

Regularized Total Least Squares Based on Eigensolvers

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Joint work with Jörg Lampe



- 1 Total Least Squares
- 2 Solving RTLS problems
 - Approach of Sima, Van Huffel, Golub
 - Approach of Renaut and Guo
- 3 Determining the regularization parameter
- 4 Numerical Examples
- 5 Conclusions

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Least Squares Problem

The ordinary Least Squares (LS) method assumes that the system matrix A of a linear model is error free, and all errors are confined to the right hand side b .

Given $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $m \geq n$

Find $x \in \mathbb{R}^n$ and $\Delta b \in \mathbb{R}^m$ such that

$$\|\Delta b\| = \min! \quad \text{subject to } Ax = b + \Delta b.$$

Obviously equivalent to: Find $x \in \mathbb{R}^n$ such that

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If the true values of the observed variables satisfy linear relations, and if the errors in the observations are independent random variables with zero mean and equal variance, then the **total least squares** (TLS) approach often gives better estimates than LS.

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Find $\Delta A \in \mathbb{R}^{m \times n}$, $\Delta b \in \mathbb{R}^m$ and $x \in \mathbb{R}^n$ such that

$$\|[\Delta A, \Delta b]\|_F^2 = \min! \quad \text{subject to } (A + \Delta A)x = b + \Delta b, \quad (1)$$

where $\|\cdot\|_F$ denotes the Frobenius norm.

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If A and $[A, b]$ are ill-conditioned, regularization is necessary.

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Lemma (Beck, Ben-Tal 2006)

Let K be an orthonormal basis of $\ker(L)$. If $\sigma_{\min}([AK, b]) < \sigma_{\min}(AK)$ holds, a solution of the RTLS problem exists.

In general there does not exist a closed form solution x_{RTLS} of the RTLS problem.

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First Order Conditions; Golub, Hansen, O'Leary 1999

Assume x_{RTLS} exists and constraint is active, then (RTLS) is equivalent to

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

First-order optimality conditions are equivalent to

$$\begin{aligned} (A^T A + \lambda_I I + \lambda_L L^T L)x &= A^T b, \\ \mu &\geq 0, \quad \|Lx\|^2 = \delta^2 \end{aligned}$$

with

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

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Two Iterative Algorithms

Two approaches for solving the first order conditions

$$\left(A^T A + \lambda_I(x) I + \lambda_L(x) L^T L \right) x = A^T b \quad (*)$$

Idea of Sima, Van Huffel, Golub [2004]:

- Iterative algorithm based on updating λ_I
- With fixed λ_I reformulate (*) into QEP
- Determine rightmost eigenvalue, i.e. the free parameter λ_L
- Use corresponding eigenvector to update λ_I

Idea of Renault, Guo [2005] is the other way round:

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A quadratic eigenproblem

For $m = 0, 1, \dots$ until convergence

Find rightmost $\lambda \in \mathbb{R}$ and x such that

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

If L is square and nonsingular: Let $z := Lx$. Then

$$Wz + \lambda z := L^{-T}(A^T A - f(x^m)I)L^{-1}z + \lambda z = L^{-T}A^T b =: h, \quad z^T z = \delta^2.$$

$$u := (W + \lambda I)^{-2}h \quad \Rightarrow \quad h^T u = z^T z = \delta^2 \quad \Rightarrow \quad h = \delta^{-2} h h^T u$$

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

If $\hat{\lambda}$ is the right-most real eigenvalue, and the corresponding eigenvector is scaled such that $h^T u = \delta^2$ then the solution of problem (*) is recovered as $x = L^{-1}(W + \hat{\lambda}I)u$.

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A quadratic eigenproblem ct.

If $L \in \mathbb{R}^{k \times n}$ with linearly independent rows and $k < n$, the first order conditions can be reduced to a quadratic eigenproblem

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

where

$$\begin{aligned} W_m &= \left(C - f(x^m)D - S(T - f(x^m)I_{n-k})^{-1}S^T \right) \\ h_m &= g - D(T - f(x^m)I_{n-k})^{-1}c \end{aligned}$$

with $C, D \in \mathbb{R}^{k \times k}$, $S \in \mathbb{R}^{k \times n-k}$, $T \in \mathbb{R}^{n-k \times n-k}$, $g \in \mathbb{R}^k$, $c \in \mathbb{R}^{n-k}$, and C, D, T are symmetric matrices.

Nonlinear maxmin characterization

Let $T(\lambda) \in \mathbb{C}^{n \times n}$, $T(\lambda) = T(\lambda)^H$, $\lambda \in J \subset \mathbb{R}$ an open interval (maybe unbounded).

For every fixed $x \in \mathbb{C}^n$, $x \neq 0$ assume that the real function

$$f(\cdot; x) : J \rightarrow \mathbb{R}, f(\lambda; x) := x^H T(\lambda) x$$

is continuous, and that the real equation

$$f(\lambda, x) = 0$$

has at most one solution $\lambda =: p(x)$ in J .

Then equation $f(\lambda, x) = 0$ implicitly defines a functional p on some subset D of \mathbb{C}^n which we call the **Rayleigh functional**.

Assume that

$$(\lambda - p(x))f(\lambda, x) > 0 \quad \text{for every } x \in D, \lambda \neq p(x).$$

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maxmin characterization (V., Werner 1982)

Let $\sup_{v \in D} p(v) \in J$ and assume that there exists a subspace $V \subset \mathbb{C}^n$ of dimension ℓ such that

$$V \cap D \neq \emptyset \quad \text{and} \quad \inf_{v \in V \cap D} p(v) \in J.$$

- Then $T(\lambda)x = 0$ has at least ℓ eigenvalues in J , and for $j = 1, \dots, \ell$ the j -largest eigenvalue λ_j can be characterized by

$$\lambda_j = \max_{\dim V=j, V \cap D \neq \emptyset} \inf_{v \in V \cap D} p(v). \quad (1)$$

- For $j = 1, \dots, \ell$ every j dimensional subspace $\tilde{V} \subset \mathbb{C}^n$ with

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Back to

$$T(\lambda)x := ((W + \lambda I)^2 - \delta^{-2}hh^T)x = 0 \quad (\text{QEP})$$

$$f(\lambda, x) = x^H T(\lambda)x = \lambda^2 \|x\|^2 + 2\lambda x^H Wx + \|Wx\|^2 - |x^H h|^2 / \delta^2, \quad x \neq 0$$

is a parabola which attains its minimum at

$$\lambda = -\frac{x^H Wx}{x^H x}.$$

Let $J = (-\lambda_{\min}, \infty)$ where λ_{\min} is the minimum eigenvalue of W . Then $f(\lambda, x) = 0$ has at most one solution $p(x) \in J$ for every $x \neq 0$. Hence, the Rayleigh functional p of (QEP) corresponding to J is defined, and the general conditions are satisfied.

