Solving Regularized Total Least Squares Problems

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Total Least Squares Problem

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

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

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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

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

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

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In statistics this approach is called errors-in-variables problem or orthogonal regression, in image deblurring blind deconvolution

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Using the orthogonal distance this problems can be rewritten as (cf. Golub, Van Loan 1980)

Find $x \in \mathbb{R}^n$ such that

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

Regularized Total Least Squares Problem ct.

Theorem 1: Let $\mathcal{N}(L)$ be the null space of L. If

$$f^* = \inf\{f(x) \,:\, \|Lx\|^2 = \delta^2\} < \min_{x\in\mathcal{N}(L),\, x\neq 0} \frac{\|Ax\|^2}{\|x\|^2} \qquad (1)$$

then

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Conversely, if problem (2) admits a global minimum, then

$$f^* \leq \min_{x \in \mathcal{N}(L),\, x \neq 0} \frac{\|Ax\|^2}{\|x\|^2}$$

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Under the condition (1) problem (2) is equivalent to the quadratic optimization problem

$$\|Ax - b\|^2 - f^*(1 + \|x\|^2) = \min! \quad \text{subject to } \|Lx\|^2 = \delta^2, \qquad (3)$$

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For fixed $y \in \mathbb{R}^n$ find $x \in \mathbb{R}^n$ such that

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

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Lemma 1 (Sima, Van Huffel, Golub 2004)
Problem (P_y) admits a global minimizer if and only if

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

RTLSQEP Method (Sima, Van Huffel, Golub 2004)

Lemma 2

Assume that y satisfies conditions of Lemma 1 and $\|Ly\| = \delta$, and let z be a global minimizer of problem (P_y). Then it holds that

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

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Proof

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

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

Require: x^0 satisfying conditions of Lemma 1 and $\|Lx^0\| = \delta$.
for $m = 0, 1, 2, \dots$ until convergence **do**
Determine global minimizer x^{m+1} of

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

end for

RTLS Method

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

RTLS Method

Theorem 2
Assume that $(\hat{\lambda}, \hat{x})$ solves the first order conditions.

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

If $\|Ly\| = \delta$ and $\hat{\lambda}$ is the maximal Lagrange multiplier then $\hat{x}$ is a global minimizer of problem (P_y).

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Proof
The statement follows immediately from the following equation which can be shown similarly as in W. Gander (1981):
If (λ_j, z^j), $j = 1, 2$, are solutions of $(*)$ then it holds that

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

A quadratic eigenproblem

$$(A^TA - f(y)I)x + \lambda L^TLx = A^Tb, \quad \|Lx\|^2 = \delta^2 \quad (*)$$

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$$Wz + \lambda z := L^{-T}(A^TA - f(y)I)L^{-1}z + \lambda z = L^{-T}A^Tb =: h, \; z^Tz = \delta^2.$$

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

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

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

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

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

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).

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

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

is continuous, and that the real equation

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

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Assume that

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

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

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

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- 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

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

$$\tilde{V} \cap D \neq \emptyset \quad \text{and} \quad \lambda_j = \inf_{v \in \tilde{V} \cap D} p(v)$$

is contained in $D \cup \{0\}$, and the maxmin characterization of λ_j can be replaced by

$$\lambda_j = \max_{\substack{\dim V = j, \\ V \setminus \{0\} \subset D}} \min_{v \in V \setminus \{0\}} p(v).$$

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

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is a parabola which attains its minimum at

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Let $J = (-\lambda_{\min}, \infty)$ where $\lambda_{\min}$ 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.

Characterization of maximal real eigenvalue

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

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

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If $h \perp V_{\min}$, and if the minimum eigenvalue $\mu_{\min}$ of $T(-\lambda_{\min})$ is negative, then for the corresponding eigenvector y_{min} it holds

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If $h \perp V_{\min}$, and $T(-\lambda_{\min})$ is positive semi-definite, then

$$f(-\lambda_{\min}, x) = x^H T(-\lambda_{\min}) x \ge 0 \quad \text{for every } x \neq 0,$$

and $D = \emptyset$.

Characterization of maximal real eigenvalue ct.

