On total least squares formulation in linear approximation problems with multiple right-hand sides

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1. Introduction

Consider an orthogonally invariant linear approximation problem

$$A\,X \approx B\,, \qquad A \in \mathbb{R}^{m\times n}\,, \quad X \in \mathbb{R}^{n\times d}\,, \quad B \in \mathbb{R}^{m\times d}$$

or, equivalently,

$$[\, B \,|\, A \,] \begin{bmatrix} -I_d \\ X \end{bmatrix} \approx 0\,.$$

With no loss of generality it is assumed:

- $A^T B \neq 0$ (otherwise the columns of B are not correlated with the columns of A, $X_{\mathrm{TLS}} \equiv 0$);
- $m \geq n + d$ (add zero rows if necessary).

The linear approximation problem specified by

$$\min_{X,E,G} \| [\, G \,|\, E \,] \|_F \quad \text{s.t.} \quad (A+E)\,X = B + G \qquad (1)$$

is called the total least squares (TLS) problem with the TLS solution $X_{\mathrm{TLS}} \equiv X$ and the correction matrix $[\, G \,|\, E \,]$.

When does the TLS solution exist?
Is it uniquely defined?

2. Single right-hand side case

With $d = 1$, the problem reduces to $A\,x \approx b$. Consider the singular value decomposition (SVD)

$$[\, b \,|\, A \,] = U \Sigma V^T$$

with the singular values of $[\, b \,|\, A \,]$

$$\sigma_1 \geq \ldots \geq \sigma_p > \sigma_{p+1} = \ldots = \sigma_{n+1} \geq 0\,,$$

and the partitioning

$$V = \left[\begin{array}{c|c} \overbrace{V_{11}}^{p} & \overbrace{V_{12}}^{n-p+1} \\ \hline V_{21} & V_{22} \end{array} \right] \begin{array}{l} \}\, 1 \\ \}\, n \end{array}.$$

(If $\sigma_1 = \sigma_{n+1}$, then $p = 0$ and σ_p, V_{11}, V_{21} are nonexistent.)

Existence and uniqueness of the TLS solution has been analyzed in [1, 4, 5, 6], which gives the following classification:

- If $V_{12} \neq 0$ with $p = n$, then
  the TLS problem has the unique (basic) solution.
- If $V_{12} \neq 0$ with $p < n$, then
  the TLS problem has infinitely many solutions, the goal is to find the minimum norm solution.
- If $V_{12} = 0$, then
  the TLS problem does not have a solution, but the TLS concept can be extended to the so called nongeneric solution (that does not solve (1)).

Core reduction:

In [6] it is shown that for any A, b there exist orthogonal matrices P, Q such that

$$P^T \,[\, b \,|\, A\,Q \,] = \left[\begin{array}{c|c|c} b_1 & A_{11} & 0 \\ 0 & 0 & A_{22} \end{array} \right].$$

The original problem and its solution are fully defined by two independent subproblems

$$A_{11}\,x_1 \approx b_1 \qquad \text{and} \qquad A_{22}\,x_2 \approx 0\,,$$

where the first one (called core problem) always *has the TLS solution* and for the second we take $x_2 \equiv 0$. Moreover,

$$x \equiv Q \begin{bmatrix} x_1 \\ 0 \end{bmatrix}$$

represents the solution of the original problem identical to one of the corresponding solutions described above (basic, minimum norm, nongeneric).

The core problem concept clarifies the meaning of the nongeneric solution.

3. Multiple right-hand sides case

Consider the SVD

$$[\, B \,|\, A \,] = U \Sigma V^T$$

with the singular values of $[\, B \,|\, A \,]$

$$\sigma_1 \geq \ldots \geq \sigma_p > \sigma_{p+1} = \ldots = \sigma_{n+1} = \ldots$$
$$= \sigma_{n+e} > \sigma_{n+e+1} \geq \ldots \geq \sigma_{n+d} \geq 0\,,$$

and the partitioning

$$V = \left[\begin{array}{c|c|c} \overbrace{V_{11}}^{p} & \overbrace{V_{12}}^{n+e-p} & \overbrace{V_{13}}^{d-e} \\ \hline V_{21} & V_{22} & V_{23} \end{array} \right] \begin{array}{l} \}\, d \\ \}\, n \end{array}.$$

(If $\sigma_1 = \sigma_{n+1}$, then $p = 0$ and σ_p, V_{11}, V_{21} are nonexistent. If $\sigma_{n+1} = \sigma_{n+d}$, then $e = d$ and σ_{n+e+1}, V_{13}, V_{23} are nonexistent.)

Classical analysis [4] gives:

- If $\mathrm{rank}\,([\, V_{12} \,|\, V_{13} \,]) = d$ with $p = n$, then
  the TLS problem has the unique (basic) solution.
- If $\mathrm{rank}\,([\, V_{12} \,|\, V_{13} \,]) = d$ with $e = d$, then
  the TLS problem has infinitely many solutions, the goal is to find the minimum norm solution.
- If $\mathrm{rank}\,([\, V_{12} \,|\, V_{13} \,]) < d$, then
  the TLS problem does not have a solution, but the TLS concept can be extended to the so called nongeneric solution (that does not solve (1)).

