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# Least squares problems with element-wise weighting

M L Rastello<sup>1</sup> and A Premoli<sup>2</sup>

<sup>1</sup> Istituto Nazionale di Ricerca Metrologica, strada delle Cacce 91, I-10135 Torino, Italy

<sup>2</sup> Dipartimento di Elettronica e Informazione, Politecnico di Milano, piazza Leonardo da Vinci 32, I-20133 Milano, Italy

E-mail: [rastello@inrim.it](mailto:rastello@inrim.it)

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## Abstract

In the conventional least squares solution of an overdetermined system of linear equations, independently distributed (i.d.) errors are assumed to affect the known terms. However, in most metrological applications, both matrix elements and known terms can be affected by errors with zero averages and different variances because they represent, in general, various physical quantities and therefore they can be measured with different accuracy. This paper reviews the least squares formulation with element-wise weighting, hereafter called element-wise weighted least squares (EWLS), applied to metrology. Formulations take into account i.d. errors in both matrix elements and known terms but relax the assumption of identical variances of element errors peculiar to the total least squares approach, while preserving their statistical independence. The variances of matrix elements and known terms are statistically independent or linked, for elements of single rows, by a generic covariance matrix. The latter statistical dependence can be accounted for successfully. Some examples compare the performances of the EWLS formulation with the more popular weighted least squares and total least squares approaches. Then, EWLS is applied for calibrating colorimeters as the devoted least-squares approach allows the uncertainties to be taken into proper account. Experimental results show the capabilities of the proposed method for accurate calibrations.

## 1. Introduction

In measurement science some unknown (output) quantity is estimated on the basis of quantitative data about a set of measured (input) quantities. The relationship between input and output quantities can be modelled mathematically. Quite often this model consists of as many relationships as the unknowns. However, in practice a relatively large number of measurements is used to infer a smaller number of measurands. In these cases, the model is inconsistent unless the data of the problem are assumed to be noisy; the model is said to be overdetermined and an adjustment procedure finds measurand values such that they are in good agreement as much as possible with the model and the experimental input data.

In metrology, the model takes the analytical form of a calibration curve. When the analytical model is not known, it consists of its approximation by combining properly chosen

parametric functions. This paper deals with linear fitting problems where the uncertainty in the input quantities is not negligible.

We consider linear models described by a linear algebraic system of equations  $AX = B$ . Here  $D := [A, B]$  contains the *measured data* and  $X \in \mathcal{R}^{n \times l}$  is the *parameter* matrix to be estimated. With fewer parameters than equations and with noisy data the model equations cannot be exactly satisfied, the residual matrix  $R = AX - B$  is considered, and an approximate solution for  $X$  is sought.

The classical least squares (LS) approach minimizes the Frobenius norm of the residual matrix, by applying the correction  $\Delta B$  with the smallest Frobenius norm to the right-hand side  $B$  in order to make the corrected system exactly solvable. The LS method is the best linear unbiased estimator when  $A$  is noise-free and  $B$  is corrupted by independent and identically distributed (i.i.d.) errors.

More general models are known in the literature as *measurement error* (also called *errors-in-variables*) models [1]. Here the assumption is that there is a true but unknown value  $D_0 = [A_0 \ B_0]$  of the measured data and a true value  $X_0$  of the parameter that satisfy the theoretical equation  $A_0 X_0 = B_0$ . The measured data  $D$  are obtained from the true value with an additive noise  $\tilde{D} := [\tilde{A} \ \tilde{B}]$ , i.e.  $D = D_0 + \tilde{D}$ .

The total least squares (TLS) technique [2–8] is a parameter estimation technique for the linear measurement error model when all elements of  $D$  are perturbed by i.i.d. errors. In this case, a correction  $\Delta D = [\Delta A \ \Delta B]$  is applied to  $D$ , so that the corrected system of equations  $(A_0 + \Delta A)X = B_0 + \Delta B$  becomes exactly solvable. Again the smallest correction, according to the Frobenius norm, is sought. Indeed, the properties of the estimator are well understood, and robust and efficient methods exist for its solution, based on the singular value decomposition (SVD). The TLS solution is given analytically in terms of the  $l$  smallest right singular vectors of the data matrix  $D$  and it provides a *consistent estimator* for the true parameter value  $X_0$  under mild additional assumptions. The TLS approach requires that all variances are coincident, so in some sense TLS requirements are stricter than the weighted least squares (WLS) ones, where the variances of each known term can be chosen independently and consequently fitted with more difficulty to the statistics of the actual data.