Back to

$$T(\lambda)x := ((W + \lambda I)^2 - \delta^{-2}hh^T)x = 0 \quad (\text{QEP})$$

$$f(\lambda, x) = x^H T(\lambda)x = \lambda^2 \|x\|^2 + 2\lambda x^H Wx + \|Wx\|^2 - |x^H h|^2 / \delta^2, \quad x \neq 0$$

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Characterization of maximal real eigenvalue

Let V_{\min} be the eigenspace of W corresponding to λ_{\min} . Then for every $x_{\min} \in V_{\min}$

$$f(-\lambda_{\min}, x_{\min}) = x_{\min}^H (W - \lambda_{\min})^2 x_{\min} - |x_{\min}^H h|^2 / \delta^2 = -|x_{\min}^H h|^2 / \delta^2 \leq 0$$

Hence, if $x_{\min}^H h \neq 0$ for some $x_{\min} \in V_{\min}$, then $x_{\min} \in D$.

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Assume that $D \neq \emptyset$. For $x^H h = 0$ it holds that

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i.e. $x \notin D$.

Hence, D does not contain a two-dimensional subspace of \mathbb{C}^n , and therefore J contains at most one eigenvalue of (QEP).

If $\lambda \in \mathbb{C}$ is a non-real eigenvalue of (QEP) and x a corresponding eigenvector, then

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Theorem

Let λ_{\min} be the minimal eigenvalue of W , and V_{\min} be the corresponding eigenspace.

- If $h \perp V_{\min}$ and $T(-\lambda_{\min})$ is positive semi-definite, then $\hat{\lambda} := -\lambda_{\min}$ is the maximal real eigenvalue of (QEP).
- Otherwise, the maximal real eigenvalue is the unique eigenvalue $\hat{\lambda}$ of (QEP) in $J = (-\lambda_{\min}, \infty)$, and it holds

$$\hat{\lambda} = \max_{x \in D} \rho(x).$$

- $\hat{\lambda}$ is the right most eigenvalue of (QEP), i.e.

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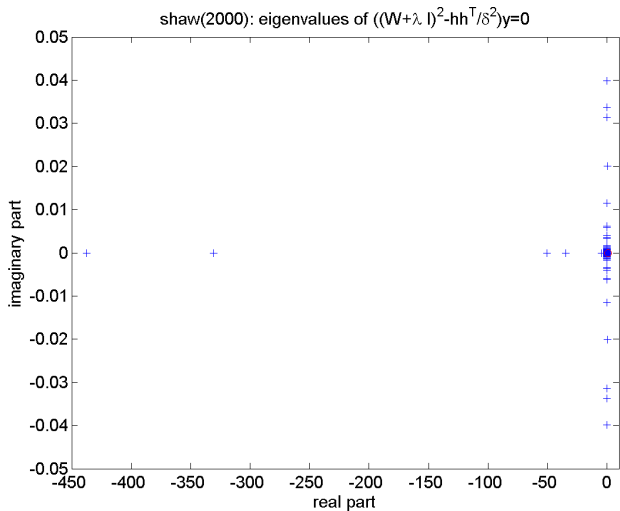
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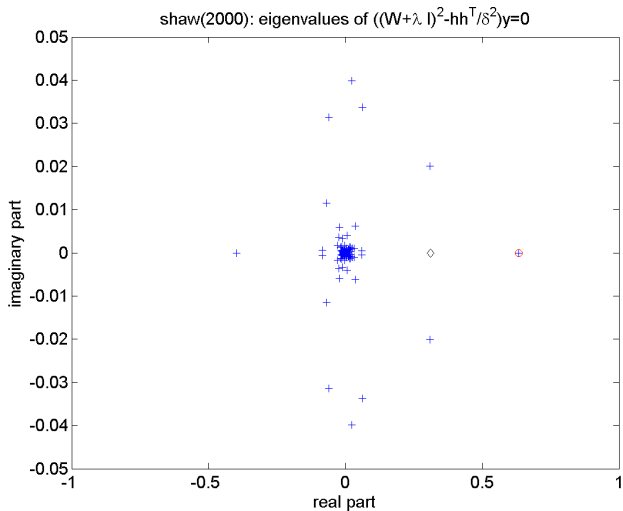
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Example



Example: close up



Positivity of $\hat{\lambda}$

Sima et al. claimed that the right-most eigenvalue problem is always positive.

Simplest counter-example: If W is positive definite with eigenvalue $\lambda_j > 0$, then $-\lambda_j$ are the only eigenvalues of the quadratic eigenproblem $(W + \lambda I)^2 x = 0$, and if the term $\delta^{-2} h h^T$ is small enough, then the quadratic problem will have no positive eigenvalue, but the right-most eigenvalue will be negative.

However, in quadratic eigenproblems occurring in regularized total least squares problems δ and h are not arbitrary, but regularization only makes sense if $\delta \leq \|Lx_{\text{TLS}}\|$ where x_{TLS} denotes the solution of the total least squares problem without regularization.

