
`baart`	DRTLS	5.7e-11	5.0e-15	1.9	14.8	0.31	2.1e-1 (3.5e-1)	3.4e-5
$\gamma = 1.1$	DRTLSnp	1.1e-01	5.4e-14	94.0	199.0	6.10	1.9e-1 (3.5e-1)	3.8e-5
	RTLSQEP	2.8e-06	3.0e-02	6.3	100.7	2.82	1.3e-1 (1.9e-1)	5.5e-5
	RTLSEVP	1.7e-12	1.8e-02	2.0	40.8	0.77	1.2e-1 (1.9e-1)	5.5e-5
`phillips`	DRTLS	1.5e-11	6.4e-15	3.4	17.8	0.33	1.0e-1 (1.0e-1)	1.4e-4
$\gamma = 1.1$	DRTLSnp	3.8e-03	5.3e-14	94.0	199.0	5.94	1.0e-1 (1.0e-1)	1.4e-4
	RTLSQEP	8.1e-05	7.1e-01	9.5	141.9	1.88	7.9e-2 (8.0e-2)	1.8e-4
	RTLSEVP	2.4e-12	1.3e-02	2.6	62.4	1.15	6.1e-2 (8.0e-2)	1.7e-4
`heat`(1)	DRTLS	1.7e-11	1.5e-13	7.3	29.6	0.58	3.1e-1 (3.0e-1)	3.0e-4
$\gamma = 1.0$	DRTLSnp	1.2e-03	2.2e-14	92.0	199.0	6.30	3.1e-1 (3.0e-1)	3.0e-4
	RTLSQEP	7.6e-07	6.4e-06	17.8	212.4	3.67	6.5e-2 (1.9e-1)	5.3e-4
	RTLSEVP	5.2e-11	1.6e-06	5.1	78.0	1.48	6.5e-2 (1.1e-1)	5.3e-4
`heat`(5)	DRTLS	1.5e-08	9.8e-15	14.0	47.0	0.87	8.9e-2 (8.8e-2)	8.5e-4
$\gamma = 1.0$	DRTLSnp	9.5e-04	2.5e-13	90.0	199.0	5.89	8.9e-2 (8.8e-2)	8.5e-4
	RTLSQEP	2.5e-04	6.1e-04	23.4	212.4	4.14	8.3e-3 (1.5e-2)	1.0e-3
	RTLSEVP	1.7e-04	8.6e-04	3.5	76.6	1.30	6.6e-3 (1.7e-2)	1.0e-3
`deriv2`(1)	DRTLS	1.1e-13	2.1e-13	3.0	17.0	0.32	3.3e-1 (2.0e-1)	4.8e-5
$\gamma = 1.0$	DRTLSnp	3.3e-02	1.8e-13	94.0	199.0	6.22	3.4e-1 (2.0e-1)	5.0e-5
	RTLSQEP	9.3e-07	1.7e-04	15.6	194.6	3.50	1.1e-1 (5.3e-2)	1.2e-4
	RTLSEVP	9.8e-13	1.4e-09	5.1	77.0	1.39	1.1e-1 (5.3e-2)	1.2e-4
`deriv2`(2)	DRTLS	2.2e-13	6.3e-13	3.0	17.0	0.34	2.9e-1 (1.7e-1)	3.7e-5
$\gamma = 0.9$	DRTLSnp	3.5e-02	6.3e-14	94.0	199.0	6.66	3.0e-1 (1.7e-1)	4.2e-5
	RTLSQEP	7.6e-07	1.9e-04	5.1	101.1	1.89	9.0e-2 (4.7e-2)	8.4e-5
	RTLSEVP	5.9e-14	1.2e-08	6.1	78.6	1.43	9.0e-2 (4.7e-2)	8.4e-5
`deriv2`(3)	DRTLS	1.6e-13	5.5e-13	3.0	17.0	0.36	2.0e-1 (2.1e-1)	2.8e-5
$\gamma = 0.9$	DRTLSnp	1.4e-01	2.6e-12	94.0	199.0	6.51	1.4e-1 (2.1e-1)	3.3e-5
	RTLSQEP	1.1e-07	2.3e-09	3.0	54.8	1.02	5.1e-2 (6.7e-2)	3.7e-5
	RTLSEVP	2.3e-13	2.8e-10	5.4	67.2	1.22	5.1e-2 (6.7e-2)	3.7e-5
`ilaplace`(2)	DRTLS	4.7e-12	5.5e-14	5.0	21.0	0.43	3.4e-1 (1.9e-1)	6.7e-5
$\gamma = 0.8$	DRTLSnp	8.8e-03	2.2e-13	94.0	199.0	6.30	7.9e-1 (5.7e-1)	1.1e-4
	RTLSQEP	2.3e-07	9.8e-07	4.0	79.4	1.44	4.2e-1 (3.0e-1)	1.5e-4
	RTLSEVP	3.5e-12	5.5e-03	1.4	46.8	0.84	4.1e-1 (3.0e-1)	1.5e-4
`ilaplace`(3)	DRTLS	9.3e-13	3.7e-11	17.7	46.4	0.98	3.9e-1 (2.3e-1)	1.4e-3
$\gamma = 0.8$	DRTLSnp	3.8e-04	1.3e-14	94.0	199.0	6.29	2.6e-1 (2.3e-1)	1.4e-3
	RTLSQEP	1.1e-06	2.0e-09	5.0	84.0	1.51	2.6e-1 (2.1e-1)	1.5e-3
	RTLSEVP	1.3e-11	2.9e-08	3.0	48.6	0.87	2.6e-1 (2.1e-1)	1.5e-3