The TLS method has also been extended to more general noise situations as the errors on the elements of  $D$  are of different sizes. This extension of the TLS method relaxes the i.i.d. assumption for the errors. In the so-called *generalized total least squares* (GTLS) estimator, the errors  $\tilde{D}$  are assumed *row-wise independent* and correlated within the rows with *identical covariance matrix*  $V$ . The method presented in [9] allows a reliable computation of the GTLS estimator. The GTLS method is still restrictive for some applications because of the assumption that all rows of  $\tilde{D}$  have equal covariance matrix.

A further generalization for the case when the elements of  $\tilde{D}$  are independent but not identically distributed with element-wise different error variances is proposed in [10]. The problem is called *element-wise weighted total least squares*. This formulation is a generalization of the TLS method.

Let the linear model be  $A_0 X_0 = B_0$ , where  $A_0, B_0$  are the true but unobservable values of the measured data  $A, B$  and  $X_0 \in \mathfrak{R}^{n \times l}$  the true value of the output quantity  $X$  of interest. The measurement model will be  $AX \approx B$ , where  $A = A_0 + \tilde{A}$ ,  $A \in \mathfrak{R}^{m \times n}$  and  $B = B_0 + \tilde{B}$ ,  $B \in \mathfrak{R}^{m \times l}$ , with  $\tilde{A}, \tilde{B}$  zero mean additive noise (measurement errors, random matrices), respectively. Every row of  $D := [A, B] \in \mathfrak{R}^{m \times (n+l)}$  corresponds to a measurement. Let rows be independent but non-identically distributed. These problems are called EWLS problems [11, 12] and turn out to be of wide interest in many measurement applications, as evidenced in [13].

## 2. Problem formulation

As stated in the introduction, every measurement corresponds to a single row of the augmented matrix  $D := [A, B] \in \mathfrak{R}^{m \times (n+l)}$ . With this notation, the measurement model becomes

$$DY = 0 \tag{1}$$

with measured data  $D = D_0 + \tilde{D}$ ,  $D \in \mathfrak{R}^{m \times (n+l)}$ , where  $D_0$  are the true but unknown data, and

$$Y := \begin{bmatrix} X \\ -I \end{bmatrix}, \quad Y \in \mathfrak{R}^{(n+l) \times l} \tag{2}$$

is the augmented matrix, associated with the true value  $Y_0 = [X_0^T \ I]^T$  satisfying  $D_0 Y_0 = 0$ ;  $\tilde{D}$  are the measurement errors, random matrices defined as  $\tilde{D} = [\tilde{A} \ \tilde{B}]$ , with zero mean and independent rows  $\tilde{d}_i$  with known  $(n+l) \times (n+l)$  covariance matrices

$$V_i^d := \text{cov}(\tilde{d}_i) = \begin{bmatrix} \text{cov}(\tilde{a}_i) & \text{cov}(\tilde{a}_i, \tilde{b}_i) \\ \text{cov}(\tilde{b}_i, \tilde{a}_i) & \text{cov}(\tilde{b}_i) \end{bmatrix} = \begin{bmatrix} V_i^{a,a} & V_i^{a,b} \\ V_i^{b,a} & V_i^{b,b} \end{bmatrix}; \quad i = 1, \dots, m. \tag{3}$$

Hereafter, column vector  $d_i$  groups the elements of the  $i$ th row of  $D$ .