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Theorem

The maximal real eigenvalue $\hat{\lambda}$ of the quadratic problem

$$(W + \lambda I)^2 x - \delta^{-2} h h^T x = 0$$

is negative if and only if W is positive definite and

$$\|W^{-1} h\| < \delta.$$

For the quadratic eigenproblem occurring in regularized total least squares it holds that

$$\|W^{-1} h\| = \|L(A^T A - f(x)I)^{-1} A^T b\|.$$

For the standard case $L = I$ the right-most eigenvalue $\hat{\lambda}$ is always nonnegative if $\delta < \|x_{TLS}\|$.

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Any limit point x^* of the sequence $\{x^m\}$ constructed by RTLSQEP is a global minimizer of

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

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Quadratic eigenproblem

The quadratic eigenproblems

$$T_m(\lambda)z = (W_m + \lambda I)^2 z - \frac{1}{\delta^2} h_m h_m^T z = 0$$

can be solved by

- linearization
- Krylov subspace method for QEP (Li & Ye 2003)
- SOAR (Bai & Su 2005)
- nonlinear Arnoldi method (Meerbergen 2001, V. 2003)

Nonlinear Arnoldi Method

Algorithm 1 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 rightmost/smallest eigenvalue λ of $V^T T_k(\lambda) V y = 0$ and corresponding eigenvector y
 - 4: Set $u = Vy$, $r = T_k(\lambda)u$
 - 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 rightmost/smallest eigenvalue λ of $V^T T_k(\lambda) V y = 0$ and corresponding eigenvector y
 - 10: Set $u = Vy$, $r = T_k(\lambda)u$
 - 11: **end while**
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Reuse of information

The convergence of W_m and h_m suggests to reuse information from the previous iterations when solving $T_m(\lambda)z = 0$.

Krylov subspace methods for $T_m(\lambda)z = 0$ can be started with the solution z^{m-1} of $T_{m-1}(\lambda)z = 0$.

The nonlinear Arnoldi method can use thick starts, i.e. the projection method for

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can be initialized by V_{m-1} where $z^{m-1} = V_{m-1}\tilde{u}$, and \tilde{u} is an eigenvector of $V_{m-1}^T T_{m-1}(\lambda) V_{m-1} u = 0$.

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Thick and early updates

$$\begin{aligned} W_m &= C - f(x^m)D - S(T - f(x^m)I_{n-k})^{-1}S^T \\ h_m &= g - D(T - f(x^m)I_{n-k})^{-1}c \end{aligned}$$

with $C, D \in \mathbb{R}^{k \times k}$, $S \in \mathbb{R}^{k \times n-k}$, $T \in \mathbb{R}^{n-k \times n-k}$, $g \in \mathbb{R}^k$, $c \in \mathbb{R}^{n-k}$.

Hence, in order to update the projected problem

$$V^T(W_{m+1} + \lambda I)^2 VU - \frac{1}{\delta^2} V^T h_{m+1} h_{m+1}^T VU = 0$$

one has to keep only CV , DV , $S^T V$, and $g^T V$.

Since it is inexpensive to obtain updates of W_m and h_m we decided to terminate the inner iteration long before convergence, namely if the residual of the quadratic eigenvalue was reduced by at least 10^{-2} . This reduced the computing time further.

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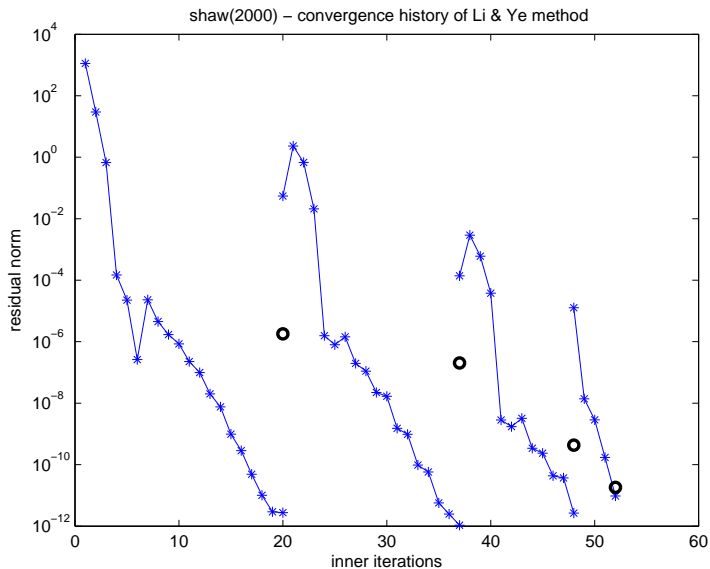
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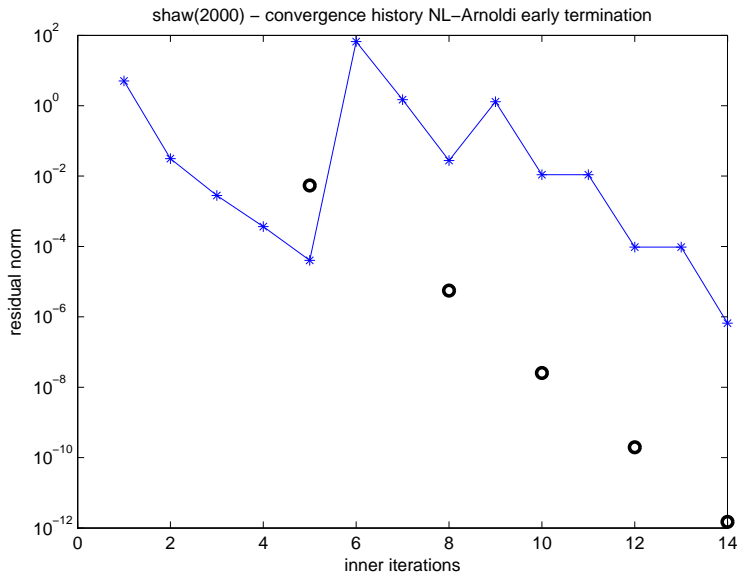
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Example: shaw(2000); Li & Ye



shaw(2000); Early updates



Necessary Condition: Guo, Renaut 2002

The RTLS solution x satisfies the linear eigenvalue problem

$$B(x) \begin{pmatrix} x \\ -1 \end{pmatrix} = -\lambda_l \begin{pmatrix} x \\ -1 \end{pmatrix}$$

where

$$B(x) = [A, b]^T [A, b] + \lambda_L(x) \begin{pmatrix} L^T L & 0 \\ 0 & -\delta^2 \end{pmatrix}$$

$$\lambda_l = -f(x)$$

$$\lambda_L = -\frac{1}{\delta^2} (b^T (Ax - b) - \lambda_l)$$

Conversely, if $\left(-\hat{\lambda}, \begin{pmatrix} \hat{x} \\ -1 \end{pmatrix}\right)$ is an eigenpair of $B(\hat{x})$, and

