# On a Quadratic Eigenproblem Occuring in Regularized Total Least Squares

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**Total Least Squares** 

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- Regularized total least squares problems
- A quadratic eigenproblem
- Nonlinear maxmin characterization
- The maximum real solution of a quadratic eigenproblem

# **Total Least Squares Problem**

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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.

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

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

 $\|(A, b) - (\tilde{A}, \tilde{b})\|_F^2 = \min!$  subject to  $\tilde{A}x = \tilde{b}$ ,

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

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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

$$\frac{\|Ax - b\|_2^2}{1 + \|x\|_2^2} = \min! \quad \text{subject to } \|Lx\|_2^2 \le \delta^2.$$

Regularized total least squres problems

# Regularized Total Least Squares Problem ct.

If  $\delta > 0$  is chosen small enough (e.g.  $\delta < \|Lx_{TLS}\|$  where  $x_{TLS}$  is the solution of the TLS problem), then the constraint  $\|Lx\|_2^2 \le \delta^2$  is active, and the RTLS problem reads

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The first order optimality conditions are

$$B(x)x + \lambda L^{T}Lx = d(x), \quad \|Lx\|_{2}^{2} = \delta^{2}$$

where

$$B(x) = \frac{1}{1 + \|x\|_2^2} \Big( A^T A - f(x) I_n \Big), \ f(x) = \frac{\|Ax - b\|_2^2}{1 + \|x\|_2^2}, \ d(x) = \frac{A^T b}{1 + \|x\|_2^2}.$$

## Algorithm RTLSQEP: Sima, Van Huffel & Golub 2004

**Initialization** Let  $x^0$  be a starting vector. Compute  $B_0 := B(x^0)$  and  $d_0 = d(x^0)$ . Set j = 0

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stopping criterion if

$$\|B_{j+1}x^{j+1} + \lambda_{j+1}L^TLx^{j+1} - d_{j+1}\|_2 < \varepsilon$$

then STOP; else  $j \leftarrow j + 1$  and go to step j.

## A quadratic eigenproblem

#### Sima, van Huffel, Golub (2004)

The first order conditions can be solved via the maximal positive eigenvalue and corresponding eigenvector of a quadratic eigenproblem

$$((W + \lambda I)^2 - \delta^{-2}hh^T)u = 0$$
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The quadratically constrained least squares problem

$$||Ax - b||_2 = \min!$$
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can be solved by via one quadratic eigenproblem (QEP) where

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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 continuously differentiable, and that the real equation

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

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

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Assume that

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 for every  $x\in D.$ 

Regularized total least squres problems

#### maxmin characterization (V., Werner 1982)

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

$$W \cap D \neq \emptyset$$
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 Then T(λ)x = 0 has at least ℓ eigenvalues in J, and for *j* = 1,...,ℓ the *j*-largest eigenvalue λ<sub>j</sub> can be characterized by

$$\lambda_{j} = \max_{\substack{\dim V=j, \\ V \cap D \neq \emptyset}} \inf_{v \in V \cap D} p(v).$$
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• For  $j = 1, ..., \ell$  every j dimensional subspace  $V \subset \mathbb{C}^n$  with  $V \cap D \neq \emptyset$  and  $\lambda_j = \inf_{v \in V \cap D} p(v)$ 

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

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

#### Back to

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

is a parabola which attains its minimum at

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

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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.

Let  $x_{\min}$  be an eigenvector of W corresponding to  $\lambda_{\min}$ . Then

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

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If  $x_{min}^{H}h = 0$ , and the minimum eigenvalue  $\mu_{min}$  of  $T(-\lambda_{min})$  is negative, then for the corresponding eigenvector  $y_{min}$  it holds

$$f(-\lambda_{\min}, y_{\min}) = y_{\min}^H T(-\lambda_{\min}) y_{\min} = \mu_{\min} \|y_{\min}\|_2^2 < 0,$$

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If  $x_{min}^{H}h = 0$ , and  $T(-\lambda_{min})$  is positive semi-definite, then

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

and  $D = \emptyset$ .

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

$$f(\lambda, x) = \|(W + \lambda I)x\|_2^2 > 0$$
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Hence, *D* does not contain a two-dimensional subspace of  $\mathbb{R}^n$ , 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

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

Hence, the real part of  $\lambda$  satisfies

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

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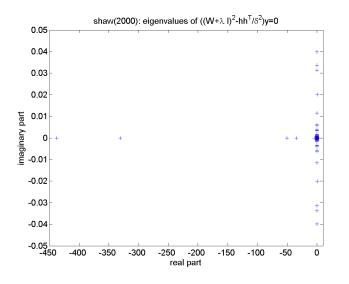
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•  $\hat{\lambda}$  is the right most eigenvalue of (QEP), i.e.

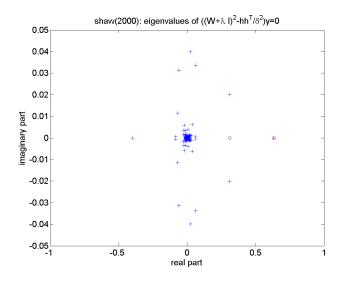
 $\operatorname{real}(\lambda) \leq -\lambda_{\min} \leq \hat{\lambda} \quad \text{for every eigenvalue } \lambda \neq \hat{\lambda} \text{ of (QEP)}.$ 

### Example



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## Example: close up



## Positivity of $\hat{\lambda}$

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  $\delta^{-2}hh^T$  is small enough, then the quadratic problem will have no positive eigenvalue, but the right–most eigenvalue will be negative.

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

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

# Positivity of $\hat{\lambda}$ ct.

#### Theorem 2

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

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

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For the standard case L = I the right-most eigenvalue  $\hat{\lambda}$  is always nonnegative if  $\delta < ||x_{TLS}||_2$ .

### Convergence

#### Theorem (Sima et al.) Assume that

$$\min_{x \neq 0: \ Lx=0} \frac{\|Ax\|_2^2}{\|x\|_2^2} \ge f(x^0). \quad (*)$$

Then the algorithm provides a sequence of vectors  $\{x^j\}$  for which the function *f* is monotonically decreasing:

$$0 \le f(x^{j+1}) \le f(x^j), \quad j = 0, 1, \ldots$$

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Beck & Teboulle (2006) proved the convergence of Sima's algorithm if the equality constraint is replaced by the inequality constraint  $\|Lx\|_2 \le \delta$ .