Solving the EWLS problem consists in finding the optimal values of the problem variables  $X$  and  $\Delta D$  minimizing the cost function

$$\min_{X, \Delta D} \sum_{i=1}^m \Delta d_i^T [V_i^d]^{-1} \Delta d_i \quad \text{subject to} \quad (D + \Delta D) \begin{bmatrix} X \\ -I \end{bmatrix} = 0, \tag{4}$$

where  $\Delta D \equiv [\Delta d_1 \ \Delta d_2 \ \dots \ \Delta d_m]^T$  are the correction on measured data to compensate for the measurement error  $\tilde{D}$ . Let  $(\hat{X}, \Delta \hat{D})$  denote the optimal solution of this minimization problem:  $\hat{X}$  will represent the EWLS estimate of  $X_0$  whereas  $D + \Delta \hat{D}$  will be the EWLS estimate of true data  $D_0$ . Note that the exact covariances  $V_i^d$  are not needed. Knowledge up to a constant factor is sufficient, as the cost function can be proved proportional to this factor and the minimum point is not affected.

If  $V_i^d = I$ , the EWLS problem reduces to a conventional TLS problem, where errors are element-wise independent and equally sized [7]. If  $V_i^d = V \ \forall i$  then we have a GTLS [9], where errors are row-wise independent and correlated within rows with identical covariance matrix  $V$ .

A more general formulation can be obtained by allowing all elements of some rows of  $D$  to be free of errors. The presence of noise-free rows can be used to reduce the size of the estimation problem. The resulting new problem is of smaller dimension, both in terms of constraints and number of variables. For the solution of this general case, see [12].

Note that the correction matrix  $\Delta D$  is an estimate of  $-\tilde{D}$ . In general, the TLS cost function is a measure of the estimated absolute error. The relative error TLS problem can be shown to be an EWLS problem with  $V_i^d = \text{diag}(d_{i1}^2, \dots, d_{i,n+1}^2)$ .

## 3. Problem solution: minimization

The solution of the EWLS problem defined in section 2 is obtained in two stages.

The first stage analytically minimizes the cost function with respect to the correction  $\Delta D$  by keeping the value of

$X \in \mathfrak{R}^{n \times l}$  constant, i.e. we find a function  $f_0(X) : \mathfrak{R}^{n \times l} \rightarrow \mathfrak{R}$

$$f_0(X) = \min_{\Delta D} \sum_{i=1}^m \Delta d_i^T [V_i^d]^{-1} \Delta d_i \quad \text{subject to} \\ [D + \Delta D]Y = 0 \quad \forall X \in \mathfrak{R}^{n \times l}. \quad (5)$$

For a fixed  $X \in \mathfrak{R}^{n \times l}$ , the constraint is a linear equation in the optimization variable  $\Delta D$ . Problem (5) is separable in  $m$  sub-problems, each for each vector  $\Delta d_i$ . Therefore, one has to solve  $m$  independent optimization problems

$$f_i(X) = \min_{\Delta d_i} \Delta d_i^T [V_i^d]^{-1} \Delta d_i \quad \text{subject to} \\ Y^T \Delta d_i = -r_i \quad i = 1, \dots, m, \quad (6)$$

where  $r_i$  is the column vector grouping the  $i$ th row of the residual matrix,  $R \equiv AX - B$ . The generic  $i$ th problem is a smooth convex optimization problem with analytical solution

$$\Delta \hat{d}_i = -V_i^d Y (Q_i)^{-1} r_i, \quad (7)$$

where for convenience we set  $Q_i(X) := Y(X)^T V_i^d Y(X)$ . The minimizer of the original problem (5) is given by

$$\Delta \hat{D} = - \begin{bmatrix} r_1^T (Q_1)^{-1} Y^T V_1^d \\ \vdots \\ r_m^T (Q_m)^{-1} Y^T V_m^d \end{bmatrix} \quad (8)$$

and the objective function assumes the value

$$f_0(X) = \sum_{i=1}^m f_i(X) = \sum_{i=1}^m r_i^T (Q_i)^{-1} r_i. \quad (9)$$

In the second stage, the EWLS problem is solved as the unconstrained optimization problem

$$\min_X f_0(X), \quad (10)$$

In general,  $f_0(X)$  is not convex. Therefore, EWLS is a non-convex optimization problem with no analytical solution, and it requires some iterative algorithms.