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

$$f(\lambda, x) = \|(W + \lambda I)x\|^2 > 0 \quad \text{for every } \lambda \in J,$$

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

$$x^H T(\lambda)x = \lambda^2 \|x\|^2 + 2\lambda x^H Wx + \|Wx\|^2 - |x^H h|^2/\delta^2 = 0.$$

Hence, the real part of λ satisfies

$$\text{real}(\lambda) = -\frac{x^H Wx}{x^H x} \leq -\lambda_{\min}.$$

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- 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

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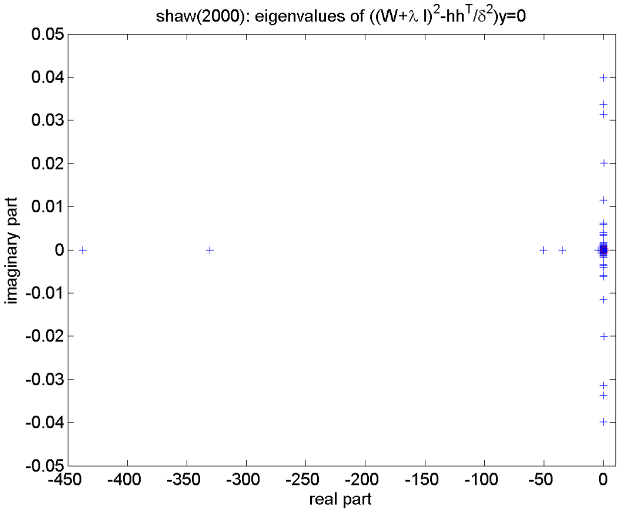
$$\hat{\lambda} = \max_{x \in D} p(x).$$

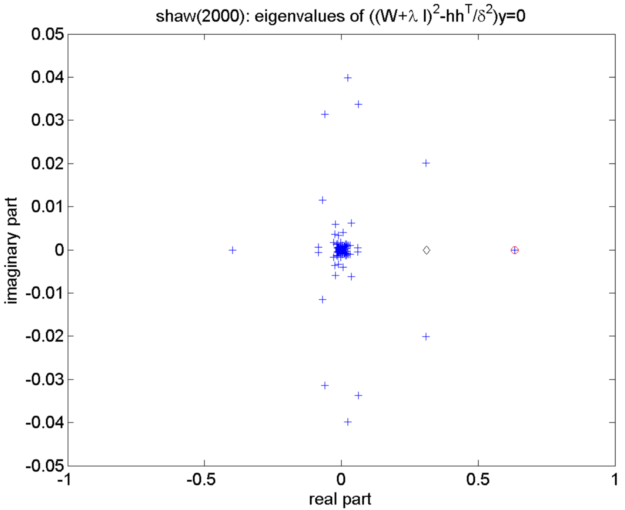
- $\hat{\lambda}$ is the right most eigenvalue of (QEP), i.e.

$$\text{real}(\lambda) \le -\lambda_{\min} \le \hat{\lambda} \quad \text{for every eigenvalue } \lambda \ne \hat{\lambda} \text{ of (QEP).}$$

Example


shaw(2000): eigenvalues of ((W+λ I)^2-hh^T/δ^2)y=0
0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
imaginary part
-450
-400
-350
-300
-250
-200
-150
-100
-50
0
real part

Example: close up



Positivity of $\hat{\lambda}$

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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.

The following theorem characterizes the case that the right–most eigenvalue is negative.

Positivity of $\hat\lambda$ ct.

Theorem 4
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

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

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

Convergence

Theorem 5
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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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

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

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From the monotonicity of $f(x^m)$ it follows that $\lim_{j\to\infty} f(x^{m_j-1}) = f(x^*)$

Proof ct.

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

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

where λ^* is the maximal Lagrange multiplier.

