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ADVANCED MATHEMATICAL & COMPUTATIONAL TOOLS IN METROLOGY V

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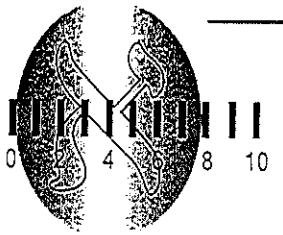
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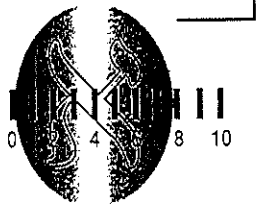
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ADVANCED MATHEMATICAL & COMPUTATIONAL TOOLS IN METROLOGY V



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ITERATIVELY REWEIGHTED TOTAL LEAST SQUARES ALGORITHMS FOR DIFFERENT VARIANCES IN OBSERVATIONS AND DATA

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Abstract

This paper generalises the Total Least Squares (TLS) problem to the cases in which the variances of data and observations are assumed to be different. Besides TLS, this formulation comprises the ordinary (OLS) and data (DLS) least squares problems by specifying a finite value of a parameter ζ depending on the ratio between data variance and observation variance. Numerical iterative techniques for finding the minimum are shown to be very efficient, when parameter ζ is suitably varied during the search path in order to stay in the convergence domain and improve the speed. Some numerical examples show the capabilities of the algorithm in dealing with large scale problems.

1 Introduction

The problem of *linear parameter estimation* consists in formulating an overdetermined set of m linear equations in n ($m > n$) unknowns ($x = [x_j] \in \Re^n$) represented in matrix form by:

$$Ax \approx b, \tag{1}$$

where $A = [a_{ij}] \in \Re^{m \times n}$ is the *data matrix* and $b = [b_i] \in \Re^m$ is the *observation vector* (unidimensional problem). In the *ordinary (classical) least squares* (OLS) approach there is the underlying assumption that errors affect only the observation vector b. This assumption is often unrealistic: matrix A is not error-free because of sampling errors, human errors, modelling errors and instrument errors. Methods for estimating the effect of such errors on the OLS solution are given elsewhere[1,2]. The method of *total least squares* (TLS) is a technique devised to compensate for data errors, when errors in A and b exhibit the same variance. It was first introduced by Golub *et al.*[3], where it has been solved by using the *singular value decomposition* (SVD), as pointed

out elsewhere[4,5]. The TLS problem can be viewed as an unconstrained perturbation problem because all columns of the *augmented matrix* $C = [A; b]$ can be affected by error perturbations. The case opposite to the OLS problem is the *Data Least Squares* (DLS) problem[6], where the errors are assumed to affect only the data matrix A.

The present problem deals with the case in which the data errors Δa_{ij} are independently and identically distributed with zero-mean and common variance σ_a and the observation errors Δb_i are also independently and identically distributed with zero-mean and common variance $\sigma_b \neq \sigma_a$. This formulation is justified in many problems of metrological interest because b and A represent different physical quantities and therefore they are often subject to different measurement methods with different accuracy. An example is the determination of the reference value for the key-comparisons in the field of photometry, where both the uncertainties declared on one hand by the participants and, in the other by the pilot laboratory have to be accounted for in a proper way.

The solution of the present problem[7] consists in minimising

$$\min_{\langle \Delta A, \Delta b, x \rangle} (1-\zeta) \|\Delta A\|_F^2 + \zeta \|\Delta b\|_F^2$$
$$\text{subject to } (A - \Delta A)x = (b - \Delta b), \tag{2}$$

where $\zeta = (1 + \sigma_b^2/\sigma_a^2)^{-1}$. By varying ζ in the range $[0, 1]$, formulation (2) comprises the OLS, TLS and DLS problems. Indeed, $\zeta = 0$ results in the OLS formulation because $\sigma_a^2 = 0$, whereas $\zeta = 0.5$ results in the TLS formulation because $\sigma_a^2 = \sigma_b^2$ and $\zeta = 1$ results in the DLS formulation because $\sigma_b^2 = 0$.

The optimal solution[3] of problem (2) is given by the minimiser of cost function with respect to x:

$$E(x, \zeta) = \frac{1}{2} \frac{(Ax - b)^T (Ax - b)}{(1-\zeta) + \zeta x^T x}. \tag{3}$$

It is apparent in equation (3) the difference with the classical weighted TLS [8] which would need a unique scalar parameter going to infinity in order to have the DLS solution. The same problem stands for the one-parameter generalisation, as pointed out by Cichocki *et al* [9]. A similar problem can be found if the augmented matrix C is pre- and post-multiplied by particular matrices[3]. As a consequence, the need for a finite parameter in the numerical algorithms limits the accuracy. This does not happen in our formulation because DLS problem is represented by a finite value, as a consequence of the fact that the parameter directly appears into the denominator of cost function $E(x, \zeta)$.