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Determine $\theta \in \mathbb{R}_+$ such that the eigenvector $(x_\theta^T, -1)^T$ of

$$B(\theta) := [A, b]^T [A, b] + \theta \begin{pmatrix} L^T L & 0 \\ 0 & -\delta^2 \end{pmatrix} \quad (*)$$

corresponding to the smallest eigenvalue satisfies the constraint $\|Lx_\theta\|^2 = \delta^2$,
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Renaut and Guo claim that (under the conditions $b^T A \neq 0$ and $\mathcal{N}(A) \cap \mathcal{N}(L) = \{0\}$) the smallest eigenvalue of $B(\theta)$ is simple, and that (under the further condition that the matrix $[A, b]$ has full rank) g is continuous and strictly monotonically decreasing.

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Renaut and Guo claim that (under the conditions $b^T A \neq 0$ and $\mathcal{N}(A) \cap \mathcal{N}(L) = \{0\}$) the smallest eigenvalue of $B(\theta)$ is simple, and that (under the further condition that the matrix $[A, b]$ has full rank) g is continuous and strictly monotonically decreasing.

Hence, $g(\theta) = 0$ has a unique root θ_0 , and the corresponding eigenvector (scaled appropriately) yields the solution of the RTLS problem.

Approach of Renault, Guo et.

Unfortunately these assertions are not true. The last component of an eigenvector corresponding to the smallest eigenvalue need not be different from zero, and then g is not defined.

Example: Let

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 0 \\ \sqrt{3} \end{pmatrix}, \quad L = \begin{pmatrix} \sqrt{2} & 0 \\ 0 & 1 \end{pmatrix}, \quad \delta = 1.$$

Then the conditions ' $[A, b]$ has full rank', ' $b^T A = (1, 0) \neq 0$ ' and ' $\mathcal{N}(A) \cap \mathcal{N}(L) = \{0\}$ ' are satisfied,

$$B(\theta) = \begin{pmatrix} 1 + 2\theta & 0 & 1 \\ 0 & 1 + \theta & 0 \\ 1 & 0 & 4 - \theta \end{pmatrix},$$

and the smallest eigenvalue $\lambda_{\min}(B(0.5)) = 1.5$ and $\lambda_{\min}(B(1)) = 2$ have multiplicity 2, and for $\theta \in (0.5, 1)$ the last component of the eigenvector $y_\theta = (0, 1, 0)^T$ corresponding to the smallest eigenvalue $\lambda_{\min}(B(\theta)) = 1 + \theta$ is equal to zero.

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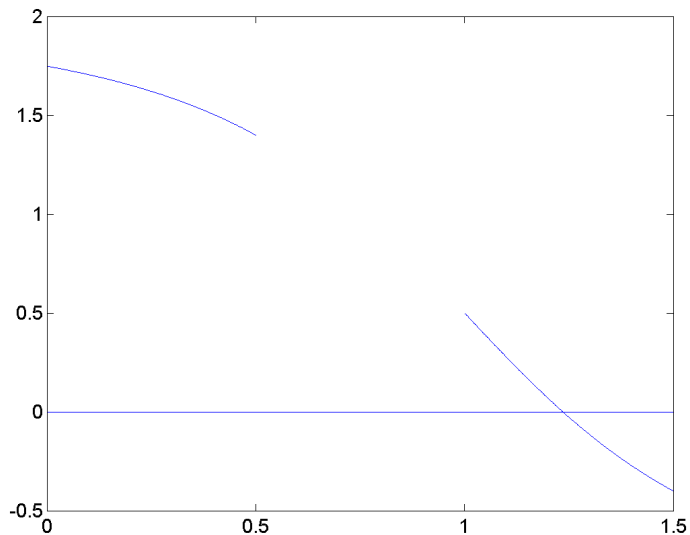
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Example 1



Modified definition of g

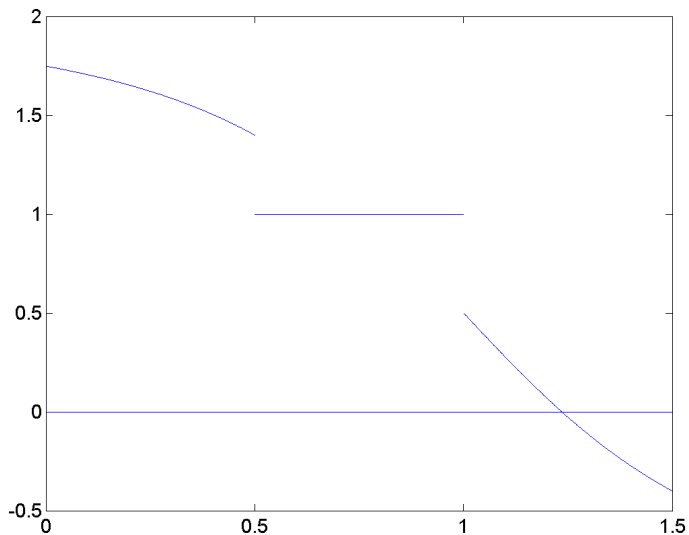
Let $\mathcal{E}(\theta)$ denote the eigenspace of $B(\theta)$ corresponding to its smallest eigenvalue, and let $N := \begin{pmatrix} L^T L & 0 \\ 0 & -\delta^2 \end{pmatrix}$.