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

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

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

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. 2004)

Krylov subspace method: Li & Ye 2003

For $A, B \in \mathbb{R}^{n\times n}$ such that some linear combination of A and B is a matrix of rank q with an Arnoldi-type process a matrix $Q \in \mathbb{R}^{n\times m+q+1}$ with orthonormal columns and two matrices $H_a \in \mathbb{R}^{m+q+1\times m}$ and $H_b \in \mathbb{R}^{m+q+1\times m}$ with lower bandwidth $q+1$ are determined such that

$$AQ(:,1:m) = Q(:,1:m+q+1)H_a \text{ and } BQ(:,1:m) = Q(:,1:m+q+1)H_b.$$

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$$(\lambda^2 I - \lambda A - B)y = 0$$

are obtained from its projection onto span$Q(:,1:m)$ which reads

$$(\lambda^2 I_m - \lambda H_a(1:m,1:m) - H_b(1:m,1:m))z = 0.$$

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For the quadratic eigenproblem $((W+\lambda I)^2 - \delta^{-2}hh^T)x = 0$ the algorithm of Li & Ye is applied with $A = -W$ and $B = hh^T$ from which the projected problem

$$(\theta^2 I - 2\theta H_a(1:m,1:m) - H_a(1:m+2,1:m)^T H_a(1:m+2,m) - \delta^{-2}H_b(1:m,1:m))z = 0$$

is easily obtained.

SOAR: Bai & Su 2005

The Second Order Arnoldi Reduction method is based on the observation that the Krylov space of the linearization

$$\begin{pmatrix} A & B \\ I & O \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = \lambda \begin{pmatrix} I & O \\ O & I \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix}$$

of $(\lambda^2 I - \lambda A - B)y = 0$ with initial vector $\begin{pmatrix} r_0 \\ 0 \end{pmatrix}$ has the form

$$\mathcal{K}_k = \left\{ \begin{pmatrix} r_0 \\ 0 \end{pmatrix}, \begin{pmatrix} r_1 \\ r_0 \end{pmatrix}, \begin{pmatrix} r_2 \\ r_1 \end{pmatrix}, \dots, \begin{pmatrix} r_{k-1} \\ r_{k-2} \end{pmatrix} \right\}$$

where

$$\begin{aligned} r_1 &= Ar_0 \\ r_j &= Ar_{j-1} + Br_{j-2}, \text{ for } j \geq 2. \end{aligned}$$

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The entire information on $\mathcal{K}_k$ is therefore contained in the Second Order Krylov Space

$$\mathcal{G}_k(A, B) = \text{span}\{r_0, r_1, \dots, r_{k-1}\}.$$

SOAR determines an orthonormal basis of $\mathcal{G}_k(A, B)$.

Nonlinear Arnoldi Method

start with initial basis V, $V^T V = I$
determine preconditioner $M \approx T(\sigma)^{-1}$, σ close to wanted eigenvalue
find largest eigenvalue μ of $V^T T(\mu) Vy = 0$ and corresponding eigenvector y
set $u = Vy$, $r = T(\mu)u$
while $\|r\|/\|u\| > \epsilon$ **do**
    $v = Mr$
    $v = v - VV^T v$
    $\tilde{v} = v/\|v\|$, $V = [V, \tilde{v}]$
    find largest eigenvalue μ of $V^T T(\mu) Vy = 0$ and corresponding eigenvector y
    set $u = Vy$, $r = T(\mu)u$
end while

Reuse of information

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

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

$$T_m(\lambda)z = 0$$

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

Thick and early updates

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

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

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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 h_m^T Vu = 0
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one has to keep only CV, DV, $S^T V$, and $g^T V$.

