

GLOBAL CONVERGENCE OF RTLSQEP: A SOLVER OF REGULARIZED TOTAL LEAST SQUARES PROBLEMS VIA QUADRATIC EIGENPROBLEMS

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Abstract. The total least squares (TLS) method is a successful approach for linear problems if both the matrix and the right hand side are contaminated by some noise. In a recent paper Sima, Van Huffel and Golub suggested an iterative method for solving regularized TLS problems, where in each iteration step a quadratic eigenproblem has to be solved. In this paper we prove its global convergence, and we present an efficient implementation using an iterative projection method with thick updates.

Key words: total least squares method, regularization, quadratic eigenvalue problem

1. Introduction

Many problems in data estimation are governed by overdetermined linear systems

$$Ax \approx b, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m, \quad m \geq n \quad (1.1)$$

where both the matrix A and the right hand side b are contaminated by some noise. A possible 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

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

where $\|\cdot\|_F$ denotes the Frobenius norm of a matrix (cf. [11, 23]).

In this paper we consider ill-conditioned problems which arise, for example, from the discretization of ill-posed problems such as integral equations of the first kind (cf. [6, 12, 15]). Then least squares or total least squares methods for

solving (1.1) often yield physically meaningless solutions, and regularization is necessary to stabilize the solution.

Motivated by Tikhonov regularization a well established approach is to add a quadratic constraint to problem (1.2) yielding the regularized total least squares (RTLS) problem

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

where (as in the whole paper) $\|\cdot\|$ denotes the Euclidean norm. δ is a regularization parameter, and $L \in \mathbb{R}^{k \times n}$, $k \leq n$ defines a (semi-) norm on the solution through which the size of the solution is bounded or a certain degree of smoothness can be imposed on the solution. Stabilization by introducing a quadratic constraint was extensively studied in [3, 4, 10, 13, 16, 17, 20, 21, 22]. Tikhonov regularization was considered in [2], and regularization by truncated total least squares in [7].

Based on the singular value decomposition of $[A, b]$ methods were developed for solving the TLS problem (1.2) [11, 23], and even a closed formula for its solution is known if $[A, b]$ has full column rank. However, this approach can not be generalized to the RTLS problem (1.3).

Assuming that the regularization parameter $\delta > 0$ is chosen such that the solution of the total least squares problem x_{TLS} satisfies $\|Lx_{TLS}\| \geq \delta$ (otherwise regularization would not be necessary) problem (1.3) can be replaced by

$$\|[\Delta A, \Delta b]\|_F^2 = \min! \quad \text{subject to } (A + \Delta A)x = b + \Delta b, \quad \|Lx\| = \delta, \quad (1.4)$$

Golub, Hansen and O’Leary [16, 10] analyzed the properties of the equality constrained TLS problem and suggested a method for solving it. Generalizing an approach of Björck [5] for TLS problems without regularization, Guo and Renault [13, 20] took advantage of the fact, that the RTLS problem (1.3) is equivalent to the minimization of the Rayleigh quotient of the augmented matrix $[A, b]^T[A, b]$ subject to the regularization constraint, and suggested an algorithm based on inverse iteration.

Inspired by the fact that quadratically constrained least squares problems can be solved by a quadratic eigenvalue problem [9], Sima, Van Huffel, and Golub [21, 22] developed an iterative method for solving (1.4) called RTL-SQEP (Regularized Total Least Squares via Quadratic Eigenvalue Problems). Here in each step the right-most eigenvalue and corresponding eigenvector of a quadratic eigenproblem has to be determined. Taking advantage of a variational characterization of eigenvalues of nonlinear symmetric eigenproblems we proved the existence of a right-most real eigenvalue which can be characterized as maximum of a Rayleigh functional [17]. For this approach Sima et al. [22] proved that every limit point of the sequence generated by RTL-SQEP solves the first order necessary conditions of (1.4). In this paper prove that it is even a global minimizer of problem (1.4).

Beck and Teboulle [4] considered the inequality constrained problem (1.3) for which they proved a global convergence result (even for a more general rational objective function). However, in this case the individual iteration steps can not be performed via quadratic eigenproblems, and are more expensive.

The paper is organized as follows. In section 2 we introduce the RTLS method and the RTLSQEP approach for solving it taking advantage of a representation due to Beck and Teboulle, and we prove its convergence to a global minimizer. Computational aspects are discussed in section 3, and we conclude the paper with numerical examples in section 4 demonstrating that the RTLSQEP method is a powerful approach.