Then

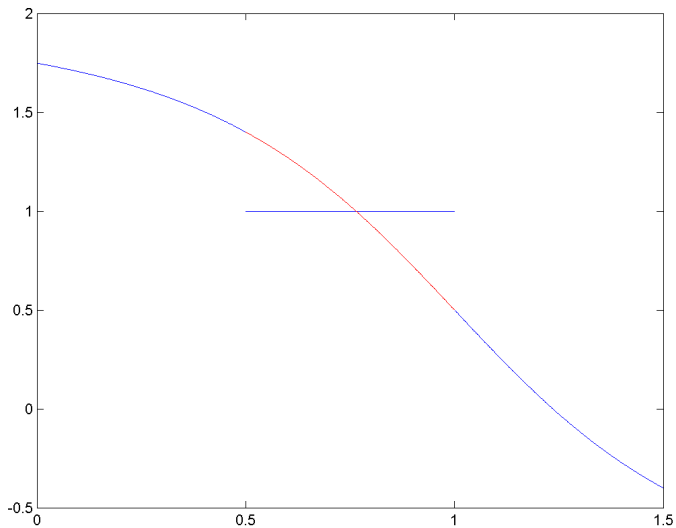
$$g(\theta) := \min_{y \in \mathcal{E}(\theta)} \frac{y^T N y}{y^T y} \quad (1)$$

is the minimal eigenvalue of the projection of N to $\mathcal{E}(\theta)$

Generalized g



Generalized g



Properties of g

Assume $\sigma_{\min}([AF, b]) < \sigma_{\min}(AF)$ holds, where the columns of $F \in \mathbb{R}^{n, n-k}$ form an orthonormal basis of the null space of L .

Then $g : [0, \infty) \rightarrow \mathbb{R}$ has the following properties:

- (i) If $\sigma_{\min}([A, b]) < \sigma_{\min}(A)$ then $g(0) > 0$
- (ii) $\lim_{\theta \rightarrow \infty} g(\theta) = -\delta^2$
- (iii) If the smallest eigenvalue of $B(\theta_0)$ is simple, then g is continuous at θ_0
- (iv) g is monotonically not increasing on $[0, \infty)$
- (v) Let $g(\hat{\theta}) = 0$ and let $y \in \mathcal{E}(\hat{\theta})$ such that $g(\hat{\theta}) = y^T N y / \|y\|^2$. Then the last component of y is different from 0.
- (vi) g has at most one root.

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Roots of g

If $\hat{\theta}$ is a positive root of g , then $x := -y(1 : n)/y(n + 1)$ solves the RTLS problem, where y denotes an eigenvector of $B(\hat{\theta})$ corresponding to its smallest eigenvalue.

However, g is not necessarily continuous.

If the multiplicity of the smallest eigenvalue of $B(\theta)$ is greater than 1 for some θ_0 , then g may have a jump discontinuity at θ_0 , and this may actually occur (cf. Example where g is discontinuous for $\theta_0 = 0.5$ and $\theta_0 = 1$). Hence, the question arises whether g may jump from a positive value to a negative one, such that it has no positive root.

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Theorem

Consider the standard case $L = I$, where $\sigma_{\min}([A, b]) < \sigma_{\min}(A)$ and $\delta^2 < \|x_{TLS}\|^2$.

Assume that the smallest eigenvalue of $B(\theta_0)$ is a multiple one for some θ_0 .

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General case

For general regularization matrices L it may happen, that g does not have root, but it jumps below zero at some θ_0 .

Example: Let

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 0 \\ \sqrt{5} \end{pmatrix}, \quad L = \begin{pmatrix} \sqrt{2} & 0 \\ 0 & 1 \end{pmatrix}, \quad \delta = \sqrt{3}.$$

Then, $1 = \sigma_{\min}(A) > \tilde{\sigma}_{\min}([A, b]) \approx 0.8986$ holds, and the corresponding TLS problem has the solution

$$x_{TLS} = (A^T A - \tilde{\sigma}_{\min}^2 I)^{-1} A^T b \approx \begin{pmatrix} 5.1926 \\ 0 \end{pmatrix}.$$

The constraint is active, because $\delta^2 = 3 < 53.9258 \approx \|Lx_{TLS}\|_2^2$ holds, and $\mathcal{N}(L) = \{0\}$, so the RTLS problem is solvable.

The corresponding function $g(\theta)$ has got two jumps, one at $\theta = 0.25$ and another one at $\theta = 1$ which jumps below zero.

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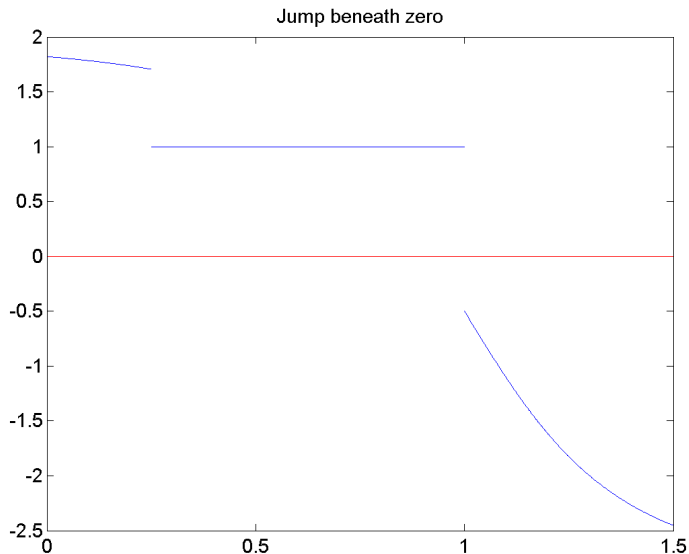
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Jump below zero



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A jump discontinuity of g only appears if $\lambda_{\min}(B(\theta_0))$ is a multiple eigenvalue of $B(\theta_0)$.