The aim of the present paper consists in considering the OLS, TLS and DLS formulations in a unique context, and in their generalisation to realistic problems with different variances in observations and data. Furthermore, the parameter ζ allowing this generalisation is exploited to design a numerical iterative algorithm which guarantees the convergence to the optimal solution of the problem. This result is obtained by investigating the bifurcation diagram of the family of the equilevel hypersurfaces of $E(x, \zeta)$.

2 Bifurcation Diagrams of Equilevel Hyperconics

For $\zeta \in [0, 1]$, the cost function in equation (3) can be written[7] as the ratio of positive definite quadratic forms $Q_N(x)$ and $Q_D(x, \zeta)$

$$E(x, \zeta) = \frac{1}{2} \frac{x^T A^T A x - 2b^T A x + b^T b}{(1-\zeta) + \zeta x^T x} = \frac{1}{2} \frac{Q_N(x)}{Q_D(x, \zeta)}. \tag{4}$$

The family of the equilevel hypersurfaces $E(x, \zeta) = \gamma$ is introduced, where γ plays the role of the family parameter. According to equation (4), this family is constituted by hyperconics and defined by the parametric equation

$$Q_N(x) - \gamma Q_D(x, \zeta) = x^T \left[A^T A - 2\gamma\zeta I_n\right] x - 2b^T A x + b^T b - 2\gamma(1-\zeta) = 0, \tag{5}$$

where I_n is the $n \times n$ identity matrix. Given the realistic assumption of $\text{rank}(A) = n$, matrix $A^T A$ is diagonaliseable in the form $A^T A = V \Lambda V^T$ where V is the eigenvector matrix of $A^T A$, and $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ orders its positive (real) eigenvalues $\lambda_1 < \lambda_2 < \cdots < \lambda_n$. Then, equation (5) can be recast as

$$z^T \left[\Lambda - 2\gamma\zeta I_n\right] z - b^T A V \left[\Lambda - 2\gamma\zeta I_n\right]^{-1} V^T A^T b + b^T b - 2\gamma(1-\zeta) = 0, \tag{6}$$

by replacing unknown vector x by vector $z = V^T[(x - x_c(\gamma, \zeta)]$ where

$$x_c(\gamma, \zeta) = V \left[\Lambda - 2\gamma\zeta I_n\right]^{-1} V^T A^T b \tag{7}$$

is the centre of the hyperconic with level γ. By introducing

$$g(\gamma, \zeta) = b^T A V \left[\Lambda - 2\gamma\zeta I_n\right]^{-1} V^T A^T b - b^T b + 2\gamma(1-\zeta)$$
$$= \sum_{i=1}^{n} \frac{q_i^2}{\lambda_i - 2\gamma\zeta} + 2\gamma(1-\zeta) - b^T b, \tag{8}$$

where $q \equiv [q_1\, q_2 \ldots q_n]^T = V^T A^T b$, equation (6) can be rewritten in the canonical form of a generic hyperconic

$$\sum_{i=1}^{n} \text{sign}(\lambda_i - 2\gamma\zeta) \left(\frac{z_i}{a_i(\gamma,\zeta)} \right)^2 = \text{sign}[g(\gamma,\zeta)], \tag{9}$$

where $a_i(\gamma,\zeta), (i = 1,\cdots,n)$, represent the lengths of the hyperconic axes

$$a_i(\gamma,\zeta) = \sqrt[2]{\frac{g(\gamma,\zeta)}{\lambda_i - 2\gamma\zeta}} \qquad (i = 1,\cdots,n). \tag{10}$$

Functions $\text{sign}(\lambda_i - 2\gamma\zeta), (i = 1,\cdots,n)$, and $\text{sign}[g(\gamma,\zeta)]$ control the bifurcation points of this family. We describe the behaviour of these hyperconics with respect to their centre $x_c(\gamma,\zeta)$. The term $g(\gamma,\zeta)$ in equation (8) exhibits n vertical asymptotes, one for each value $\hat{\gamma}_i = \lambda_i/(2\zeta), (i = 1,\cdots,n)$, corresponding to the commutation of $\text{sign}(\lambda_i - 2\gamma\zeta)$. Moreover $g(0,\zeta) < 0, \forall\zeta$, as shown in Ref. 7. The term $g(\gamma,\zeta)$ monotonically increases in each of $n+1$ intervals $[0,\hat{\gamma}_1), (\hat{\gamma}_1,\hat{\gamma}_2),\ldots,(\hat{\gamma}_{n-1},\hat{\gamma}_n)$ and $(\hat{\gamma}_n,\infty)$. This monotonicity assures that one and only one zero exists in each of these intervals. Due to its role, the zero in the first interval $[0,\hat{\gamma}_1)$ will be denoted hereafter as γ_{min}.