2. Regularized total least squares via quadratic eigenproblems

We briefly introduce the RTLS problem and the approach of Sima, Van Huffel, and Golub for solving it. It is well known (cf. [23], and [3] for a different derivation) that the RTLS problem (1.3) is equivalent to

$$\frac{\|Ax - b\|^2}{1 + \|x\|^2} = \min! \quad \text{subject to } \|Lx\|^2 \leq \delta^2. \quad (2.1)$$

We assume that the regularization parameter $\delta > 0$ is less than $\|Lx_{TLS}\|$, where x_{TLS} denotes the solution of the total least squares problem (1.2) (otherwise no regularization would be necessary). Then at the optimal solution of (2.1) the constraint $\|Lx\| \leq \delta$ holds with equality, and we may replace (2.1) by

$$f(x) := \frac{\|Ax - b\|^2}{1 + \|x\|^2} = \min! \quad \text{subject to } \|Lx\|^2 = \delta^2. \quad (2.2)$$

Obviously, problem (2.2) is equivalent to the quadratic optimization problem

$$\|Ax - b\|^2 - f^*(1 + \|x\|^2) = \min! \quad \text{subject to } \|Lx\|^2 = \delta^2, \quad (2.3)$$

where

$$f^* = \inf\{f(x) : \|Lx\|^2 = \delta^2\},$$

i.e. x^* is a global minimizer of problem (2.2) if and only if it is a global minimizer of (2.3).

More generally we consider for fixed $y \in \mathbb{R}^n$ the quadratic optimization problem

$$g(x; y) := \|Ax - b\|^2 - f(y)(1 + \|x\|^2) = \min! \quad \text{subject to } \|Lx\|^2 = \delta^2. \quad (2.4)$$

The following existence result was proven in Sima et al. [22]:

Lemma 1. *Problem (2.4) admits a global minimizer if and only if*

$$f(y) \leq \min_{x \in \mathcal{N}(L), x \neq 0} \frac{x^T A^T A x}{x^T x}, \quad (2.5)$$

where $\mathcal{N}(L)$ denotes the null space of L .

Lemma 2. *Assume that y satisfies condition (2.5) and $\|Ly\| = \delta$, and let z be a global minimizer of problem (2.4). Then it holds that*

$$f(z) \leq f(y). \quad (2.6)$$

Proof.

$$(1 + \|z\|)^2(f(z) - f(y)) = g(z; y) \leq g(y; y) = (1 + \|y\|^2)(f(y) - f(y)) = 0.$$

□

This monotonicity result suggests the following method for solving the optimization problem (2.2):

Algorithm 1 Regularized Total Least Squares

Require: x^0 satisfying condition (2.5) and $\|Lx^0\| = \delta$.

for $m = 0, 1, 2, \dots$ **until convergence do**

Determine global minimizer x^{m+1} of

$$g(x; x^m) = \min! \quad \text{subject to } \|Lx\|^2 = \delta^2. \quad (2.7)$$

end for

By Lemma 1 the sequence $\{x^m\}$ is defined, and from Lemma 2 it follows that

$$0 \leq f(x^{m+1}) \leq f(x^m). \quad (2.8)$$

The quadratic optimization problem (2.4) can be solved via the first order necessary optimality conditions

$$(A^T A - f(y)I)x + \lambda L^T Lx = A^T b, \quad \|Lx\|^2 = \delta^2. \quad (2.9)$$

Although $g(\cdot; y)$ in general is not convex these conditions are even sufficient if the Lagrange parameter is chosen maximal.

Theorem 1. *Assume that $(\hat{\lambda}, \hat{x})$ solves the first order conditions (2.9). If $\|Ly\| = \delta$ and $\hat{\lambda}$ is the maximal Lagrange multiplier then \hat{x} is a global minimizer of (2.4)*

Proof. The statement follows immediately from the following equation which can be shown similarly as Theorem 1 in Gander [8]: If (λ_j, z^j) , $j = 1, 2$, are solutions of (2.9) then it holds that

$$g(z^2; y) - g(z^1; y) = \frac{1}{2}(\lambda_1 - \lambda_2)\|L(z^1 - z^2)\|^2.$$