Hence, there exists $v \in \mathcal{E}(\theta_0)$ with vanishing last component, and clearly the Rayleigh quotient $R_N(v)$ of N at v is positive.

Since $g(\theta_0) < 0$, there exists some $w \in \mathcal{E}(\theta_0)$ with $R_N(w) = g(\theta_0) < 0$ and non vanishing last component.

Hence, for some linear combination of v and w we have $R_N(\alpha v + \beta w) = 0$, and scaling the last component to -1 yields a solution of the RTLS problem

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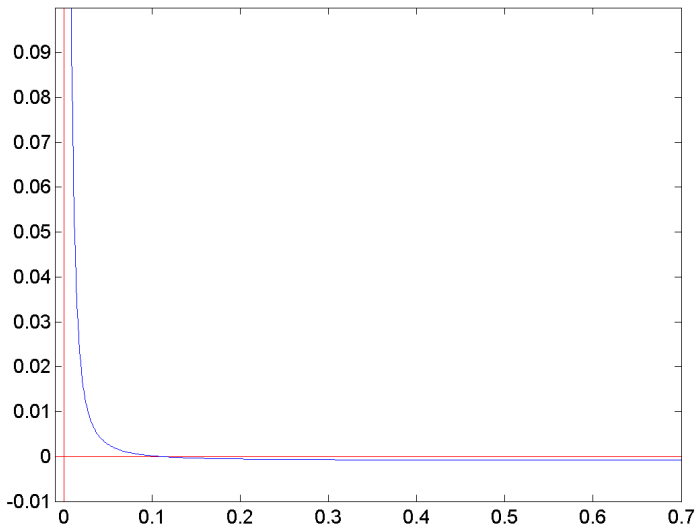
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Typical g

Typical behaviour of g



Method of Renaut and Guo

Assuming that g is continuous and strictly monotonically decreasing Renaut and Guo derived the following update

$$\theta_{k+1} = \theta_k + \frac{\theta_k}{\delta^2} g(\theta_k)$$

for solving

$$g(\theta) = \frac{\|Lx\|^2 - \delta^2}{\|x\|^2 + 1} = 0,$$

where at step k , $(x_{\theta_k}^T, -1)^T$ is the eigenvector of $B(\theta_k) = M + \theta_k N$ corresponding to $\lambda_{\min}(B(\theta_k))$.

Additionally, back tracking was introduced to make the method converge, i.e. the update was modified to

$$\theta_{k+1} = \theta_k + \iota \frac{\theta_k}{\delta^2} g(\theta_k)$$

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RTLSEVP

Require: Initial guess $\theta_0 > 0$

- 1: compute the smallest eigenvalue $\lambda_{\min}(B(\theta_0))$, and the corresponding eigenvector $(x_0^T, -1)^T$
- 2: compute $g(\theta_0)$, and set $k = 1$
- 3: **while** not converged **do**
- 4: $\iota = 1$
- 5: **while** sign condition not satisfied **do**
- 6: update θ_{k+1}
- 7: compute the smallest eigenvalue $\lambda_{\min}(B(\theta_{k+1}))$, and the corresponding eigenvector $(x_{k+1}^T, -1)^T$
- 8: **if** $g(\theta_k)g(\theta_{k+1}) < 0$ **then**
- 9: $\iota = \iota/2$
- 10: **end if**
- 11: **end while**
- 12: **end while**
- 13: $X_{RTLS} = X_{k+1}$

Although in general the assumptions are not satisfied, the algorithm may be applied to the modified function g since generically the smallest eigenvalue of $B(\theta)$ is simple and solutions of the RTLS problem correspond to the root of g . However, the method as suggested by Renault and Guo suffers two drawbacks:

The suggested eigensolver in line 7 of algorithm for finding the smallest eigenpair of $B(\theta_{k+1})$ is the Rayleigh quotient iteration. Due to the required LU factorizations in each step this method is very costly. An approach like this does not turn to account the fact that the matrices $B(\theta_k)$ converge as θ_k approaches the root $\hat{\theta}$ of g . We suggest a method which takes advantage of information acquired in previous iteration steps by thick starts.

Secondly, the safeguarding by back tracking hampers the convergence of the method considerably. We propose to replace it by an algorithm which encloses the root in bounds and utilizes the asymptotic behaviour of g .

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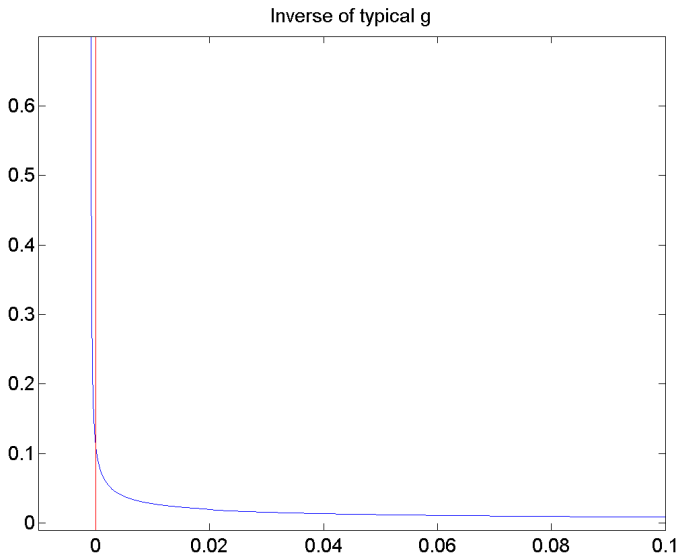
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Typical g^{-1} 

Root finding

Given three pairs $(\theta_j, g(\theta_j))$, $j = 1, 2, 3$ with

$$\theta_1 < \theta_2 < \theta_3 \quad \text{and} \quad g(\theta_1) > 0 > g(\theta_3) \quad (*)$$

we determine the rational interpolation

$$h(\gamma) = \frac{p(\gamma)}{\gamma + \delta^2}, \quad \text{where } p \text{ is a polynomial of degree 2,}$$

and p is chosen such that $h(g(\theta_j)) = \theta_j$, $j = 1, 2, 3$.