method, the 94 iterations directly correspond to $2\cdot(\text{MaxIters}+6)-1 = 199$ MatVecs; see Section 3. Similarly for the variant with preconditioner, the relation $2\cdot(\text{Iters}+6)-1 = \text{MatVecs}$ holds. Thus, for Algorithms 4 the dimension of the search space is the size of the initial space plus the number of iterations. For the RTLSQEP method we are in need of four MatVecs to increase the size of the search space by one, whereas the RTLSEVP method requires only two MatVecs. Hence, despite the large number of MatVecs required for RTLSQEP, the dimension of the search space often is smaller than for RTLSEVP.

The CPU times in the seventh column are given in seconds. They are closely related to the number of MatVecs since these are the most expensive operations within all four algorithms. Thus, the main part of the CPU time is required for computing the MatVecs, i.e., roughly 60% for the GKS-DRTLS method without preconditioner and 80–90% for the other three algorithms. Note that the CPU time for simply computing 100 matrix vector multiplications with $A \in \mathbb{R}^{4000\times 2000}$ is about 1.7 seconds. The DRTLS method outperforms the other three algorithms, i.e., in almost all cases, the highest accuracy is obtained with the smallest number of MatVecs. In the next to last column, the relative error with respect to the true solution x_{true} can be found together with a value given in brackets stating the relative error of a reduced discretization level (by a factor of 10) of the same problem, i.e., using a system matrix of size 400×200. Note that the relative error is not suited for directly comparing the DRTLS and RTLS methods since they are solving different problems. More meaningful is the comparison between the two variants of the DRTLS and RTLS methods on the one hand and the comparison of the relative error of a specific method to its correspondent small-scale value. The relative errors of small- and large-scale problems are throughout very similar, differing by a factor of two at most. The same holds true when comparing DRTLS and DRTLSnp as well as RTLSEVP and RTLSQEP, i.e., often the relative errors are almost identical and the maximum difference is given by a factor of two. In the last column, the norm of $\widetilde{L}x$ at the computed solution is given. Since this is the quantity which is minimized in the dual RTLS approach, one would expect this value to be less compared to the value at the computed RTLS solutions. This is indeed the case for all problems of Table 4.3. Notice that in none of these examples, the DRTLSnp method has achieved a smaller norm $\widetilde{L}x$ compared to the DRTLS variant with preconditioner.

The smallest relative errors are obtained with $\gamma = 1$. Values of γ larger than 1 corresponds to a certain degree of under-regularization, whereas $\gamma < 1$ corresponds to over-regularization.