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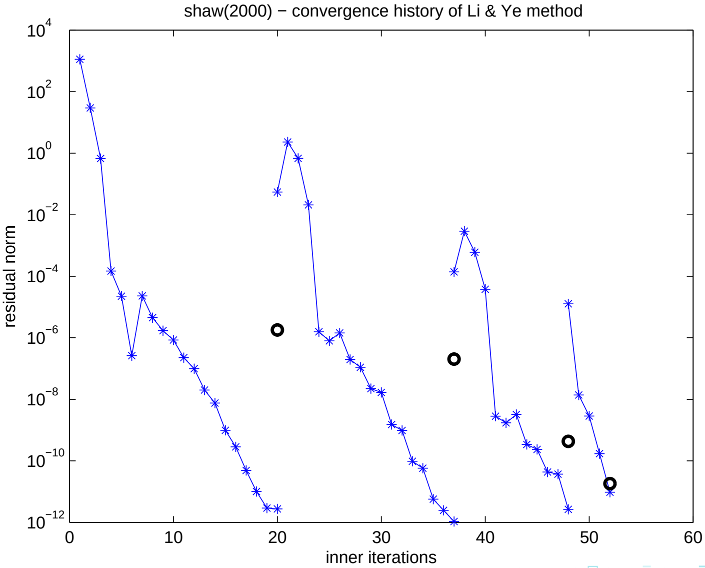
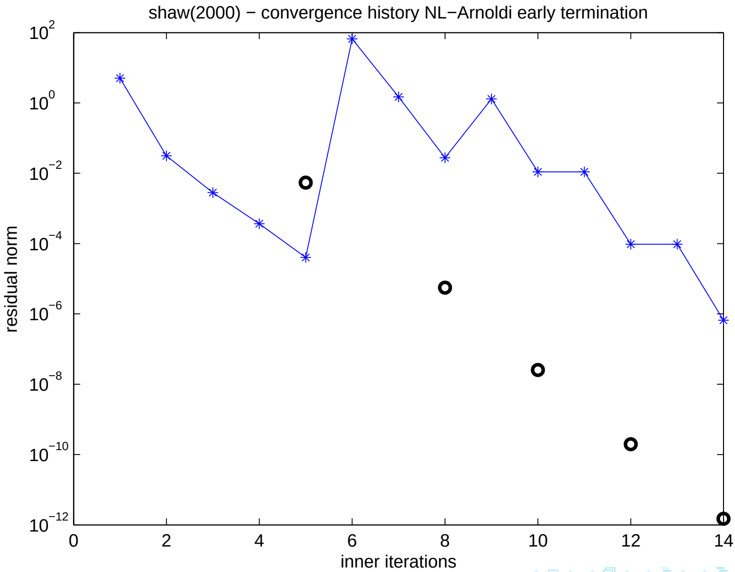
Since it is inexpensive to obtain updates of W_m and h_m we decided to terminate the inner iteration long before convergence, namely if the residual of the quadratic eigenvalue was reduced by at least 10^{-2}. This reduced the computing time further.

Example: shaw(2000); Li & Ye



shaw(2000); Early updates



Necessary Condition: Golub, Hansen, O'Leary 1999

The RTLS solution x satisfies

$$(A^TA + \lambda_I I + \lambda_L L^T L)x = A^T b, \quad \|Lx\|^2 = \delta^2$$

where

$$\begin{aligned} \lambda_I &= -f(x) \\ \lambda_L &= -\frac{1}{\delta^2}(b^T(Ax - b) - \lambda_I) \end{aligned}$$

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Eliminating λ_I:

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

iterating on $f(x^m)$, and solving via quadratic eigenproblems yields the method of Sima, Van Huffel and Golub.

Necessary Condition: Renaut, Guo 2002,2005

The RTLS solution x satisfies the eigenproblem

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

where

$$\begin{aligned} B(x) &= [A,b]^T[A,b] + \lambda_L(x)\begin{pmatrix} L^TL & 0 \\ 0 & -\delta^2 \end{pmatrix} \\ \lambda_I &= -f(x) \\ \lambda_L &= -\frac{1}{\delta^2}(b^T(Ax-b)-\lambda_I) \end{aligned}$$

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Conversely, if $\left(-\hat{\lambda}, \begin{pmatrix} \hat{x} \\ -1 \end{pmatrix}\right)$ is an eigenpair of $B(\hat{x})$, and $\lambda_L(\hat{x}) = -\frac{1}{\delta^2}(b^T(A\hat{x}-b)+f(\hat{x}))$, then $\hat{x}$ satisfies the necessary conditions of the last slide, and the eigenvalue is given by $\hat{\lambda} = -f(\hat{x})$.