Difficulty:

The case $[\, V_{12} \,|\, V_{13} \,]$ of full row rank (equal to d) with $p < n$ and $e < d$, is not analyzed in the literature, and a TLS solution is not defined. The TLS algorithm [4] by Van Huffel, however computes some X for any problem $A\,X \approx B$.

Remember that the block V_{12} corresponds to the singular value σ_{n+1}, while the block V_{13} corresponds to singular values $\sigma_j < \sigma_{n+1}$. In the further analysis we look at *individual ranks* of the matrices V_{12} and V_{13}.

Notation:

When $[\, V_{12} \,|\, V_{13} \,]$ is of full row rank (equal to d), this rank can be "divided" between blocks V_{12} and V_{13} in three different ways, see [7].

Denote $\mathcal{F}_1$ the set of problems (1) for which
$\mathrm{rank}\,([\, V_{12} \,|\, V_{13} \,]) = d$ with
$\mathrm{rank}\,(V_{12}) = e$ and $\mathrm{rank}\,(V_{13}) = d - e$ (maximal).
(Special cases $p = n$ and $e = d$.)

Denote $\mathcal{F}_2$ the set of problems (1) for which
$\mathrm{rank}\,([\, V_{12} \,|\, V_{13} \,]) = d$ with
$\mathrm{rank}\,(V_{12}) > e$ and $\mathrm{rank}\,(V_{13}) = d - e$ (maximal).

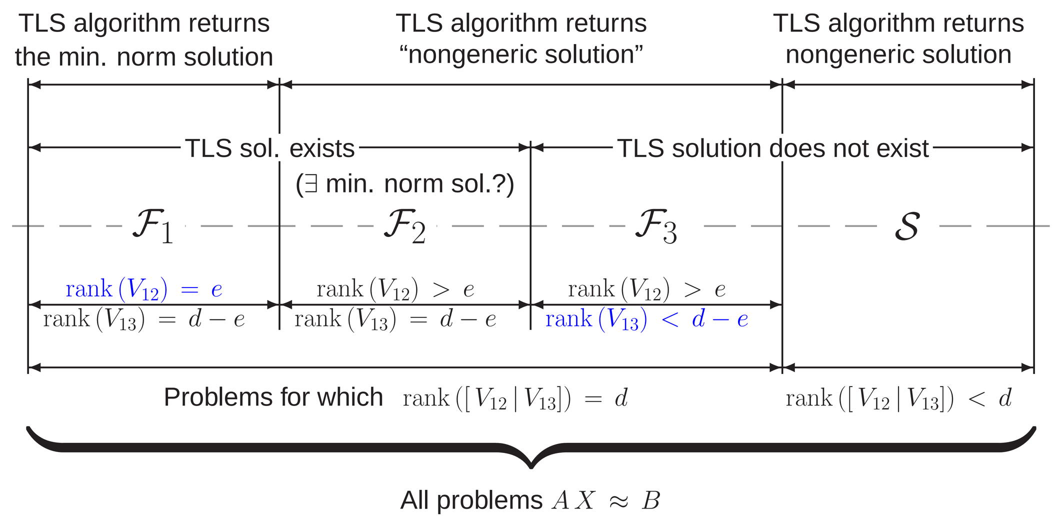
Denote $\mathcal{F}_3$ the set of problems (1) for which
$\mathrm{rank}\,([\, V_{12} \,|\, V_{13} \,]) = d$ with
$\mathrm{rank}\,(V_{12}) > e$ and $\mathrm{rank}\,(V_{13}) < d - e$.

Denote $\mathcal{S}$ the set of problems (1) for which
$\mathrm{rank}\,([\, V_{12} \,|\, V_{13} \,]) < d$.

The sets $\mathcal{F}_j$, $j = 1, 2, 3$, and $\mathcal{S}$, are mutually disjoint and cover all cases that can occur.

Complete classification of TLS problems, see [7]:

- If the problem belongs in $\mathcal{F}_1$, then
  the TLS problem has a solution.
  If $p = n$, then the solution is unique, otherwise the goal is to find the minimum norm solution.
- If the problem belongs in $\mathcal{F}_2$, then
  the TLS problem has a solution, but the TLS algorithm [4] does not compute it.
- If the problem belongs in $\mathcal{F}_3$, then
  the TLS problem does not have a solution.
- If the problem belongs in $\mathcal{S}$, then
  the TLS problem does not have a solution, but the TLS concept can be extended to the so called nongeneric solution (that does not solve (1)).



4. Conclusions

The analysis of the multiple right-hand side problems is complicated. In particular, in the set $\mathcal{F}_2$ two different "solutions" can be defined – the solution of the minimization problem (1), and the solution given by the TLS algorithm [4]. Extension of the core reduction to multiple right-hand side problems is in progress, see [7].

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