Table 4.4 contains the results of the problems considered in Table 4.3 but now with the noise level reduced to $\sigma = 10^{-3}$. The results are similar to those in Table 4.3. The GKS-DRTLS with preconditioner outperforms DRTLSnp, RTLSQEP, and RTLSEVP in all examples, i.e., the relative residual is computed to almost machine precision within a search space of fairly small dimension. For the examples $\texttt{heat}(1)$ and $\texttt{heat}(5)$, the dimension of the initial search space was now increased to 12 and 16 and for both examples *ilaplace* to 9 to ensure the function $g_{V_0}(\alpha;\beta_0^0)$ having a positive root. Note that for problem $\texttt{heat}(5)$ with the noise level $\sigma = 10^{-3}$, the DRTLSnp method converges for several noise realizations to the required accuracy, whereas for all other examples the maximum number of iterations is reached. For most examples the number of MatVecs of Algorithm 4 with $M = \widetilde{L}^T\widetilde{L}$ is often only about 10–50% of the MatVecs required for the RTLSQEP and RTLSEVP method. The DRTLSnp method is clearly inferior to the other three methods in terms of accuracy and number of MatVecs. The relative error in the next to last column of Table 4.4 indicates again suitable computed approximations for all algorithms.

Notice that in the last column there is one case, for *ilaplace(3)*, where the norm of $\widetilde{L}x$ at the dual RTLS solution is larger than the norm of $\widetilde{L}x$ at the RTLS solution. This might appear implausible at first sight but can be explained by the special problem setup: the choice of constraint parameters has been defined as $\delta = \gamma\|\widetilde{L}x_{true}\|$ for RTLS and $h_A = \gamma\|E\|_F$, $h_b = \|e\|$. The norm of $\widetilde{L}x$ at the RTLS solution is directly given by δ. Hence, for all values $\gamma \geq 1$, the norm at the RTLS solution is not smaller than $\|\widetilde{L}x_{true}\|$, whereas the DRTLS solution has a norm of $\widetilde{L}x$ which is not larger than $\|\widetilde{L}x_{true}\|$ since this is already contained in the feasible region. But for values of γ less than 1, as in the last row of Table 4.4

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TABLE 4.4
Problems from Regularization Tools, noise level $\sigma = 10^{-3}$.