□

Sima et al. [22] suggested to solve the first order conditions (2.9) via a quadratic eigenvalue problem

$$(W + \lambda I)^2 u - \delta^{-2} h h^T u = 0. \quad (2.10)$$

where $W \in \mathbb{R}^{k \times k}$ is a symmetric matrix and $h \in \mathbb{R}^k$ (the detailed form of W and h will be given in Section 3 when we discuss a numerical method; notice however, that $W = W(y)$ and $h = h(y)$ depend continuously on y). In [17] we studied this quadratic eigenproblem, and we proved that (2.10) always has a right-most real eigenvalue $\hat{\lambda}$ such that

$$\hat{\lambda} \geq \operatorname{real}(\lambda) \quad \text{for every eigenvalue } \lambda \text{ of (2.10)}. \quad (2.11)$$

It is this right-most eigenvalue which corresponds to the global minimizer of problem (2.4).

To prove the global convergence of the method defined by Algorithm 1 we need the boundedness of the generated sequence.

Lemma 3. *The sequence $\{x^m\}$ constructed by the Algorithm 1 is bounded.*

Proof. If L is quadratic and nonsingular, then the admissible set is bounded and the lemma is trivial.

For $\operatorname{rank}(L) = k < n$ assume that x^m is unbounded. x^m can be uniquely written as $x^m = y^m + z^m$ where $y^m \in \operatorname{Range}(L^T L)$ and $z^m \in \mathcal{N}(L^T L)$, and trivially $\{y^m\}$ is bounded and $\{z^m\}$ inherits the unboundedness from $\{x^m\}$.

Without loss of generality we assume that $t_m := \|z^m\| \rightarrow \infty$, and that the sequence $w^m := z^m/t_m$ converges to some w^* . Then it follows that

$$\begin{aligned} f(x^m) &= \frac{\|Ax^m - b\|^2}{1 + \|x^m\|^2} = \frac{\|Az^m + Ay^m - b\|^2}{1 + \|z^m\|^2 + \|y^m\|^2} \\ &= \frac{\|Aw^m\|^2 + 2(Aw^m)^T(Ay^m - b)/t_m + \|Ay^m - b\|^2/t_m^2}{1/t_m^2 + \|w^m\|^2 + \|y^m\|^2/t_m^2} \\ &\rightarrow \frac{(w^*)^T A^T A w^*}{\|w^*\|^2} \quad \text{for } m \rightarrow \infty \end{aligned}$$

contradicting (2.5) with $y = x^0$ and (2.8). \square

We are now in the position to prove the convergence of Algorithm 1.

Theorem 2. *Any limit point x^* of the sequence $\{x^m\}$ constructed by Algorithm 1 is a global minimizer of the optimization problem (2.2).*

Proof. Let x^* be a limit point of $\{x^m\}$, and let $\{x^{m_j}\}$ be a subsequence converging to x^* . Then x^{m_j} solves the first order conditions

$$(A^T A - f(x^{m_j-1})I)x^{m_j} + \lambda_{m_j} L^T L x^{m_j} = A^T b.$$

By Lemma 3 $\{x^{m_j-1}\}$ is bounded. Hence, it contains a subsequence $\{x^{m_{j'}}\}$ converging to some limit point \tilde{x} , and from (2.8) it follows that $f(\tilde{x}) = f(x^*)$.

Since $W(y)$ and $h(y)$ depend continuously on y the sequence of right-most eigenvalues $\{\lambda_{m_{j'}}\}$ converges to some λ^* , and x^* satisfies

$$(A^T A - f(x^*)I)x^* - \lambda^* L^T L x^* = A^T b, \quad \|Lx^*\|^2 = \delta^2,$$

where λ^* is the maximal Lagrange multiplier. Hence, by Theorem 1 x^* is a global minimizer of

$$g(x; x^*) = \min! \quad \text{subject to } \|Lx\|^2 = \delta^2, \quad (2.12)$$

and for $y \in \mathbb{R}^n$ with $\|Ly\|^2 = \delta^2$ it follows that

$$\begin{aligned} 0 &= g(x^*; x^*) \leq g(y; x^*) \\ &= \|Ay - b\|^2 - f(x^*)(1 + \|y\|^2) \\ &= (f(y) - f(x^*))(1 + \|y\|^2), \quad \text{i.e. } f(y) \geq f(x^*). \end{aligned}$$

□

Remark 1. Sima et al. [22] proved the weaker convergence result, that every limit point of $\{x^m\}$ satisfies the first order conditions (2.9). Beck and Teboulle [4] considered problem (2.1) with inequality constraints (even for a more general objective function) for which they proved global convergence. Notice however, that the minimization problem for $g(\cdot; x^m)$ with inequality constraint can not be solved via a quadratic eigenvalue problem, whereas it is much more expensive to solve problem (2.7) with inequality constraint.