### 4. Iterative procedure

The iterative algorithm is based on an approximation of the first order optimality condition of (10):

$$f'_0(X) = 0. \quad (11)$$

The derivative of  $f_0$  with respect to  $X$  is given by

$$f'_0(X) = 2 \sum_{i=1}^m \{a_i r_i(X)^T Q_i^{-1}(X) - [V_i^a, V_i^{a,b}] Y(X) \\ \times Q_i^{-1}(X) r_i(X) r_i(X)^T Q_i^{-1}(X)\}. \quad (12)$$

Equation (11) is a necessary condition for a minimum of (10); i.e. a solution of (11) corresponds to the global minimum of (10). Solving (11) is, however, a difficult non-linear problem and we approach the solution by an iterative procedure. Let  $X^{(k)}$  be the approximation on the  $k$ th step: the approximation  $X^{(k+1)}$  on the next step is defined as the solution of equation

$$F(X^{(k+1)}, X^{(k)}) = 0, \quad (13)$$

where  $F$  is a linear approximation of  $f'_0(X^{(k+1)})$ , evaluated in  $X^{(k)}$ , given by

$$F(X^{(k+1)}, X^{(k)}) = 2 \sum_{i=1}^m \{a_i (X^{(k+1)})^T a_i - b_i\}^T Q_i^{-1}(X^{(k)}) \\ - (V_i^a X^{(k+1)} - V_i^{a,b}) Q_i^{-1}(X^{(k)}) r_i(X^{(k)}) r_i^T(X^{(k)}) \\ \times Q_i^{-1}(X^{(k)}\}. \quad (14)$$

On the  $k$ th step of the iterative algorithm, we solve equation (13). The iteration is repeated until the weighted Frobenius norm (WFN) of the relative difference between the new estimate and the previous one is smaller than a given tolerance. The algorithm is a successive approximation-type algorithm. It is heuristic because equation (11) is only a necessary condition for optimality of (10), and the iteration of the solution of equation (13) does not guarantee the global convergence to a solution of (11). Note that the proposed algorithm is not a Gauss-Newton type algorithm for solving equation (13) because the proposed approximation is not the first-order truncated Taylor series of  $f'_0$ .

As for local convergence, if the initial approximation is sufficiently close to the EWLS estimator, the algorithm based on linear approximation almost surely converges to the estimator. Moreover, for a fixed sample size, the convergence is linear.

The EWLS estimator generalizes the TLS estimator and improves its statistical accuracy under more general noise assumptions but makes the problem computationally more difficult. Indeed, while the TLS problem has one closed form analytical solution and can be computed reliably via the SVD, a solution in a closed form is not known for generic EWLS problems. This paper proposes a robust iterative algorithm solving this class of problems. It is based on the minimization of the WFN of residual matrix [11, 12]. WFN turns out to be equal to the sum of ratios of suitable quadratic forms versus  $X$ . This objective function is convex-constrained to a finite sub-region including the expected minimum and requires an iterative algorithm to find the solution. In principle, there can be multiple solutions; essentially they are due to the covariance matrix  $V$  depending on the row, as it affects the denominator of any ratio appearing in the objective function. The choice of a good starting point may be critical because the boundary of the convexity sub-region of  $\mathfrak{R}^{n \times l}$  cannot be easily determined. Anyway, the user's experience helps this choice. In many EWLS problems of practical interest the objective function appears to exhibit a unique minimum and so the convergence to this minimum is assured. This non-linearity does not appear in TLS and GTLS because denominators in the ratios are coincident.

### 5. Algorithm

In detail, the algorithm steps are as follows.

- (i) Read the data matrix  $\tilde{D}$ , the covariance matrix  $V^{\tilde{d}}$  and the maximum allowed number of iterations  $K$ .
- (ii) Set the iteration counter  $k = 0$  and choose the starting value  $X^{(0)}$ .
- (iii) Increase  $k = k + 1$ .
- (iv) Set  $X^1 = X^{(0)}$ .

