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Brief Paper

On the Accuracy of Total Least Squares and Least Squares Techniques in the Presence of Errors on all Data*

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Key Words—Linear algebra; matrix algebra; numerical methods; statistics; system identification; least-squares estimation; total least-squares estimation; singular value decomposition.

Abstract—Every linear parameter estimation problem gives rise to an overdetermined set of linear equations $\mathbf{AX} \approx \mathbf{B}$ which is usually solved with the ordinary least squares (LS) method. Often, both $\mathbf{A}$ and $\mathbf{B}$ are inaccurate. For these cases, a more general fitting technique, called total least squares (TLS), is devised. This paper investigates, via simulations how perturbations on both $\mathbf{A}$ and $\mathbf{B}$ affect the accuracy of the TLS and LS solution. Several important factors are discussed, as well as the consistency properties of the TLS solution in the presence of uncorrelated and equally sized errors.

1. *Introduction*

THIS PAPER compares least squares (LS) and total least squares (TLS) methods for solving overdetermined sets of linear equations arising in any linear parameter estimation problem.

TLS formulation. Consider a set of m linear equations in $n \times d$ unknowns $\mathbf{X}$

$$\mathbf{AX} \approx \mathbf{B}, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{B} \in \mathbb{R}^{m \times d} \text{ and } \mathbf{X} \in \mathbb{R}^{n \times d} \tag{1}$$

then, a **TLS solution** is any solution $\mathbf{X}$ of the set

$$\hat{\mathbf{A}}\mathbf{X} = \hat{\mathbf{B}} \tag{2}$$

where $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ are determined such that

$$R(\hat{\mathbf{B}}) \subset R(\hat{\mathbf{A}}) \tag{3}$$

$$\|[\Delta\hat{\mathbf{A}}; \Delta\hat{\mathbf{B}}]\|_F = \|[\mathbf{A}; \mathbf{B}] - [\hat{\mathbf{A}}; \hat{\mathbf{B}}]\|_F \text{ is minimal.} \tag{4}$$

$\|\mathbf{M}\|_F$ denotes the Frobenius norm and $R(\mathbf{M})$ the range of a matrix $\mathbf{M}$. The problem of finding $[\Delta\hat{\mathbf{A}}; \Delta\hat{\mathbf{B}}]$ such that (3) and (4) are satisfied, is referred to as the **TLS problem**. Whenever the solution is not unique, TLS singles out the minimum norm solution, denoted by $\hat{\mathbf{X}}$.

It is important to observe that the LS problem is in fact a "**constrained**" TLS problem (2)–(4) subject to the additional constraint that $\hat{\mathbf{A}} = \mathbf{A}$ is fixed. TLS has a long history in the statistical literature where the method is known as orthogonal regression or **errors-in-variables regression** (Gleser, 1981). More recently, the TLS approach to fitting has also attracted interest outside statistics, e.g. in numerical analysis, beamforming, experimental modal analysis, in system identification where TLS is known as the **eigenvector method** or the **Koopmans–Levin** method (see, e.g. Van Huffel and Vandewalle (1989) for a list of references), . . . and several algorithms have been suggested see, e.g. Golub and Van Loan (1983), Van Huffel and Vandewalle (1988, 1989), and Fernando and Nicholson (1985).

This paper examines, via simulations, how perturbations on both $\mathbf{A}$ and $\mathbf{B}$ affect the accuracy of the TLS and LS problem. The difference in sensitivity of the singular subspaces related to the TLS and LS problem (see Section 2), as well as the consistency properties of the TLS solution in the presence of uncorrelated and equally sized errors (see Section 3), explain the better performance of TLS.

2. *Sensitivity of singular subspaces*

We first introduce some additional notation used throughout this paper.

(a) The singular value decomposition (SVD) of the matrix $\mathbf{A}$ in (1), given by its dyadic decomposition (Golub and Van Loan, 1983), is denoted by

$$\mathbf{A} = \sum_{i=1}^{n} \tilde{\sigma}_i' \tilde{\mathbf{u}}_i' \tilde{\mathbf{v}}_i'^{\mathrm{T}} \quad \tilde{\mathbf{u}}_i' \in \mathbb{R}^m, \tilde{\mathbf{v}}_i' \in \mathbb{R}^n$$

$$\text{and} \quad \tilde{\sigma}_1' \geq \cdots \geq \tilde{\sigma}_n' \geq 0. \tag{5}$$