3. Computational considerations

By Theorem 1 one has to solve

$$(A^T A - f(x^m)I)x + \lambda L^T Lx = A^T b, \quad \|Lx\|^2 = \delta^2 \quad (3.1)$$

for (λ, x) to implement Algorithm 1, and according to Sima et al. [22], this can be obtained via the quadratic eigenvalue problem

$$T_m(\lambda)u := ((W_m + \lambda I)^2 - \delta^{-2} h_m h_m^T)u = 0. \quad (3.2)$$

Here,

$$W_m := L^{-T}(A^T A - f(x^m)I)L^{-1}, \quad h_m := L^{-T}A^T b, \quad (3.3)$$

if L is square and nonsingular. u has to be scaled such that $u^T h_m = \delta^2$ and $x = L^{-1}(W_m + \lambda I)u$.

For $k < n$ it holds that (cf. [17])

$$W_m := S_1^{-1/2}(X_1 - f(x^m)I_k - X_2(X_4 - f(x^m)I_{n-k})^{-1}X_2^T)S_1^{-1/2} \quad (3.4)$$

$$h_m := S_1^{-1/2}(c_1 - X_2(X_4 - f(x^m)I_{n-k})^{-1}c_2) \quad (3.5)$$

where $L^T L = USU^T$ is an eigen decomposition of $L^T L$,

$$(AU)^T(AU) = \begin{pmatrix} X_1 & X_2 \\ X_2^T & X_4 \end{pmatrix}, \quad S = \begin{pmatrix} S_1 & 0 \\ 0 & 0 \end{pmatrix}, \quad U^T A^T b = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad (3.6)$$

and the leading blocks have dimension k . Again u is scaled such that $u^T h_m = \delta^2$, $z := (W_m + \lambda I)u$, and

$$x := U \begin{pmatrix} S_1^{-1/2} z \\ (X_4 - f(x^m)I)^{-1}(c_2 - X_2^T S_1^{-1/2} z) \end{pmatrix}.$$

Algorithm 1 where the quadratic eigenvalue problem (2.9) is solved via the quadratic eigenvalue problem (3.2) was called RTLSQEP.

An obvious approach for solving the quadratic eigenvalue problems (3.2) in the m -th iteration step is linearization, i.e. solving the liner eigenproblem

$$\begin{pmatrix} -2W_m & -W_m^2 + \delta^{-2}h_m h_m^T \\ I & 0 \end{pmatrix} \begin{pmatrix} v \\ u \end{pmatrix} = \lambda \begin{pmatrix} v \\ u \end{pmatrix} \quad (3.7)$$

and choosing the maximal real eigenvalue, and the corresponding u -part of the eigenvector, which is an eigenvector of (3.2). This approach is reasonable if the dimension n of problem (2.2) is small.

For larger dimensions it is not efficient to determine the entire spectrum of (3.2), and to choose the eigenpair that is needed afterwards. In this case the right-most eigenvalue and corresponding eigenvector of (2.2) can be determined via the implicitly restarted Arnoldi method implemented in ARPACK [18] (and included in MATLAB as function `eigs`) or a Krylov subspace solver tailored for quadratic eigenvalue problems like the one proposed by Li and Ye [19] or the SOAR method suggested by Bai and Su [1].

Notice however, that in the RTLS Algorithm 1 we have to solve a sequence of quadratic eigenvalue problems which suggests to use as much information as possible from previous steps. For Krylov subspace methods the only degree of freedom is the choice of the initial vector, and therefore the best one can do is to start the eigensolver in step m with the eigen solution u^{m-1} of the preceding step.

A method which is able to take advantage of the complete information gathered in the previous steps is the nonlinear Arnoldi [24] method which allows thick starts, i.e. arbitrary initial search spaces. Hence, solving $T_m(\lambda)u = 0$ in step m of the RTLS Algorithm 1 one may start with an orthonormal basis V of the search space that was used in the preceding step when determining the solution $u^{m-1} = Vz$ of the projected problem $V^T T_{m-1}(\lambda)Vz = 0$.