If g is strictly monotonically decreasing in $[\theta_1, \theta_3]$ then this is a rational interpolation of $g^{-1} : [g(\theta_3), g(\theta_1)] \rightarrow \mathbb{R}$.

As our next iterate we choose $\theta_4 = h(0)$. In exact arithmetic $\theta_4 \in (\theta_1, \theta_3)$, and we replace θ_1 or θ_3 by θ_4 such that the new triple satisfies $(*)$.

It may happen that due to nonexistence of the inverse g^{-1} on $[g(\theta_3), g(\theta_1)]$ or due to rounding errors very close to the root $\hat{\theta}$, θ_4 is not contained in the interval (θ_1, θ_3) . In this case we perform a bisection step such that the interval definitely still contains the root.

If a discontinuity at or close to the root is encountered, then a very small $\epsilon = \theta_3 - \theta_1$ appears with relatively large $g(\theta_1) - g(\theta_3)$. In this case we terminate the iteration and determine the solution as described before.

Root finding

Given three pairs $(\theta_j, g(\theta_j))$, $j = 1, 2, 3$ with

$$\theta_1 < \theta_2 < \theta_3 \quad \text{and} \quad g(\theta_1) > 0 > g(\theta_3) \quad (*)$$

we determine the rational interpolation

$$h(\gamma) = \frac{p(\gamma)}{\gamma + \delta^2}, \quad \text{where } p \text{ is a polynomial of degree 2,}$$

and p is chosen such that $h(g(\theta_j)) = \theta_j$, $j = 1, 2, 3$.

If g is strictly monotonically decreasing in $[\theta_1, \theta_3]$ then this is a rational interpolation of $g^{-1} : [g(\theta_3), g(\theta_1)] \rightarrow \mathbb{R}$.

As our next iterate we choose $\theta_4 = h(0)$. In exact arithmetic $\theta_4 \in (\theta_1, \theta_3)$, and we replace θ_1 or θ_3 by θ_4 such that the new triple satisfies $(*)$.

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Solving sequence of eigenproblems

To evaluate g one has to solve an eigenproblem

$$B(\theta_k)y = (M + \theta_k N)y = \lambda y$$

with $M = [A, b]^T [A, b]$ and $N = \begin{pmatrix} L^T L & 0 \\ 0 & -\delta^2 \end{pmatrix}$.

As for the sequence of quadratic eigenproblems in the approach of Sima, Golub, Van Huffel this can be done with the Nonlinear Arnoldi method and thick starts taking advantage of the information gathered in previous iteration steps.

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Numerical example

Numerical examples are obtained from Hansen's regularization tool box:

We added white noise to the data of `heat(1)` with noise level 1% and 10%, and chose L_1 to be an approximate first order derivative (marked 'a') and a nonsingular approximation (marked 'b').

The following table contains the average CPU time for 100 test problems of dimensions $n = 1000$, $n = 2000$, and $n = 4000$ (CPU: Pentium D, 3.4 GHz).

	n	LY 1a	LY 1b	SO 1a	SO 1b	NLA 1a	NLA 1b	NLA 2a
1%	1000	0.53	0.47	0.52	0.63	0.35	0.36	0.19
	2000	1.28	1.19	1.13	1.02	1.08	0.99	0.60
	4000	4.94	4.68	4.37	3.78	4.21	3.88	2.65
10%	1000	0.55	0.46	0.48	0.45	0.36	0.32	0.19
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Numerical example 2: tomo

'tomo' is a discretization of a Fredholm integral equation of the first kind with 2D domain. $L_2 = \begin{pmatrix} L_1 \otimes I \\ I \otimes L_1 \end{pmatrix}$ is an approximation of the first order derivative.

The following tabel contains the average CPU time for 100 test problems.

	n	Li&Ye 1a	SOAR 1a	NL Arn. 1a	NL Arn. 1b	NL Arn. 2a
1%	30x30	0.77	1.01	1.02	1.24	0.20
	40x40	2.62	2.55	2.07	2.81	0.54
	50x50	6.93	6.44	4.78	6.03	3.86
10%	30x30	0.77	1.02	1.00	1.23	0.21
	40x40	2.63	2.56	2.02	2.88	0.56
	50x50	6.89	6.38	4.80	5.98	3.83

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L-curve

Several methods are available for determining the regularization parameter δ :
 Discrepancy principle, Cross validation, Information Criteria, L-curve

Idea of the L-curve:

- Developed to balance $\|Ax_\lambda - b\|^2$ and $\|Lx_\lambda\|^2$ in Tikhonov approach
 $\|Ax - b\|^2 + \lambda\|Lx\|^2 = \min_x$
- Works as well for $\|Ax_\delta - b\|^2 = \min_x$ subject to $\|Lx_\delta\| \leq \delta$
- Can be extended to $f(x_\delta) = \frac{\|Ax_\delta - b\|^2}{1 + \|x_\delta\|^2} = \min_x$ s.t. $\|Lx_\delta\| \leq \delta$
- Choose set of $\delta_i, i = 1, \dots, \ell$ and solve one RTLS problem for each δ_i

Note, there is no discrete Picard condition for RTLS problems,
 nor there exists a tool like GSVD to obtain L-curve analytically.

We simply try to balance the function value $f(x_\delta)$ and the size of the norm $\|Lx_\delta\|$, which seems to work fine in most cases.