The elements $\tilde{\sigma}_i'$, organized in decreasing order of magnitude, are the singular values of $\mathbf{A}$. The vectors $\tilde{\mathbf{u}}_i'$ (resp., $\tilde{\mathbf{v}}_i'$) are orthonormal and represent the associated ith left (resp., right) singular vectors. The spaces generated by some subset of left (resp., right) singular vectors are called left (resp., right) **singular subspaces** of the matrix $\mathbf{A}$. Analogously, the SVD of the augmented matrix $[\mathbf{A}; \mathbf{B}]$ in (1) is represented by (omit primes)

$$[\mathbf{A}; \mathbf{B}] = \sum_{i=1}^{n+d} \tilde{\sigma}_i \tilde{\mathbf{u}}_i \tilde{\mathbf{v}}_i^{\mathrm{T}} \quad \tilde{\mathbf{u}}_i \in \mathbb{R}^m, \tilde{\mathbf{v}}_i \in \mathbb{R}^{n+d}$$

$$\text{and} \quad \tilde{\sigma}_1 \geq \cdots \geq \tilde{\sigma}_{n+d} \geq 0. \tag{6}$$

(b) Analogous to the perturbed counterparts (5) and (6), the SVD of the corresponding unperturbed matrices $\mathbf{A}_0$ and $[\mathbf{A}_0; \mathbf{B}_0]$ are obtained by omitting the tilde in (5) and (6).

(c) The **distance** between any two subspaces S_1 and S_2, defined by (Golub and Van Loan, 1983)

$$\text{dist}(S_1, S_2) = \|\mathbf{P}_1 - \mathbf{P}_2\|_2 \tag{7}$$

where $\mathbf{P}_i$ is the orthogonal projection onto S_i ($\|\mathbf{M}\|_2$ denotes the two-norm), describes the closeness between S_1 and S_2 and is just the sine of the largest canonical angle.

In order to make the set of equations (1) compatible, LS projects the data $\mathbf{A}$, $\mathbf{B}$ into the singular subspaces $R([\tilde{\mathbf{u}}_1', \ldots, \tilde{\mathbf{u}}_n'])$ and $R([\tilde{\mathbf{v}}_1', \ldots, \tilde{\mathbf{v}}_n'])$ of the matrix $\mathbf{A}$ of numerical rank $r \leq n$, while TLS projects $\mathbf{A}$, $\mathbf{B}$ into the singular subspaces $R([\tilde{\mathbf{u}}_1, \ldots, \tilde{\mathbf{u}}_r])$ and $R([\tilde{\mathbf{v}}_1, \ldots, \tilde{\mathbf{v}}_r])$ of $[\mathbf{A}; \mathbf{B}]$. Indeed from their respective definitions, the LS

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solution $\mathbf{X}'$ is the minimum norm solution (Golub and Van Loan, 1983) of

$$\mathbf{A}_r\mathbf{X} = \mathbf{B}' \quad \text{with} \quad \mathbf{A}_r = \sum_{i=1}^{r} \bar{\sigma}_i' \bar{\mathbf{u}}_i' \bar{\mathbf{v}}_i'^{\mathrm{T}} \quad \text{and} \quad \mathbf{B}' = \sum_{i=1}^{r} \bar{\mathbf{u}}_i' \bar{\mathbf{u}}_i'^{\mathrm{T}} \mathbf{B} \tag{8}$$

and the TLS solution $\hat{\mathbf{X}}$ is the minimum norm solution of

$$\hat{\mathbf{A}}\mathbf{X} = \hat{\mathbf{B}} \quad \text{with} \quad [\hat{\mathbf{A}}; \hat{\mathbf{B}}] = \sum_{i=1}^{r} \bar{\sigma}_i \bar{\mathbf{u}}_i \bar{\mathbf{v}}_i^{\mathrm{T}} \quad \text{the TLS approximation.} \tag{9}$$

The differences in sensitivity of these singular subspaces explain the better performance of TLS in the presence of perturbations, as shown below.