Method of Renaut, Guo 2005

For $\theta \in \mathbb{R}_+$ let $(x_\theta^T, -1)^T$ be the eigenvector corresponding to the smallest eigenvalue of

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

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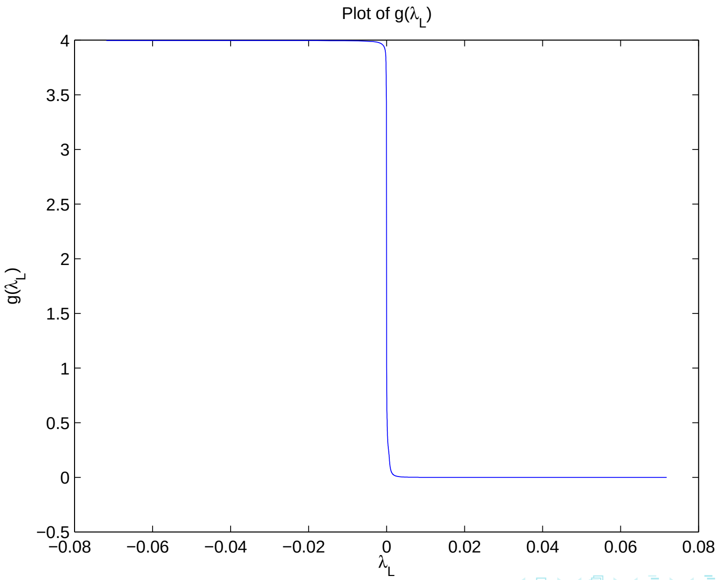
Problem Determine θ such that $g(\theta) = 0$ where

$$g(\theta) := \frac{\|Lx_\theta\|^2 - \delta^2}{1 + \|x_\theta\|^2}.$$

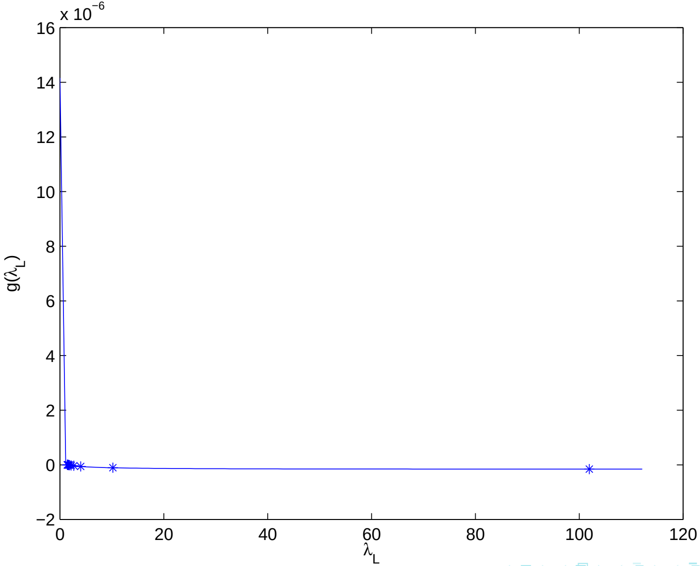
Given θ_k, the eigenvalue problem (*) is solved by the Rayleigh quotient iteration, and θ_k is updated according to

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

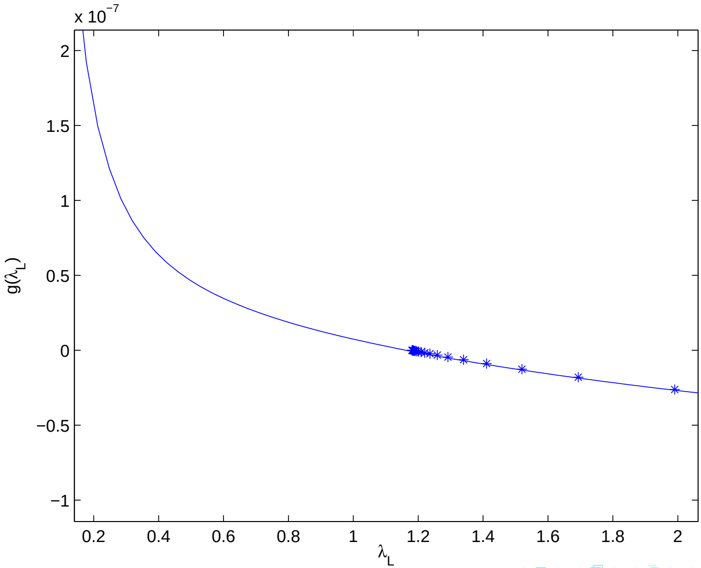
Typical g


Plot of g(λ_L)
4
3.5
3
2.5
2
1.5
1
0.5
0
−0.5
−0.08
−0.06
−0.04
−0.02
0
0.02
0.04
0.06
0.08
λ_L
g(λ_L)