Algorithm 2 Nonlinear Arnoldi

- 1: start with initial basis V , $V^T V = I$
 - 2: determine preconditioner $M \approx T(\sigma)^{-1}$, σ close to wanted eigenvalue
 - 3: find right-most eigenvalue μ of $V^T T(\mu)Vy = 0$ and corresponding eigenvector y
 - 4: set $u = Vy$, $r = T(\mu)u$
 - 5: **while** $\|r\|/\|u\| > \epsilon$ **do**
 - 6: $v = Mr$
 - 7: $v = v - VV^T v$
 - 8: $\tilde{v} = v/\|v\|$, $V = [V, \tilde{v}]$
 - 9: find right-most eigenvalue μ of projected problem $V^T T(\mu)Vy = 0$ and corresponding eigenvector y
 - 10: set $u = Vy$, $r = T(\mu)u$
 - 11: **end while**
-

In the RTLS algorithm a sequence of quadratic eigenvalue problems has to be solved, and the convergence of the matrices and vectors

$$W_m = \left(C - f(x^m)\tilde{S} - D(X_4 - f(x^m)I_{n-k})^{-1}D^T \right) \quad (3.8)$$

$$h_m = \left(g_1 - D(X_4 - f(x^m)I_{n-k})^{-1}c_2 \right). \quad (3.9)$$

with $C := S_1^{-1/2}X_1S_1^{-1/2}$, $\tilde{S} = S_1^{-1}$, $D = S_1^{-1/2}X_2$ and $g_1 = S_1^{-1/2}c_1$ suggest to reuse information from the previous steps when solving problem (3.1) in step m .

The projected problem

$$V^T T_m(\lambda) V z = ((W_m + \lambda I)V)^T ((W_m + \lambda I)V) z - \delta^{-2} (h_m^T V)^T (h_m^T V) z = 0 \quad (3.10)$$

can be determined efficiently, if the matrices CV , SV , $D^T V$ and $g_1^T V$ are known. These are obtained on-the-fly appending one column and component to the current matrix and vector, respectively, in every iteration step of the nonlinear Arnoldi method. Notice, that the explicit form of the matrices C , D and g_1 are not needed to execute these multiplications. Moreover we can take advantage of further updates multiplying $((W_m + \lambda I)V)^T ((W_m + \lambda I)V)$.

Since it is very inexpensive to obtain updates of $W_m V$ and $h_m^T V$ from the preceding matrices $W_{m-1} V$ and $h_{m-1}^T V$ (cf. (3.8) and (3.9)) we decided to terminate the inner iteration long before convergence. Our numerical experiments demonstrated that computing time could be reduced substantially terminating the inner iteration if the residual of the quadratic eigenvalue was diminished at least by a factor 10^{-2} .

4. Numerical experiments

In order to evaluate the performance of the RTLSQEP method for large dimensions where the quadratic eigenproblems are solved by the nonlinear Arnoldi method we use test examples from Hansen's *Regularization Tools* [14]. Two functions, *baart* and *shaw*, which are both discretizations of Fredholm integral equations of the first kind, are used to generate matrices $A_{\text{true}} \in \mathbb{R}^{n \times n}$, right hand sides $b_{\text{true}} \in \mathbb{R}^n$ and solutions $x_{\text{true}} \in \mathbb{R}^n$ such that

$$A_{\text{true}} x_{\text{true}} = b_{\text{true}}.$$

In all cases the matrices A_{true} and $[A_{\text{true}}, b_{\text{true}}]$ are ill-conditioned.

To construct a suitable TLS problem, the norm of b_{true} is scaled such that $\|b_{\text{true}}\| = \max \|A_{\text{true}}(:, i)\|$ holds. x_{true} is scaled by the same factor. The noise added to the problem is put in relation to the maximal element of the augmented matrix, $maxval = \max(\max(abs[A_{\text{true}}, b_{\text{true}}]))$. We add white noise of level 5-50%, i.e. $\sigma = maxval \cdot (0.05 \dots 0.5)$ to the data, and obtained the systems $Ax \approx b$ to be solved where $A = A_{\text{true}} + \sigma E$ and $b = b_{\text{true}} + \sigma e$, and the elements of E and e are independent random variables with zero

mean and variance σ . The matrix $L \in \mathbb{R}^{n-1 \times n}$ approximates the first order derivative, and δ is chosen to be $\delta = 0.9 \|Lx_{\text{true}}\|$.