First consider the unperturbed **TLS problem** $\mathbf{A}_0\mathbf{X} \approx \mathbf{B}_0$. Let the m by $n+d$ matrix $[\mathbf{A}_0; \mathbf{B}_0]$ be perturbed by $[\Delta\mathbf{A}; \Delta\mathbf{B}]$ such that $[\mathbf{A}; \mathbf{B}] = [\mathbf{A}_0; \mathbf{B}_0] + [\Delta\mathbf{A}; \Delta\mathbf{B}]$. Denote by r ($\leq n$) the rank of the TLS approximation $[\hat{\mathbf{A}}_0; \hat{\mathbf{B}}_0]$ (defined by (9)) of $[\mathbf{A}_0; \mathbf{B}_0]$. Applying the generalized sin θ theorem of Wedin (1972) to $[\mathbf{A}_0; \mathbf{B}_0]$ and $[\mathbf{A}; \mathbf{B}]$ and the TLS condition (3) (i.e. $R(\hat{\mathbf{A}}) = R([\hat{\mathbf{A}}; \hat{\mathbf{B}}])$), one obtains

$$\operatorname{dist}(R(\hat{\mathbf{A}}), R(\hat{\mathbf{A}}_0)) \leq \|[\Delta\mathbf{A}; \Delta\mathbf{B}]\|_2/(\bar{\sigma}_r - \sigma_{r+1}) \tag{10}$$

$$\operatorname{dist}(R([\hat{\mathbf{A}}; \hat{\mathbf{B}}]^{\mathrm{T}}), R([\hat{\mathbf{A}}_0; \hat{\mathbf{B}}_0]^{\mathrm{T}})) \leq \|[\Delta\mathbf{A}; \Delta\mathbf{B}]\|_2/(\bar{\sigma}_r - \sigma_{r+1}). \tag{11}$$

If $\mathbf{A}_0X = \mathbf{B}_0$ represents an **exact** relationship as assumed in the errors-in-variables model (Gleser, 1981), then $[\hat{\mathbf{A}}_0; \hat{\mathbf{B}}_0] = [\mathbf{A}_0; \mathbf{B}_0]$ and thus $\sigma_{r+1} = 0$ in (10) and (11). Usually **full rank** problems are considered, i.e. $\mathbf{A}_0$ has maximal rank $r = n$. Then (10) and (11) reduce to

$$\operatorname{dist}(R(\hat{\mathbf{A}}), R(\mathbf{A}_0)) \leq \|[\Delta\mathbf{A}; \Delta\mathbf{B}]\|_2/\bar{\sigma}_n \tag{12}$$

$$\operatorname{dist}(R([\hat{\mathbf{A}}; \hat{\mathbf{B}}]^{\mathrm{T}}), R([\mathbf{A}_0; \mathbf{B}_0]^{\mathrm{T}})) \leq \|[\Delta\mathbf{A}; \Delta\mathbf{B}]\|_2/\bar{\sigma}_n. \tag{13}$$

This means that the TLS solution space approaches the exact solution if the perturbations $\|[\Delta\mathbf{A}; \Delta\mathbf{B}]\|_2$ are kept **small** and if the **gap** between the rth and $(r+1)$th singular value of $[\mathbf{A}; \mathbf{B}]$ is **large**.

Consider now **LS problems**. Let the m by n matrix $\mathbf{A}_0$ of rank r (i.e. $\sigma_{r+1}' = 0$) be perturbed by $\Delta\mathbf{A}$ such that $\mathbf{A} = \mathbf{A}_0 + \Delta\mathbf{A}$. Applying Wedin's generalized sin θ theorem to $\mathbf{A}_0$ and $\mathbf{A}$, one obtains

$$\operatorname{dist}(R(\mathbf{A}), R(\mathbf{A}_0)) \leq \|\Delta\mathbf{A}\|_2/\bar{\sigma}_r' \tag{14}$$

$$\operatorname{dist}(R(\mathbf{A}^{\mathrm{T}}), R(\mathbf{A}_0^{\mathrm{T}})) \leq \|\Delta\mathbf{A}\|_2/\bar{\sigma}_r'. \tag{15}$$

Usually, $\mathbf{A}_0$ has maximal rank $r = n$. Then (14) reduces to

$$\operatorname{dist}(R(\mathbf{A}), R(\mathbf{A}_0)) \leq \|\Delta\mathbf{A}\|_2/\bar{\sigma}_n'. \tag{16}$$

Comparing the sensitivity of the singular subspaces associated with the LS and TLS problem from the expressions above, the following important observations are made.