Problem *factor* γ	Method	$\frac{\|r^j\|}{\|A^Tb\|}$	Constr.	Iters	Mat-Vecs	CPU time	$\frac{\|x-x_{true}\|}{\|x_{true}\|}$ (small-scale)	$\|\widetilde{L}x\|$
shaw	DRTLS	2.5e-14	3.9e-13	3.0	17.0	0.32	2.3e-1 (2.4e-1)	7.8e-5
$\gamma = 1.2$	DRTLSnp	6.1e-04	2.4e-12	94.0	199.0	6.12	2.1e-1 (2.4e-1)	8.0e-5
	RTLSQEP	4.3e-08	6.5e-08	15.2	183.4	1.51	9.6e-2 (1.1e-1)	1.3e-4
	RTLSEVP	5.3e-13	1.2e-01	1.0	44.6	0.81	5.7e-2 (7.8e-2)	1.1e-4
baart	DRTLS	8.7e-14	1.2e-12	1.9	14.8	0.28	9.5e-2 (1.3e-1)	4.1e-5
$\gamma = 1.1$	DRTLSnp	2.3e-03	1.8e-12	94.0	199.0	6.06	1.2e-1 (1.3e-1)	4.3e-5
	RTLSQEP	8.2e-08	3.9e-07	11.2	150.6	1.61	1.1e-1 (1.6e-1)	5.5e-4
	RTLSEVP	1.5e-12	1.1e-01	1.0	31.4	0.54	7.9e-2 (1.4e-1)	5.1e-5
phillips	DRTLS	1.3e-13	1.1e-13	4.8	22.6	0.43	2.7e-2 (2.7e-2)	1.6e-4
$\gamma = 1.1$	DRTLSnp	1.6e-04	1.5e-14	94.0	199.0	6.04	2.7e-2 (2.7e-2)	1.6e-4
	RTLSQEP	2.3e-08	1.1e-06	20.0	228.2	4.01	3.8e-2 (5.1e-2)	1.8e-4
	RTLSEVP	4.5e-10	3.3e-02	1.0	62.0	1.12	3.8e-2 (5.2e-2)	1.8e-4
heat(1)	DRTLS	8.7e-13	4.1e-12	11.1	45.2	0.81	1.1e-1 (1.1e-1)	4.5e-4
$\gamma = 1.0$	DRTLSnp	4.7e-06	2.1e-13	88.0	199.0	5.91	1.1e-1 (1.1e-1)	4.5e-4
	RTLSQEP	8.0e-09	2.3e-10	23.4	261.6	4.68	2.7e-2 (3.7e-2)	5.3e-4
	RTLSEVP	5.7e-09	4.7e-02	3.2	87.0	1.42	4.9e-2 (4.2e-2)	5.6e-4
heat(5)	DRTLS	7.3e-09	2.3e-12	23.8	78.6	1.59	1.3e-2 (1.4e-2)	9.9e-4
$\gamma = 1.0$	DRTLSnp	1.4e-06	9.8e-12	82.1	195.2	5.36	1.3e-2 (1.4e-2)	9.9e-4
	RTLSQEP	1.1e-03	4.3e-02	24.0	301.4	5.78	2.1e-2 (2.4e-2)	1.1e-3
	RTLSEVP	1.4e-05	9.6e-04	2.0	78.0	1.29	2.1e-3 (5.4e-3)	1.0e-3
deriv2(1)	DRTLS	3.3e-14	2.2e-13	7.0	25.0	0.47	1.7e-1 (8.7e-2)	6.9e-5
$\gamma = 1.0$	DRTLSnp	4.6e-04	3.6e-14	94.0	199.0	5.97	1.9e-1 (8.7e-2)	7.1e-5
	RTLSQEP	3.5e-08	3.9e-07	22.2	238.8	3.91	5.3e-2 (2.6e-2)	1.2e-4
	RTLSEVP	3.5e-11	3.2e-05	5.3	84.6	1.42	4.9e-2 (2.6e-2)	1.2e-4
deriv2(2)	DRTLS	1.8e-14	2.7e-13	7.0	25.0	0.50	1.5e-1 (7.3e-2)	5.4e-5
$\gamma = 0.9$	DRTLSnp	5.1e-04	7.1e-14	94.0	199.0	6.41	1.7e-1 (7.3e-2)	5.9e-5
	RTLSQEP	4.9e-08	2.3e-06	18.8	217.4	4.22	4.2e-2 (3.0e-2)	8.4e-5
	RTLSEVP	7.4e-12	5.9e-06	4.5	80.6	1.48	4.2e-2 (3.0e-2)	8.4e-5
deriv2(3)	DRTLS	1.0e-13	6.4e-14	4.0	19.0	0.37	7.3e-2 (8.5e-2)	3.5e-5
$\gamma = 0.9$	DRTLSnp	2.0e-03	2.6e-13	94.0	199.0	5.99	4.5e-2 (8.5e-2)	3.7e-5
	RTLSQEP	4.0e-09	3.8e-09	3.0	52.0	0.96	4.9e-2 (4.5e-2)	3.7e-5
	RTLSEVP	1.4e-13	2.1e-10	5.0	63.2	1.15	4.9e-2 (4.5e-2)	3.7e-5
ilaplace(2)	DRTLS	2.5e-13	2.5e-13	4.9	26.8	0.51	3.8e-1 (2.6e-1)	1.3e-4
$\gamma = 0.8$	DRTLSnp	2.4e-04	2.2e-13	91.0	199.0	6.01	7.7e-1 (5.6e-1)	1.5e-4
	RTLSQEP	2.6e-08	1.5e-07	9.2	128.6	2.39	4.1e-1 (3.0e-1)	1.5e-4
	RTLSEVP	4.5e-13	1.4e-03	1.0	44.6	0.80	4.1e-1 (3.0e-1)	1.5e-4
ilaplace(3)	DRTLS	1.3e-13	1.2e-12	12.7	42.4	0.85	1.4e-1 (8.4e-1)	1.8e-3
$\gamma = 0.8$	DRTLSnp	4.9e-06	1.8e-13	91.0	199.0	6.05	1.0e-1 (1.8e-1)	1.8e-3
	RTLSQEP	7.5e-07	2.2e-09	5.0	83.2	1.50	2.5e-1 (2.1e-1)	1.5e-3
	RTLSEVP	3.7e-11	2.8e-08	3.0	45.0	0.81	2.5e-1 (2.1e-1)	1.5e-3

with $\gamma = 0.8$, there is no guarantee that the DRTLS method yields seminorms less than δ. (Especially for small values $\gamma \ll 1$.)