- (v) If  $k = K$ , the algorithm does not converge. End.
- (vi) Calculate  $Q_i(X^{(k)})$ .
- (vii) Calculate  $R(X^{(k)})$ .
- (viii) Solve  $F(X^{(k+1)}, X^{(k)}) = 0$ .
- (ix) If  $\|X^{(k+1)} - X^{(k)}\| \geq \varepsilon X^{(0)}$ , go to step (iii).
- (x) The value  $X^{(k+1)}$  in step (viii) approximates the minimizer  $\hat{X}$  with a relative accuracy less than  $\varepsilon$ . End.

Note that the numerical convergence is controlled by the distance between two successive values in step (ix).

For the initial approximation  $X_0$  one can use the GTLS estimate with weighting matrix  $V = \sum_{i=1}^m V_i/m$ . Alternatively, one can use the computationally cheaper WLS estimate. The choice between them depends on the noise covariance information. If errors in  $B$  are larger than errors in  $A$  then WLS should be used.

If the elements of any row of  $\tilde{D}$  are uncorrelated, i.e. if  $V_i^d = \text{diag}(\sigma_{i,1}^2, \dots, \sigma_{i,n}^2, \sigma_{i,n+1}^2, \dots, \sigma_{i,n+l}^2)$  for any  $i$ , one can simplify  $Q_i = \sum_{j=1}^n \sigma_{ij}^2 x_j + \sum_{j=n+1}^{n+l} \sigma_{ij}^2$ .

### 6. Consistency of the estimator

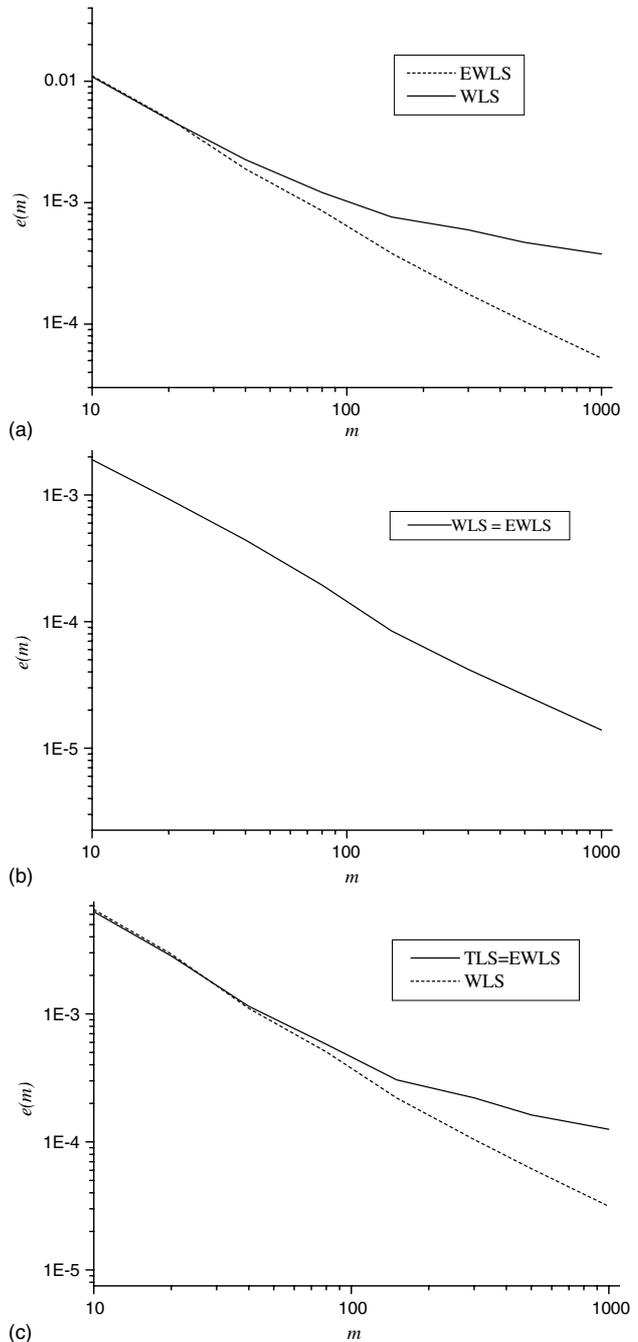
In this section some simulation results illustrate the consistency of the EWLS estimator. Consistency is indicated by the convergence of the relative error of the estimation to zero for increasing number  $m$  of rows. The simulated example corresponds to the measurement error model (1) with  $n = 3$ ,  $l = 1$  and  $m \in [10, 1000]$ . The elements of random matrix  $\tilde{D}$  are statistically normal and independent, with variances  $\text{var}(\tilde{D}_{ii}) = \sigma_i^2$  and  $\text{var}(\tilde{D}_{ij}) = 0$  for  $i \neq j$ .