(a) First assume that the data $\mathbf{A}$ and $\mathbf{B}$ are measured samples of an exact relation $\mathbf{A}_0\mathbf{X} = \mathbf{B}_0$. The measurement errors $\Delta\mathbf{A}$ and $\Delta\mathbf{B}$ may be arbitrarily distributed provided $\|\Delta\mathbf{A}\|_2 \approx \|[\Delta\mathbf{A}; \Delta\mathbf{B}]\|_2$ (e.g. when all data are equally perturbed). Then, using the interlacing property for singular values, i.e. $\bar{\sigma}_i \geq \bar{\sigma}_i'$, $i = 1, \ldots, n$ (Golub and Van Loan, 1983), it is concluded that the singular subspaces related to the TLS problem are **less noise sensitive** than those related to the LS problem. This implies that the former are expected to be "closer" to their corresponding unperturbed subspaces. Hence, the TLS solution is expected to be more accurate than the LS solution. This is also the case for problems $\mathbf{A}_0\mathbf{X} \approx \mathbf{B}_0$ where $\bar{\sigma}_r - \sigma_{r+1} > \bar{\sigma}_r'$ in (10) and (14). Or in other words, the corresponding unperturbed problem $\mathbf{A}_0\mathbf{X} \approx \mathbf{B}_0$ must be **sufficiently compatible**.

(b) Since the difference in sensitivity depends on the ratio $(\bar{\sigma}_r - \sigma_{r+1})/\bar{\sigma}_r'$ the better accuracy of TLS as opposed to LS will be more pronounced when this ratio is larger. This ratio is mainly influenced by the length (Frobenius norm), the column dimension and the orientation of the observation matrix $\mathbf{B}_0$ (or equivalently, of the solution $\mathbf{X}$) w.r.t. the singular vectors of $\mathbf{A}_0$. These observations are now confirmed by simulations.

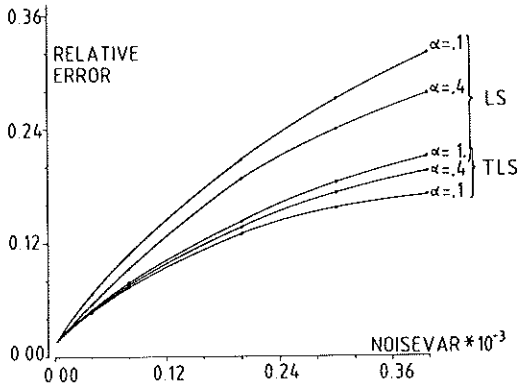


FIG. 1. Comparison of the average relative error of the LS and TLS solution vs the variance of the noise added to the set $(\mathbf{A}_0)_{18\times5}\mathbf{X} = (\mathbf{B}_0)_{18\times1}$ with $\sigma'(\mathbf{A}_0) = \{10, 8, 4, 1, 0.1\}$ and $\mathbf{B}_0 = \sum_{i=1}^{5} \beta_i \mathbf{u}_i'(\mathbf{A}_0)$ **for different coefficient ratios** $\alpha = \max_{i=1,4} (\beta_i/\sigma_i')/(\beta_5/\sigma_5')$. The values 1, 0.4 and 0.1 of α correspond with a ratio $\sigma_5([\mathbf{A}_0; \mathbf{B}_0])/\sigma_5'(\mathbf{A}_0)$ equal to 1.1, 1.6 and 3.6, respectively.

Simulation procedure. We start from an exact, overdetermined set of m equations $\mathbf{A}_0\mathbf{X} = \mathbf{B}_0$ in $n \times d$ unknowns $\mathbf{X}$ with d observation vectors in $\mathbf{B}_0$ and $\mathbf{A}_0$ of full rank. Random errors $\Delta\mathbf{A}_{ij}$ and $\Delta\mathbf{B}_{ij}$, normally distributed with zero mean and variance s^2, are then added to the entries of the exact data matrix $[\mathbf{A}_0; \mathbf{B}_0]$. Call the perturbed matrix $[\mathbf{A}; \mathbf{B}] = [\mathbf{A}_0; \mathbf{B}_0] + [\Delta\mathbf{A}; \Delta\mathbf{B}]$. We then solve the perturbed set of equations (1) to obtain the TLS solution $\hat{\mathbf{X}}$ and the LS solution $\mathbf{X}'$. The relative errors $\|\mathbf{X}' - \mathbf{X}\|_{\mathrm{F}}/\|\mathbf{X}\|_{\mathrm{F}}$ and $\|\hat{\mathbf{X}} - \mathbf{X}\|_{\mathrm{F}}/\|\mathbf{X}\|_{\mathrm{F}}$ are averaged over 100 sets of equations affected by random errors with zero mean and equal variance s^2. We repeat the simulation for progressively larger noise variances s^2. The average relative errors are then plotted vs the noise variance s^2 (see Figs 1–3).