The numerical tests were run on a PentiumR4 computer with 3.4 GHz and 3GB RAM under MATLAB R2006b. Tables 1 and 2 contain the CPU times in seconds averaged over 100 random simulations for dimensions $n = 1000$, $n = 2000$, and $n = 4000$ with noise levels 5% and 50% for *baart* and *shaw*, respectively. The quadratic eigenproblems were solved by the Krylov subspace methods for quadratic eigenproblems presented by Li and Ye and by Bai and Su, and by the nonlinear Arnoldi method with early updates. We also tried early updates for the Krylov spaces solvers, but this even delayed the convergence. Solving the quadratic eigenvalue problems by linearization and the restarted Arnoldi method (callings eigs) took much more time although in this case the precompiled FORTRAN routine ARPACK is used. The outer iteration was terminated if the residual norm of the first order condition was less than 10^{-10} .

Table 1. Average CPU time; Noise level 5%

problem	n	SOAR	Li & Ye	NL Arn.
baart	1000	0.28	0.15	0.10
	2000	0.92	0.45	0.31
	4000	3.51	1.62	1.16
shaw	1000	0.40	0.23	0.12
	2000	1.33	0.60	0.37
	4000	5.09	1.89	1.39

Table 2. Average CPU time; Noise level 50%

problem	n	SOAR	Li & Ye	NL Arn.
baart	1000	0.19	0.11	0.10
	2000	0.61	0.35	0.31
	4000	2.45	1.18	1.14
shaw	1000	0.27	0.14	0.11
	2000	1.01	0.44	0.35
	4000	4.10	1.73	1.31

Figures 1 and 2 show the typical convergence behaviour of the RTLSQEP where the quadratic eigenproblems are solved by method presented by Li and Ye (the SOAR method behaves similarly) and by the nonlinear Arnoldi method, respectively. An asterisk marks the residual norm of a quadratic eigenvalue problem in an inner iteration, and a circle denotes the residual

norm of the first order condition in an outer iteration. Notice, however, that the method presented by Li and Ye requires only one matrix vector product in every inner iteration, whereas the nonlinear Arnoldi method needs roughly two matrix vector products. However, due to the early updates the nonlinear Arnoldi method requires significantly less matrix-vector products than the Krylov subspace methods.

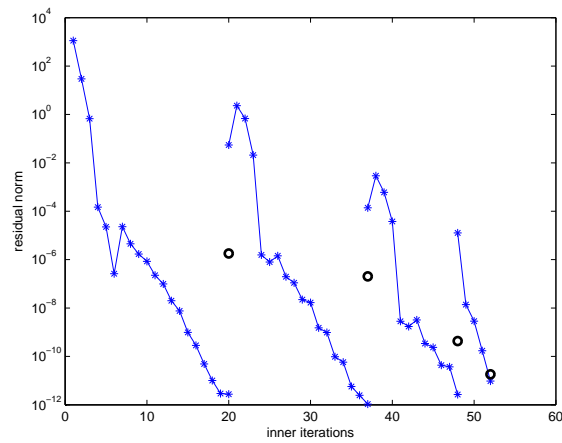


Figure 1. Convergence history; quadratic eigenproblems by the Li & Ye algorithm

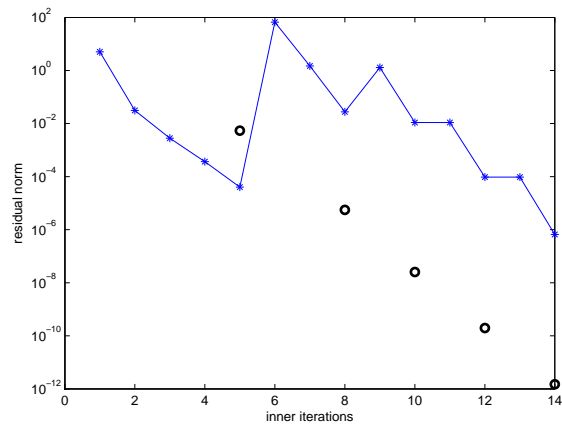


Figure 2. Convergence history; quadratic eigenproblems by Arnoldi algorithm

5. Conclusions

Regularized total least squares problems can be solved efficiently by the RTLSQEP method introduced by Sima, Van Huffel and Golub [22] via a sequence of quadratic eigenvalue problems. We proved its convergence to a global minimizer. For problems of high dimension the quadratic eigenvalue problems can be solved efficiently by the nonlinear Arnoldi method with early updates.

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