# On a Quadratic Eigenproblem Occuring in Regularized Total Least Squares 

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## Outline

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


## Total 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 $b$. In practical applications it may happen that all data are contaminated by noise.

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

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

where $\|\cdot\|_{F}$ denotes the Frobenius norm.

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Let $L \in \mathbb{R}^{k \times n}, k \leq n$ and $\delta>0$. Then the quadratically constrained formulation of the Regularized Total Least Squares (RTLS) problems reads:
Find $\tilde{A} \in \mathbb{R}^{m \times n}, \tilde{b} \in \mathbb{R}^{m}$ and $x \in \mathbb{R}^{n}$ such that

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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

$$
\frac{\|A x-b\|_{2}^{2}}{1+\|x\|_{2}^{2}}=\min !\quad \text { subject to }\|L x\|_{2}^{2} \leq \delta^{2}
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If $\delta>0$ is chosen small enough (e.g. $\delta<\left\|L x_{T L S}\right\|$ where $x_{T L S}$ is the solution of the TLS problem), then the constraint $\|L x\|_{2}^{2} \leq \delta^{2}$ is active, and the RTLS problem reads
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$$

The first order optimality conditions are

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

where

$$
B(x)=\frac{1}{1+\|x\|_{2}^{2}}\left(A^{T} A-f(x) I_{n}\right), f(x)=\frac{\|A x-b\|_{2}^{2}}{1+\|x\|_{2}^{2}}, d(x)=\frac{A^{T} b}{1+\|x\|_{2}^{2}}
$$

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

Initialization Let $x^{0}$ be a starting vector. Compute $B_{0}:=B\left(x^{0}\right)$ and $d_{0}=d\left(x^{0}\right)$. Set $j=0$

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step $j$ Find $x^{j+1}$ and $\lambda_{j+1}$ which solves

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Compute $B_{j+1}=B\left(x^{j+1}\right)$ and $d_{j+1}=d\left(x^{j+1}\right)$
stopping criterion if

$$
\left\|B_{j+1} x^{j+1}+\lambda_{j+1} L^{T} L x^{j+1}-d_{j+1}\right\|_{2}<\varepsilon
$$

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

$$
\left((W+\lambda I)^{2}-\delta^{-2} h h^{T}\right) u=0 \quad(Q E P)
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where $W \in \mathbb{R}^{k \times k}$ is symmetric, and $h \in \mathbb{R}^{k}$.

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can be solved by via one quadratic eigenproblem (QEP) where

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W=A^{T} A \quad \text { and } \quad h=A^{T} b
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For every fixed $x \in \mathbb{C}^{n}, x \neq 0$ assume that the real function

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

$$
\left.\frac{\partial}{\partial \lambda} f(\lambda ; x)\right|_{\lambda=p(x)}>0 \quad \text { for every } x \in D
$$

## 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

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W \cap D \neq \emptyset \quad \text { and } \quad \inf _{v \in W \cap D} p(v) \in J .
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- Then $T(\lambda) x=0$ has at least $\ell$ eigenvalues in $J$, and for $j=1, \ldots, \ell$ the $j$-largest eigenvalue $\lambda_{j}$ can be characterized by

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\begin{equation*}
\lambda_{j}=\max _{\substack{\operatorname{dim} \\ V \cap D=j \\ V \neq D}} \inf _{v \in V \cap D} p(v) . \tag{1}
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- For $j=1, \ldots, \ell$ every $j$ dimensional subspace $V \subset \mathbb{C}^{n}$ with

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V \cap D \neq \emptyset \text { 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{\text { dimb } \\ V\{\{ \} \in j}} \min _{V \in \mathcal{V} \backslash\{0\}} p(v) .
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is a parabola which attains its minimum at

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Let $J=\left(-\lambda_{\text {min }}, \infty\right)$ where $\lambda_{\text {min }}$ 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 $x_{\text {min }}$ be an eigenvector of $W$ corresponding to $\lambda_{\text {min }}$. Then
$f\left(-\lambda_{\text {min }}, x_{\text {min }}\right)=x_{\text {min }}^{H}\left(W-\lambda_{\text {min }}\right)^{2} x_{\text {min }}-\left|x_{\text {min }}^{H} h\right|^{2} / \delta^{2}=-\left|x_{\text {min }}^{H} h\right|^{2} / \delta^{2} \leq 0$

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Hence, if $x_{\min }^{H} h \neq 0$ then $x_{\text {min }} \in D$.
If $x_{\text {min }}^{H} h=0$, and the minimum eigenvalue $\mu_{\text {min }}$ of $T\left(-\lambda_{\min }\right)$ is negative, then for the corresponding eigenvector $y_{\text {min }}$ it holds

$$
f\left(-\lambda_{\min }, y_{\min }\right)=y_{\min }^{H} T\left(-\lambda_{\min }\right) y_{\min }=\mu_{\min }\left\|y_{\min }\right\|_{2}^{2}<0,
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and $y_{\text {min }} \in D$.
If $x_{\text {min }}^{H} h=0$, and $T\left(-\lambda_{\text {min }}\right)$ is positive semi-definite, then

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

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}^{2}>0 \quad \text { for every } \lambda \in J
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i.e. $x \notin D$.

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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

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

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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- If $x_{\text {min }}^{H} h=0$ and $T\left(-\lambda_{\text {min }}\right)$ is positive semi-definite, then $\hat{\lambda}:=-\lambda_{\min }$ is the maximal real eigenvalue of (QEP).


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- Otherwise, the maximal real eigenvalue is the unique eigenvalue $\hat{\lambda}$ of (QEP) in $J=\left(-\lambda_{\min }, \infty\right)$, and it holds

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

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

## Example



## 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 $\delta^{-2} h h^{T}$ 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 $\delta \leq\left\|L x_{\mathrm{TLS}}\right\|$ where $x_{\text {TLS }}$ 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 $\hat{\lambda} \mathrm{ct}$.

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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is negative if and only if $W$ is positive definite and

$$
\left\|W^{-1} h\right\|_{2}<\delta
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For the quadratic eigenproblem occuring in regularized total least squares it holds that

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For the standard case $L=I$ the right-most eigenvalue $\hat{\lambda}$ is always nonnegative if $\delta<\left\|x_{T L S}\right\|_{2}$.

## Convergence

Theorem (Sima et al.) Assume that

$$
\begin{equation*}
\min _{x \neq 0: L x=0} \frac{\|A x\|_{2}^{2}}{\|x\|_{2}^{2}} \geq f\left(x^{0}\right) \tag{*}
\end{equation*}
$$

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

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0 \leq f\left(x^{j+1}\right) \leq f\left(x^{j}\right), \quad j=0,1, \ldots
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Under the condition (*) every limit point of $\left\{x^{j}\right\}$ is a global minimizer of

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f(x):=\frac{\|A x-b\|_{2}^{2}}{1+\|x\|_{2}^{2}}, \quad \text { subject to }\|L x\|_{2}=\delta
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Beck \& Teboulle (2006) proved the convergence of Sima's algorithm if the equality constraint is replaced by the inequality constraint $\|L x\|_{2} \leq \delta$.