From the previous discussion and since $\mathbf{A}_0\mathbf{X} = \mathbf{B}_0$ (i.e. $\sigma_{n+1} = 0$), it is clear that the difference in accuracy depends on the ratio $\bar{\sigma}_n/\bar{\sigma}_n'$ of the nth singular values of $[\mathbf{A}; \mathbf{B}]$ and $\mathbf{A}$ or equivalently, on the **ratio** σ_n/σ_n'. Let us investigate the parameters which **influence** this ratio.

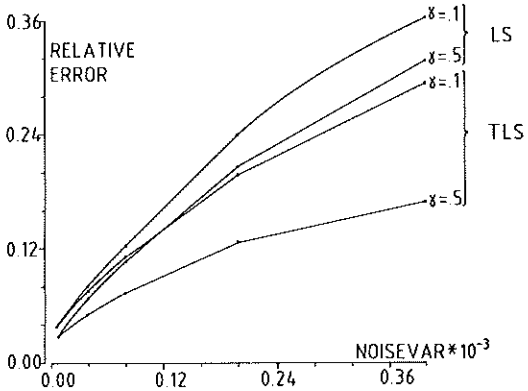


FIG. 2. Comparison of the average relative error of the LS and TLS solution vs the variance of the noise added to the set $(\mathbf{A}_0)_{18\times5}\mathbf{X} = (\mathbf{B}_0)_{18\times1}$ with $\sigma'(\mathbf{A}_0) = \{10, 8, 4, 1, 0.1\}$ and $\mathbf{B}_0 = \gamma\mathbf{u}_5'$ **for different lengths** γ **of** $\mathbf{B}_0$. The values 0.1 and 0.5 of γ correspond with a ratio $\sigma_5([\mathbf{A}_0; \mathbf{B}_0])/\sigma_5'(\mathbf{A}_0)$ equal to 1.4 and 5.1, respectively.

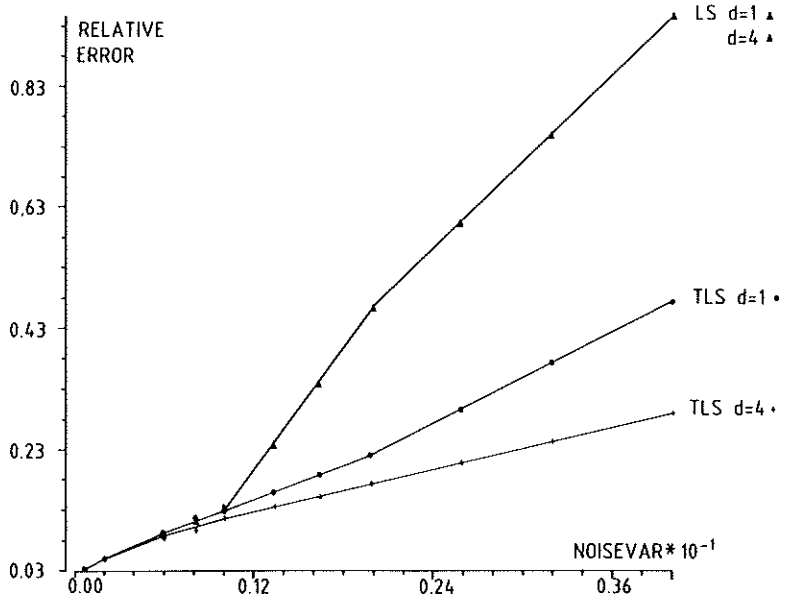


FIG. 3. Comparison of the average relative error of the LS and TLS solution vs the variance of the noise added to the set $(\mathbf{A}_0)_{14\times 4}\mathbf{X} = (\mathbf{B}_0)_{14\times d}$ with $\sigma'(\mathbf{A}_0) = \{264, 9.7, 2.7, 0.75\}$ **for different numbers** d **of observation vectors.** All d columns of $\mathbf{B}_0$ are equal to $\sum_{i=1}^{4} \mathbf{u}_i'(\mathbf{A}_0)$. The values 1 and 4 of d correspond with a ratio $\sigma_4([\mathbf{A}_0; \mathbf{B}_0])/\sigma_4'(\mathbf{A}_0)$ equal to 1.6 and 2.2, respectively.