4.3. Large 2-D example. We consider the restoration of a greyscale image that is represented by an array of 197×197 pixels. The pixels are stored columnwise in a vector in $\mathbb{R}^{38809}$. The vector x_{true} represents the uncontaminated image. A block Toeplitz blur-

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ring matrix $A_{true} \in \mathbb{R}^{38809\times 38809}$ with Toeplitz blocks is determined with the function `blur` from [10] using the parameter values $band = 3$ (which is the half-bandwidth of each 197×197 Toeplitz block) and $sigma = 1.5$ (which determines the width of the underlying Gaussian point spread function). The matrix A_{true} has $9.6 \cdot 10^5$ nonzero entries. The right hand side b_{true} is determined by $A_{true}x_{true}$ and the scaling described in the beginning of Section 4 has been applied. We add Gaussian noise corresponding to the noise level $\sigma = 10^{-4}$ to b_{true} and the nonzero entries of A_{true} to keep the number of nonzeros of $A = A_{true} + A_{\text{noise}}$ at a manageable level (a full matrix from $\mathbb{R}^{38809\times 38809}$ requires more than 11GB storage). Please note that this kind of disturbance does not entirely reflect the underlying basic idea of total least squares problems, where the complete matrix and right-hand side are assumed to be contaminated by noise.

We would like to determine an accurate restoration of x_{true} given A and b and some information about the noise. The factor γ is set to 1.

Different regularization matrices L and zero-finders are compared. We use the first order discrete derivative operator for two space dimensions

$$L_{1,2D} = \begin{bmatrix} L_1 \otimes I_n \\ I_n \otimes L_1 \end{bmatrix}$$

with L_1 defined by (4.1) with $n = 197$ and I_n the identity matrix of order 197. The second order discrete derivative operator in two space dimensions

$$L_{2,2D} = \begin{bmatrix} L_2 \otimes I_n \\ I_n \otimes L_2 \end{bmatrix}$$

is also considered where

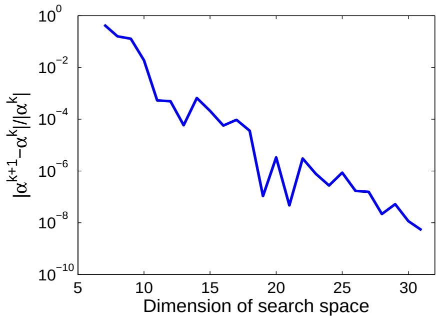
$$L_2 = \begin{bmatrix} -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \end{bmatrix} \in \mathbb{R}^{(n-2)\times n}, \qquad n = 197.$$

We compare the performance of Algorithm 4 to the RTLSEVP algorithm (for solving the correspondent RTLS problem) for the regularization matrices $L_{1,2D}$, $L_{2,2D}$, and $L = I$. For the latter regularization matrix, the generalized Krylov subspaces $\mathcal{V}$ determined by Algorithm 4 reduce to the standard Krylov subspaces $\mathcal{K}_k(A^TA, A^Tb)$.

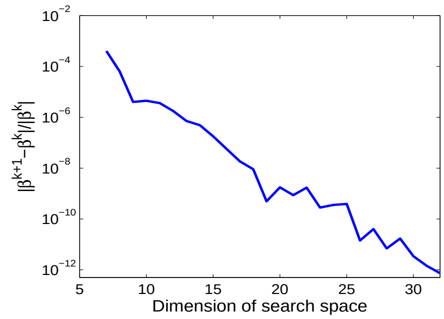
Initial search spaces and stopping criteria for the GKS-DRTLS and RTLSEVP algorithms have been chosen as in the previous Section 4.2 together with the additional criterion of a maximum search space dimension of 50. For the GKS-DRTLS method, no preconditioner has been applied, i.e., $M = I$. The convergence history of the most interesting quantities when using the regularization matrix $L = L_{1,2D}$ is shown in Figure 4.4. The graphs are similar for the regularization matrices $L = L_{2,2D}$ and $L = I$, therefore the latter graphs are not shown.