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L-curve

- Use Nonlinear Arnoldi to solve sequence of RTLS problems
- This means solving a sequence of a sequence of QEPs or EVPs
- Updating projected problems is trivial, because all stored matrices are independent of parameter δ_j
- Reusing search space V during sequence of sequence of eigenproblems
- If search space grows too large, include restart strategy

Restart strategy:

- If dimension $p \ll n$ of search space $\text{span}(V)$ is reached, restart Nonlinear Arnoldi by subspace of $q < p$ eigenvectors corresponding to rightmost/smallest eigenvalues of $T_k(\lambda)$.
- Values can be set in advance (e.g. $p = 45, q = 5$), nice for memory allocation purposes
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Example 1 – RTLSQEP solves 20 RTLS problem

Problem: *phillips*(2000)

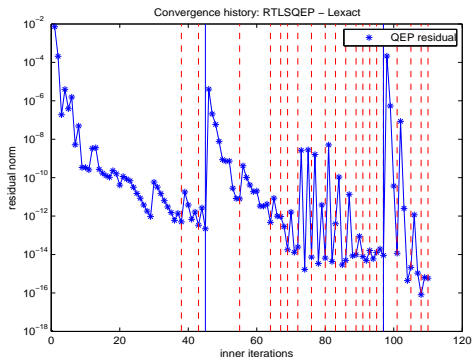


Figure: Convergence history of RTLSQEP for different δ_i

- Restart performed if dimension of search space exceeds $p = 45$
- With subspace corresponding to $q = 5$ rightmost eigenvalues
- Each RTLS problem is solved by very few QEPs

Example 1 – L-curve of 20 RTLS problem

- $\delta_i = \delta_{true} \cdot (0, 0001 \dots 100)$, $\delta_{true} = \|Lx_{true}\|$, $i = 1, \dots, 20$

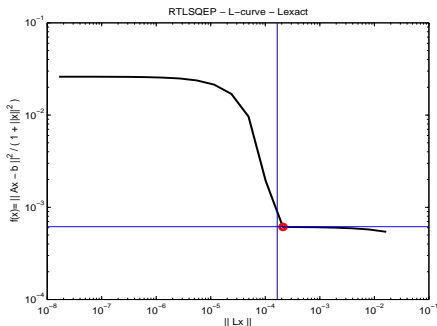


Figure: L-curve of RTLSQEP

- L-curve of RTLS looks similar to L-curve of RLS
- 120 inner iterations for 20 RTLS problems (\rightarrow 500 MatVecs)
- 70 inner iterations for 20 RLS problems (\rightarrow 280 MatVecs)
- Computation time 4,2sec for RTLS, and 2,4sec for RLS

Example 2 – RTLSQEP solves 20 RTLS problem

- Problem *deriv2(2000)*, discretized Fredholm integral equation of first-kind
- $\delta_i = \delta_{true} \cdot (0, 0001 \dots 100)$, $\delta_{true} = \|Lx_{true}\|$, $i = 1, \dots, 20$

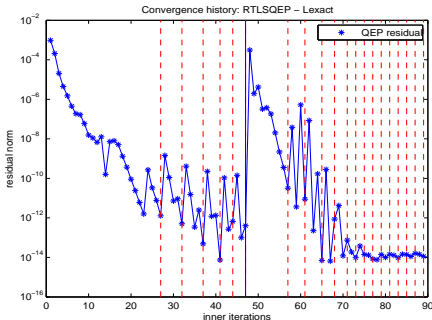


Figure: Convergence history of RTLSQEP for different δ_i

- 90 inner iterations for 20 RTLS problems (\rightarrow 360 MatVecs)
- Computation time 3sec (resp. 2, 3sec for 20 RLS problems)

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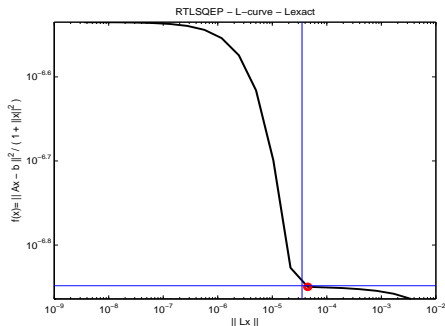


Figure: L-curve of RTLSQEP

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Example 5 – Solution at corner of L

$$L = \begin{pmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix} \quad \text{or} \quad \tilde{L} = \begin{pmatrix} \varepsilon & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix}$$

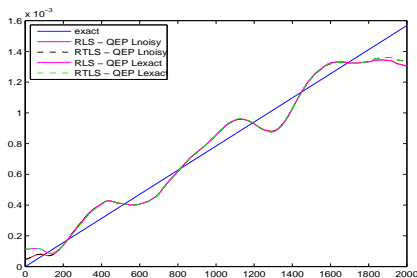


Figure: Solution curves for RLS and RTLS

- Not much difference between RLS and RTLS approach
- Little difference between approaches with different regularization matrices L and \tilde{L}

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Conclusions

- RTLS problems can be solved efficiently by sequence of EVPs or QEPs
- Nonlinear Arnoldi can reuse all previous information
- Determine hyperparameter δ via L-curve
- Restart strategy necessary
- Computational complexity stays $\mathcal{O}(mn)$, if number of MatVecs smaller than n

References

- R. Renaut and H. Guo, Efficient Algorithms for Solution of Regularized Total Least Squares, SIAM J. Matrix Anal. Appl., 2005, vol. 26, p. 457 – 476
- D. Sima, S. Van Huffel and G.H. Golub, Regularized total least squares based on quadratic eigenvalue problem solvers, 2004, BIT Numerical Mathematics, vol. 44, p. 793 – 812
- J. Lampe and H. Voss, On a Quadratic Eigenproblem Occuring in Regularized Total Least Squares, Comput. Stat. Data Anal., 2007, vol. 52/2, p. 1090 – 1102
- J. Lampe and H. Voss, Global convergence of RTLSQEP: a solver of regularized total least squares problems via quadratic eigenproblems, 2008, Math. Modelling Anal., vol. 13, p. 55 – 66
- J. Lampe and H. Voss, A fast algorithm for solving regularized total least squares problems, 2008, Electr. Trans. Numer. Anal., vol. 31, p. 12 – 24
- J. Lampe and H. Voss, Solving Regularized Total Least Squares Problems Based on Eigenproblems, 2008, to appear in Taiwanese Journal of Mathematics
- J. Lampe and H. Voss, Efficient determination of the Hyperparameter in Regularized Total Least Squares Problems, 2009, submitted