(a) The **orientation of the observation matrix** $\mathbf{B}_0$, or equivalently the orientation of the solution $\mathbf{X}$, w.r.t. the lowest singular vectors $\mathbf{u}_n'$ or $\mathbf{v}_n'$ of $\mathbf{A}_0$, respectively, plays an important role. From the interlacing property for singular values (Golub and Van Loan, 1983), it is clear that the singular values of $[\mathbf{A}_0; \mathbf{B}_0]$ are always larger than the corresponding ones of $\mathbf{A}_0$, i.e. $\sigma_i \geq \sigma_i'$, $i = 1, \ldots, n$. However the extent to which σ_i is larger, depends on the orientation of $\mathbf{B}_0$ w.r.t. $\mathbf{u}_i'$ of $\mathbf{A}_0$. It is not difficult to see that those directions $\mathbf{u}_i'$ of $\mathbf{A}_0$ onto which $\mathbf{B}_0$ has a larger projection, will be "**favored**" and have the largest ratio σ_i/σ_i'. Hence, the ratio σ_n/σ_n' increases when $\mathbf{B}_0$ becomes closer and closer to the direction of $\mathbf{u}_n'$. As shown in Fig. 1, the better accuracy of TLS as opposed to LS is then more pronounced. This happens not only if $\mathbf{B}_0$ is "close" to the lowest singular vector $\mathbf{u}_n'$, but also if the **condition number** σ_1'/σ_n' of $\mathbf{A}_0$ is **large**. Indeed, a large condition number implies a small σ_n'. If

$$\mathbf{B}_0 = \sum_{i=1}^{n} \beta_i \mathbf{u}_i'$$

then the exact solution

$$\mathbf{X} = \sum_{i=1}^{n} (\beta_i/\sigma_i')\mathbf{v}_i'.$$

Hence, the component β_n/σ_n' of $\mathbf{X}$ in the direction of $\mathbf{v}_n'$ is large whenever σ_n' is small (provided the projection β_n of $\mathbf{B}_0$ onto $\mathbf{u}_n'$ is not too small). The better accuracy of TLS w.r.t. LS is most pronounced when each column of $\mathbf{B}_0$ is parallel with $\mathbf{u}_n'$. In this case, the ratio σ_n/σ_n' reaches its maximal value for a given $\|\mathbf{B}_0\|_F$ and σ_n' is given by

$$\sigma_n = \sqrt{(\sigma_n'^2 + \|\mathbf{B}_0\|_F^2)}. \tag{17}$$

Observe that the accuracy of the LS solution is then mostly affected, according to Wedin's $\sin\theta$ theorem with complementary residuals applied to singular vectors (Wedin, 1972).

(b) The **length of each observation vector** in $\mathbf{B}_0$ influences the ratio σ_n/σ_n'. This is clear from (17). Making $\|\mathbf{B}_0\|_F$ larger, increases the ratio σ_n/σ_n' if $\mathbf{B}_0 // \mathbf{u}_n$ (as long as $\sigma_{n-1} > \sqrt{(\sigma_n'^2 + \|\mathbf{B}_0\|_F^2)}$) and hence, the better accuracy of the TLS solution w.r.t. the LS solution will be more pronounced, as shown in Fig. 2.

(c) The ratio σ_n/σ_n' depends on the **number** d **of observation vectors** in $\mathbf{B}_0$. Indeed, if now all d vectors of $\mathbf{B}_0$ (instead of one) are close to the lowest singular vector $\mathbf{u}_n'$ of $\mathbf{A}_0$, the singular value σ_n of $[\mathbf{A}_0; \mathbf{B}_0]$ increases. Since d observation vectors together have a larger norm than one vector, the ratio σ_n/σ_n' increases with increasing number d of observation vectors. The better accuracy of the TLS solution as opposed to LS is most pronounced, not only if all observation vectors are equally oriented along the lowest singular vector $\mathbf{u}_n'$ of $\mathbf{A}_0$, but also if the condition number of $\mathbf{A}_0$ is large (as explained before). This is illustrated in Fig. 3. Observe that the accuracy of the TLS solution improves with increasing number d of observation vectors while the accuracy of LS is independent of d.

3. *Consistency*

Furthermore, the difference in accuracy between TLS and LS also depends on the number m of equations. Since the "errors-in-variables" regression estimator coincides with the TLS solution, Gleser's consistency analysis can be straightforwardly applied to the TLS problem.