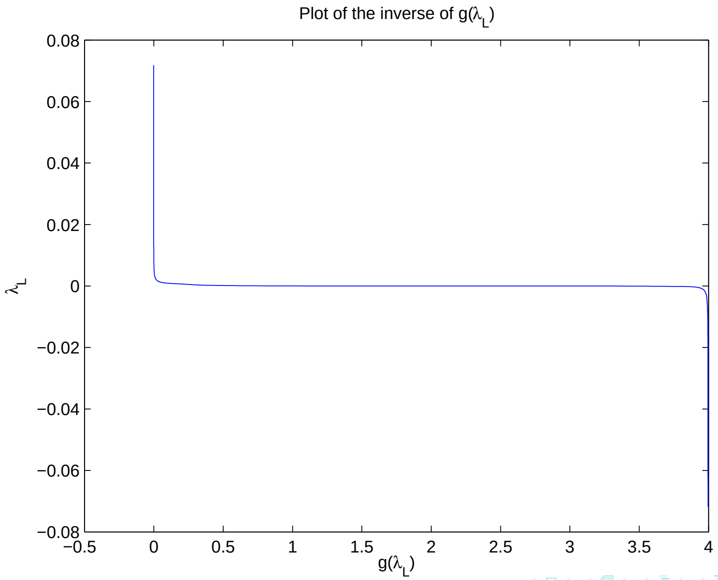
Back tracking



Close up



Typical g^{-1}



Plot of the inverse of g(λL)
0.08
0.06
0.04
0.02
0
−0.02
−0.04
−0.06
−0.08
λL
−0.5
0
0.5
1
1.5
2
2.5
3
3.5
4
g(λL)

Rational interpolation

Assumption A: Let $\theta_1 < \theta_2 < \theta_3$ such that $g(\theta_3) < 0 < g(\theta_1)$.

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Let $p_1 < p_2$ be the poles of g^{-1}, let

$$h := \frac{\alpha + \beta x + \gamma x^2}{(p_2 - x)(x - p_1)}$$

be the interpolation of g^{-1} at $(g(\theta_j), \theta_j)$, $j = 1, 2, 3$, and set $\theta_4 = h(0)$.

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Drop θ_1 or θ_3 such that the remaining θ values satisfy assumption A, and repeat until convergence.

To evaluate $g(\theta)$ one has to solve the eigenvalue problem $B(\theta)x = \mu x$ which can be done efficiently by the nonlinear Arnoldi method starting with the entire search space of the previous step.

Numerical example

We added white noise to the data of phillips(n) and deriv2(n) with noise level 1%, and chose L to be an approximate first derivative.

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

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problem	n	SOAR	Li & Ye	NL Arn.	R & G
phillips	1000	0.11	0.13	0.05	0.07
	2000	0.38	0.39	0.15	0.19
	4000	1.30	1.30	0.66	0.70
deriv2	1000	0.12	0.09	0.06	0.05
	2000	0.31	0.28	0.18	0.17
	4000	1.25	1.06	0.69	0.38

Numerical example ct.

We added white noise to the data of phillips(n) and deriv2(n) with noise level 10%, and chose L to be an approximate first derivative.

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

problem	n	SOAR	Li & Ye	NL Arn.	R & G
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	2000	0.45	0.44	0.16	0.23
	4000	1.16	1.39	0.64	0.74
deriv2	1000	0.10	0.08	0.05	0.05
	2000	0.27	0.24	0.16	0.18
	4000	0.99	0.93	0.64	0.43

Conclusions

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THANK YOU FOR YOUR ATTENTION