For any $\gamma \in (\gamma_{\text{min}},\hat{\gamma}_1)$, all sign functions equal 1 and the hyperconics in equation (9) are hyperellipsoides. Moreover, since n lengths $a_i(\gamma,\zeta)$ increase with γ, we can characterise a region centered on $x_c(\gamma,\zeta)$, in which $E(x,\zeta)$ is convex $\forall\zeta$. For $\gamma = \gamma_{\text{min}}$, all lengths $a_i(\gamma,\zeta)$ are null and the hyperconic collapses in a single point. So, for $\gamma = \gamma_{\text{min}}$ we obtain the global minimum of $E(x,\zeta)$ coincident with the centre of the collapsed hyperellipsoid:

$$\tilde{x}(\zeta) = x_c(\gamma_{\text{min}},\zeta) = \left[A^TA - 2\gamma_{\text{min}}\zeta I_n\right]^{-1} A^Tb \tag{11}$$

As γ increase past each of the values $\hat{\gamma}_1,\hat{\gamma}_2,\ldots,\hat{\gamma}_n$, the corresponding value of $\text{sign}(\lambda_i - 2\gamma\zeta)$ changes from $+1$ to -1 and so the structure and behaviour of the hyperconic changes. In particular, the zeroes of $g(\gamma,\zeta)$ within $(\hat{\gamma}_1,\hat{\gamma}_n)$ correspond to saddle points of $E(x,\zeta)$. Indeed, in these cases, some functions $\text{sign}(\lambda_i - 2\gamma\zeta), (i = 1,\cdots,n)$, are equal to 1 and others are equal to -1. The last zero, greater than $\hat{\gamma}_n$, corresponds to the maximum of $E(x,\zeta)$ where all functions $\text{sign}(\lambda_i - 2\gamma\zeta) = -1$.

3 Iterative Algorithm

The ζ parametrisation has been conceived in order to unify and generalise the three basic regression problems, OLS, TLS and DLS. The continuity of the solutions versus ζ, i.e. locus $\tilde{x}(\zeta)$ in equation (11), suggests a novel numerical technique for the solution of the basic problems, which further motivates the

interest about intermediary ζ cases. This technique requires a predefined programmation of the parameter ζ: it uses the solution locus just like an *attraction locus* for the trajectory of the solution estimate in the $(n+1)$-dimensional space (x,ζ) due to the convexity of the region centered on $\tilde{x}(\zeta)$ and is especially conceived for solving the DLS problem, which can be the most troublesome, or, more generally, for solving problems with ζ close to 1.

From a computational point of view, the different regression problems can be unified in a common framework by introducing a single scalar parameter, as in the Weighted TLS [8] approach, which is limited by the requirement of a non finite value of the parameter for the DLS problem. Once introduced this formulation, the problem can be solved by resorting to direct analytical techniques (SVD and partial SVD computation [10]). However, iterative methods can also be used: they allow one to control the convergence and should be preferred when a good starting guess is available (slowly varying systems in time, frequency and space), for moderate dimensions of the data matrix and when high accuracy is not required. At this time, the best iterative technique is the inverse iteration (II) method, which is more robust and works for generic and nongeneric problems [10]. The region of convergence of the iterative methods depends on the regression problem at hand. It is unbounded for the OLS problem (global convergence), but becomes smaller and smaller for increasing ζ (DLS being the worst case). However, the availability of a parameter can be exploited for assuring the convergence for any ζ. By increasing ζ from 0 to the value required by the problem in a predefined or adaptive way, it is always possible to keep the estimate in the convexity region of $E(x,\zeta)$ around $\tilde{x}(\zeta)$, which is equivalent to the creation of an *attraction locus* [11]. Furthermore, unlike WTLS, ζ is always finite (positive and smaller or equal to 1). This approach has to be associated with a specific numerical method [12] for minimising cost function (3), e.g. steepest descent, conjugate gradient, Newton and quasi-Newton methods. The next section shows that this use of parameter ζ is advantageous in solving large and very large sets of equations. For the sake of brevity, we do not report on the details of the specific gradient-based algorithm implemented but compare the performance with other well-known methods.