Theorem 1 (*Gleser*, 1981). Assume that the data $[\mathbf{A}; \mathbf{B}]$, given by $[\mathbf{A}_0 + \Delta\mathbf{A}; \mathbf{B}_0 + \Delta\mathbf{B}]$, are measured samples of an exact relationship $\mathbf{A}_0\mathbf{X} = \mathbf{B}_0$ and that the rows of the error matrix $[\Delta\mathbf{A}; \Delta\mathbf{B}]$ are independent and identically distributed with zero mean and common covariance matrix $s^2\mathbf{I}$ ($\mathbf{I}$ is the identity matrix, s is an unknown scalar).

If

$$\lim_{m\to\infty} \frac{1}{m} \mathbf{A}_0^T\mathbf{A}_0$$

exists and is positive definite, then $\hat{\mathbf{X}}$ is a **strongly consistent estimate** of $\mathbf{X}$, i.e.

$$\lim_{m\to\infty} \hat{\mathbf{X}} = \mathbf{X}$$

with probability one.

This means that the TLS solution $\hat{\mathbf{X}}^{(m)}$, computed from m measurements (1) of the exact but unobservable relation $\mathbf{A}_0\mathbf{X} = \mathbf{B}_0$, converges with probability one to the true parameter values $\mathbf{X}$ as m tends to infinity. As is well known in linear regression, the ordinary LS solution $\mathbf{X}'$ is always inconsistent in this case.

In many problems of system identification and parameter estimation, the matrix $[\mathbf{A}; \mathbf{B}]$ consists of Toeplitz or Hankel expansions of input and/or output sequences, e.g. in ARMA modelling. A well-known estimator of the parameters in these models is the Koopmans–Levin method (Fernando and

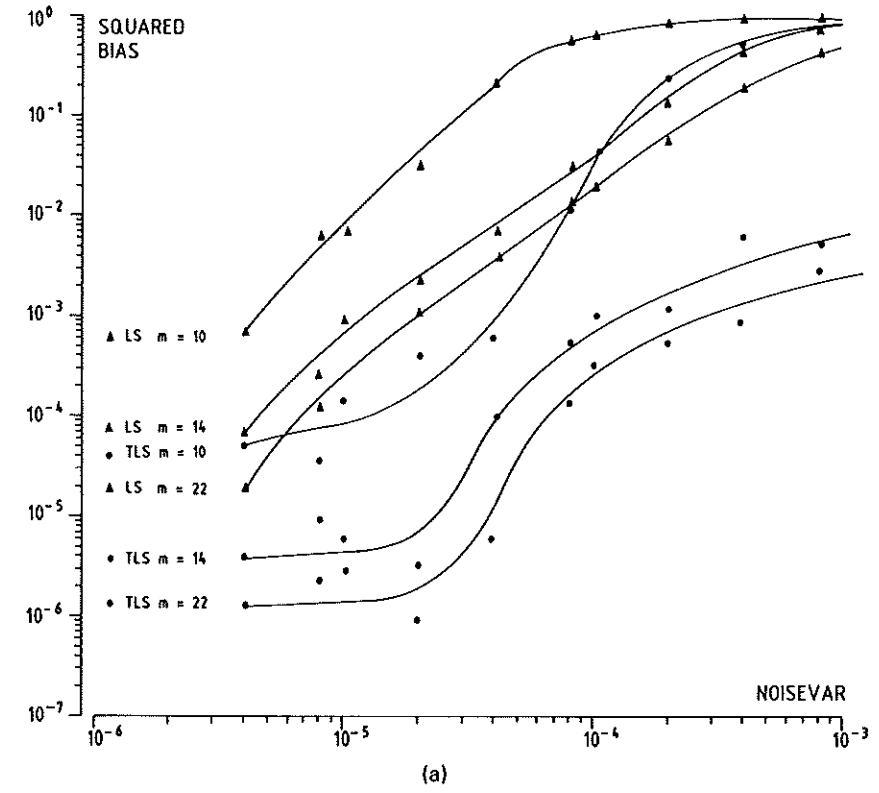


FIG. 4. Comparison of (a) the squared bias and (b) the mean squared error (MSE) of the LS and TLS solution (all values divided by $\|\mathbf{X}\|_F^2$) vs the variance of the noise added to the set $(\mathbf{A}_0)_{m\times 5}\mathbf{X} = (\mathbf{B}_0)_{m\times 1}$ **for different row dimensions** $m = 10$, 14 and 22. The 22×5 matrix $\mathbf{A}_0$ has singular values 10, 8, 4, 1, 0.1 and $\mathbf{B}_0 = 0.5\mathbf{u}_5$ where $\mathbf{u}_5$ is the left singular vector of $\mathbf{A}_0$ corresponding to 0.1. By deleting the last rows in this 22×6 matrix $[\mathbf{A}_0; \mathbf{B}_0]$, the other $m \times 6$ matrices $[\mathbf{A}_0; \mathbf{B}_0]$ are derived.