Similarly as in the small-scale example in Section 4.1, the parameters α and β stagnate quite quickly; see Figures 4.4(a) and (b), respectively. Other quantities on which a stopping criterion for Algorithm 4 can be based are displayed in Figures 4.4(c)–(e). The relative change of two consecutive approximations x^k and the corresponding relative residual norm $\|r(x^k)\|/\|A^Tb\|$ are shown in Figure 4.4(c) and (d), respectively. Both quantities decrease by 7 orders of magnitude. The absolute value of the entries of the vector y^{32} is displayed in Figure 4.4(e). They decrease by 8 orders of magnitude but not monotonically.

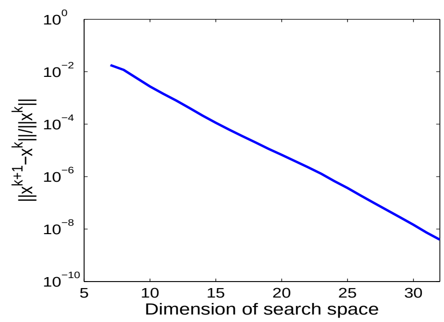
Figure 4.5 shows the original (blur- and noise-free) image, the blurred and noisy image, and several restorations. The first row of Figure 4.5 depicts the original image as well as the



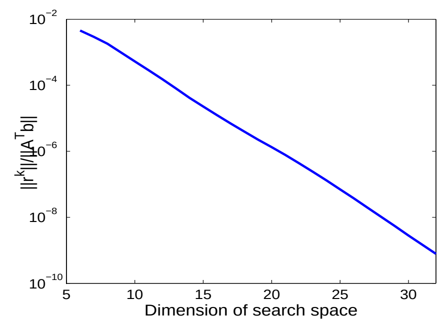
(a) Relative change of α^k.



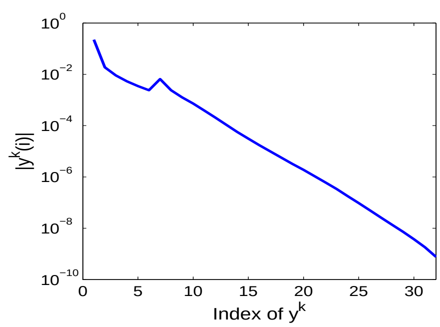
(b) Relative change of β^k.



(c) Relative change of two subsequent x^k.



(d) Relative error of residual norm r^k.



(e) Absolute values of y^k over the index.

FIGURE 4.4. *Convergence histories for the restoration of Lothar using the regularization matrix* $L_{1,2D}$.

blur- and noise-contaminated image. The relative error of the blurred and noisy image is

$$\frac{\|b - x_{true}\|}{\|x_{true}\|} = 20.46\%\,.$$

The images restored in the second row are obtained by using $L = I$ as regularization matrix and applying the RTLSEVP algorithm in Figure 4.5(c) and the GKS-DRTLS algorithm in Figure 4.5(d) using search spaces of dimension $\dim(\mathcal{V}) = 43$ and 50 at termination. The relative errors in the computed restorations are 5.24% and 5.37%. The restorations shown by the images in row three are for the discrete first order derivative operator $L_{1,2D}$. The termination criterion is the same as above. The computed restorations have relative errors $\|x_{RTLS}^{L_{1,2D}} - x_{true}\|/\|x_{true}\| = 7.45\%$ and $\|x_{DRTLS}^{L_{1,2D}} - x_{true}\|/\|x_{true}\| = 6.20\%$ by using a

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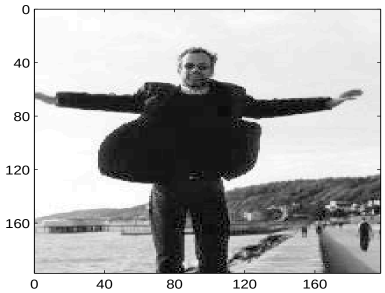
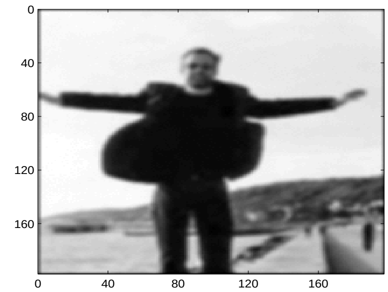
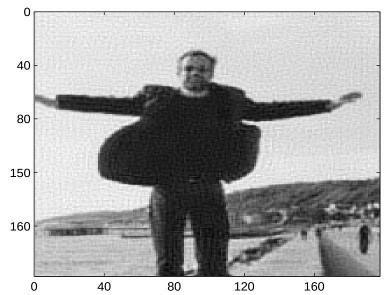