4 Examples and Numerical Considerations

Define $C = [A;b] \in \Re^{m\times(n+1)}$ and consider the (one-dimensional) TLS solution. The total number of operations (flops) required by the method proposed here after the presentation of all the rows of C is given by $2m(3n+1)$. The ratio $k(m,n)$ of the operation counts of the partial SVD (as pointed out else-

where [10,4] with $s = 2$, where s is the average number of required QR/QL iteration steps for convergence to one basis vector) to those of the method proposed here is given by:

$$k(m,n) = \begin{cases} \dfrac{\left(2mn^2 - \frac{2}{3}n^3 + 11n^2 + \frac{128}{3}n - 2m - 55\right)}{2m(3n+1)} & \text{for } m < \frac{5}{3}n \\ \dfrac{\left(mn^2 + n^3 + \frac{23}{2}n^2 + mn + \frac{83}{2}n - 62\right)}{2m(3n+1)} & \text{for } m \geq \frac{5}{3}n \end{cases} \quad (12)$$

and the analogous ratio for the II method[10] is given by :

$$k(m,n) = \frac{\left(\frac{1}{6}n^3 + \frac{3}{4}n^2 + \frac{7}{3}n + n(n+7)K_i\right)}{2m(3n+1)} \quad (13)$$

where K_i is the number of II steps for given C. Formulae (12) and (13) are tabulated in Tables 1 and 2, respectively.

Table 1. Ratio of the operation counts of the partial SVD method to those of the method proposed here.

$m \downarrow n \rightarrow$	20	50	100	200	500	1000	2000
20	5.79	–	–	–	–	–	–
50	5.63	12.7	–	–	–	–	–
100	4.54	13.6	23.9	–	–	–	–
200	3.99	11.0	26.1	46.2	–	–	–
500	3.66	9.48	20.5	47.5	112.9	–	–
1000	3.55	8.96	18.6	40.5	126.0	224.0	–
2000	3.50	8.70	17.7	37.0	104.7	251.0	446.2

Table 2. Ratio of the operation counts of the inverse iteration method to those of the method proposed here,by assuming $K_i = 2$.

$m \downarrow n \rightarrow$	20	50	100	200	500	1000	2000
20	1.13	–	–	–	–	–	–
50	0.45	1.89	–	–	–	–	–
100	0.23	0.94	3.25	–	–	–	–
200	0.11	0.47	1.63	6.02	–	–	–
500	0.05	0.19	0.65	2.41	14.3	–	–
1000	0.02	0.09	0.33	1.20	7.17	28.2	–
2000	0.01	0.05	0.16	0.60	3.59	14.1	56.0

The comparison with the partial SVD method (Table 1) is in favour to the method proposed here for any value of m and n. The comparison with the II method (Table 2) is in favour for increasing m and n not too far from m.

Consider, as an example, the following benchmark problem [13]: a line model $a_1x_1 + a_2x_2 = 1$ is fitted to an observation data set by the estimation of its parameters. Here, $a_1 = 0.25$ and $a_2 = 0.5$ ($n = 2$). First, m points are taken from this line with $0 < x < 5$ by uniform sampling. Then, the noisy observation set is generated by adding Gaussian noise with zero mean and variance $\sigma^2 = 0.005$ to these points. The II method requires fewer iterations, but the cost per iteration is much larger. It is apparent in Table 3 where the problem is solved for several values of m. The technique proposed here works far better for large m: for $m \geq 400$ the computational cost remains nearly the same for a given accuracy. This phenomenon can be easily explained by the observation that the cost function (3) is derived from the (weighted) Rayleigh Quotient of C^TC and then its minimisation operates on the column space of C, implying that it mainly depends [11] on n and not on m. This is an important advantage for large and very large systems of linear equations.

Table 3. Total computational cost (flops) of the inverse iteration method and the method proposed here for the benchmark problem.

m	50	100	250	400	1000
inverse iteration (II)	31123	122596	756316	1928876	12022016
here proposed	46175	313799	451397	632009	632747

5 Conclusions

This paper has considered the generalisation of the Total Least Squares (TLS) problems by introducing a wider class of problems comprehensive also of the OLS and DLS ones as particular cases. This generalisation is aimed to the unification of the previous problems and the formulation of a class of iterative algorithms characterised by a robust convergence. These algorithms are based on a geometrical and mathematical analysis of the parametrised cost function. This approach also requires a finite value of the parameter and guarantees the convergence for an appropriate choice of the parameter. Until now the parameter ζ has been defined in advance. Future work will imply its definition in an adaptive way in order to track the changing convergence domain with respect to ζ and to accelerate the algorithm without damaging the robustness of the method.

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