Nicholson, 1985) the statistical properties of which have been studied by Aoki and Yue (1970). Since this estimator coincides with the TLS solution, their results also apply to the TLS problem. Necessary and sufficient conditions for consistency, similar to those given by Gleser, have been derived. See Aoki and Yue (1970) for more details.

The consistency properties of the TLS solution are fairly well approximated in applications of **moderate sample sizes**, as confirmed by simulations now. We therefore compare the accuracy of the TLS and LS solution with respect to their squared bias and mean squared error (MSE). These quantities are related as follows (E is the expected value operator)

$$\begin{aligned}\text{MSE}(\hat{X}) &= E\{(\hat{X}-X)^{\mathrm{T}}(\hat{X}-X)\}\\ &= E\{(\hat{X}-E(\hat{X}))^{\mathrm{T}}(\hat{X}-E(\hat{X}))\}\\ &\quad + \{(E(\hat{X})-X)^{\mathrm{T}}(E(\hat{X})-X)\}\\ &= \text{total variance}(\hat{X}) + \text{squared bias}(\hat{X})\end{aligned}$$

with $\mathbf{X}$ the exact solution of $\mathbf{A}_0\mathbf{X}=\mathbf{B}_0$ (assume $d=1$). For reasons of conciseness, the total variance is not discussed here (see, e.g. Van Huffel (1987)). We use the same simulation procedure of Section 2 but instead of relative errors, the squared bias and MSE of the solution are estimated (from the sample mean). These estimated values are divided by $\|\mathbf{X}\|_{\mathrm{F}}^2$ and then plotted in a log–log diagram vs the noise variance.

Figure 4 illustrates the difference in accuracy between TLS and LS with **increasing** degree m of **overdetermination**.

(a) The **bias of TLS** is much **smaller** then the bias of LS and decreases with increasing m, conformal to the asymptotic unbiasedness property of TLS implied by Theorem 1. Observe that the squared bias does not exceed the noise variance for $m=22$.

(b) The **MSE combines** the effects of **bias and variance**. At the smallest noise variances, the LS bias is rather low (and usually substantially smaller than the variance). The variance of TLS is always larger than the LS variance, as shown in Ketellapper (1983) and Van Huffel (1987). These two effects annihilate each other, producing comparable MSE for TLS and LS. By increasing the noise on the data, the bias of LS becomes more important and even the dominating term. Hence, the differences in MSE are more pronounced, showing the advantages of TLS. Especially when the sets of equations are more overdetermined, the TLS solution is clearly more accurate since the TLS estimator approaches then its asymptotic properties. Figure 4 confirms that these properties are already fairly well reached for **moderate sample size** m.

4. *Conclusions*

In this paper, we compare, via simulations, the accuracy of total least squares (TLS) and least squares (LS) methods in solving overdetermined sets of linear equations $\mathbf{AX}\approx\mathbf{B}$ where both $\mathbf{B}$ and $\mathbf{A}$ are perturbed. Assume that the perturbations added to the corresponding unperturbed set $\mathbf{A}_0\mathbf{X}\approx\mathbf{B}_0$ have approximately the same size. Then the better accuracy of the TLS solution w.r.t. the LS solution is more pronounced if the number of observation vectors in $\mathbf{B}_0$ and their length increase and if $\mathbf{B}_0$, or equivalently the solution $\mathbf{X}$, is "close" to the singular vector of $\mathbf{A}_0$, associated with its smallest singular value. Moreover, assume that $\mathbf{A}$, $\mathbf{B}$ are observations of an exact relationship $\mathbf{A}_0\mathbf{X}=\mathbf{B}_0$ with $\mathbf{A}_0$ of full rank and that the errors are uncorrelated with zero mean and all have the same variance. Then TLS computes a strongly consistent estimate of the true parameters $\mathbf{X}$ of the unperturbed set $\mathbf{A}_0\mathbf{X}=\mathbf{B}_0$. The LS solution is always inconsistent in this case. This consistency property is fairly well approximated in moderately sized problems.

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