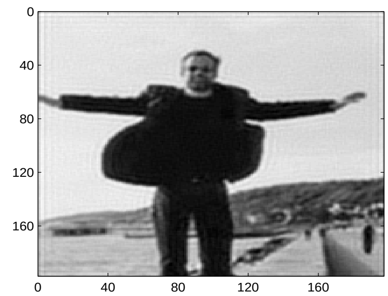
(a) Original picture



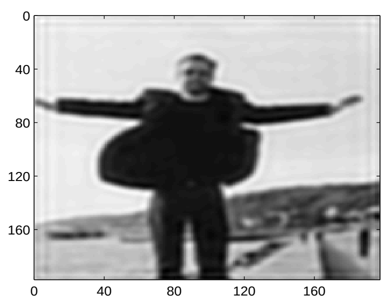
(b) Blurred and noisy picture



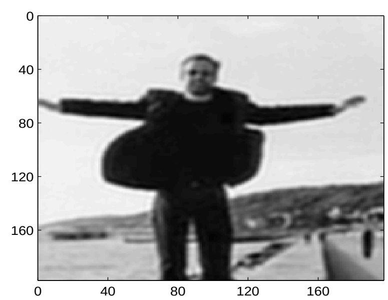
(c) Restored by RTLS with $L = I$



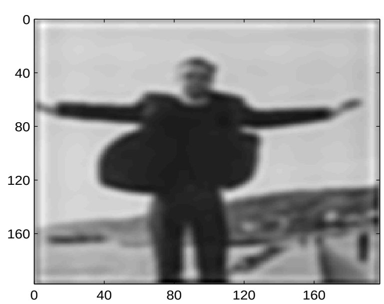
(d) Restored by DRTLS with $L = I$



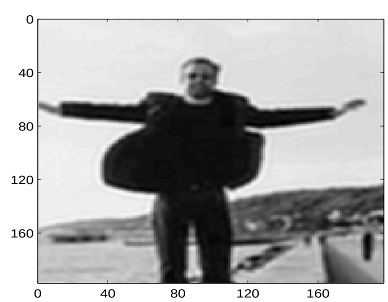
(e) Restored by RTLS with $L = L_{1,2D}$



(f) Restored by DRTLS with $L = L_{1,2D}$



(g) Restored by RTLS with $L = L_{2,2D}$



(h) Restored by DRTLS with $L = L_{2,2D}$

FIGURE 4.5. *Original, blurred, and restored Lothar.*

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search space of dimension 42 for RTLSEVP and of 32 for GKS-DRTLS. The last row displays two restored images obtained with the discrete Laplace operator $L = L_{2,2D}$; the first one corresponds to RTLSEVP with $\dim(\mathcal{V}) = 41$ and an relative error of 9.55%, while the DRTLS restoration used in the second image has required a search space of $\dim(\mathcal{V}) = 42$ with a relative error of $\|x_{DRTLS}^{L_{2,2D}} - x_{true}\|/\|x_{true}\| = 6.34\%$.

Figure 4.5 shows that the regularization matrix $L = I$ gives the best restoration although the restored images can be seen to contain a lot of "freckles". The quality of the restorations obtained by the DRTLS method with $L_{1,2D}$ and $L_{2,2D}$ is about the same, whereas the corresponding restorations by RTLS are clearly inferior. We find the images obtained with $L_{1,2D}$ to be slightly sharper than the image determined with $L_{2,2D}$. Also the relative error is slightly smaller. Since only the DRTLS method with $L = I$ has been terminated by the condition on the search space dimension (with visually indistinguishable restorations in the last few outer iterations), we conclude that it typically suffices to use low-dimensional search spaces $\mathcal{V}$ of dimension 40.

5. Conclusions. A new method based on orthogonal projection for solving dual regularized total least squares problems is presented. The proposed iterative method solves a convergent sequence of projected two-parameter linear systems with a minimization constraint. Due to convergence of this sequence, it turns out to be highly advantageous to reuse the information gathered while solving one system for the solution of the next. Several numerical examples demonstrate that the computed search space is highly suitable. Typically, search spaces of fairly small dimension are sufficient.

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