We generated a noiseless matrix vector  $A_0$  and determined the corresponding  $B_0$  so that the overdetermined system (1) admits the exact solution  $X_0 = [1 \ 2 \ 3]$ . Then we added to each element of matrix  $D_0$  an independently distributed (i.d.) error with a variance depending on a given scenario.

Four noise scenarios are considered. Each scenario is characterized by the matrix of the error variances  $\Sigma = \sigma_{ij}^2$ , specified element by element. We generate  $N = 500$  different noise realizations (but with the same statistics) for each fixed  $m \in [10, 1000]$  and compute the EWLS estimates  $\hat{x}(m, N)$  and the relative error of estimation  $e(m, N) := \|\hat{x}(m, N) - x_0\|/\|x_0\|$ . Figure 1 shows the behaviour of the average  $e(m) := \sum_{i=1}^N e(m, i)/N$  for three of the considered scenarios.

In the first EWLS scenario, the variances of errors in  $D$  are independently and uniformly chosen in  $[0.01, 0.26]$  for  $A$  and in  $[0.01, 0.035]$  for  $B$ . Figure 1(a) shows the behaviour of the EWLS solution, obtained by choosing all the variances coincident with those of the scenario, and the behaviour of the WLS solution, obtained by setting the variances of  $A$  to zero and the variances of  $B$  coincident with the scenario. Table 1 shows the true value  $X_0$  in the first column, the starting point (WLS) in the second column and the EWLS solution in the last column in the case  $m = 1000$ .

In the second EWLS scenario, the variances of errors in  $D$  are independently and uniformly chosen in  $[0.01, 0.026]$  for  $A$  and in  $[0.01, 0.35]$  for  $B$ . In this case, the behaviour of the EWLS solution, obtained by choosing all the variances coincident with those of the scenario, and the behaviour of the WLS solution, obtained by setting the variances of  $A$  to zero



**Figure 1.** (a) Behaviour of  $e(m)$  versus  $m$  for the first EWLS scenario: WLS solution (—) and EWLS solution (- - -). (b) Behaviour of  $e(m)$  versus  $m$  for the WLS scenario: WLS and EWLS solutions. (c) Behaviour of  $e(m)$  versus  $m$  for the TLS scenario: WLS solution (- - -) and EWLS solution (—), coincident with TLS solution.

**Table 1.** True value, starting point and EWLS solution for the first EWLS scenario and  $m = 1000$ .

| Scenario | $X_0$        | WLS solution     | EWLS solution    |
|----------|--------------|------------------|------------------|
| EWLS     | 1.000 000 00 | 0.984 744 963 94 | 1.000 234 998 63 |
|          | 2.000 000 00 | 1.961 338 205 16 | 1.998 773 507 39 |
|          | 3.000 000 00 | 2.946 968 668 02 | 3.000 638 171 99 |

**Table 2.** True value, starting point and EWLS solution for the TLS scenario and  $m = 1000$ .

| Scenario | $X_0$        | WLS solution     | EWLS solution    |
|----------|--------------|------------------|------------------|
| TLS      | 1.000 000 00 | 0.991 894 589 76 | 1.000 391 581 93 |
|          | 2.000 000 00 | 1.978 951 403 17 | 1.998 912 329 90 |
|          | 3.000 000 00 | 2.971 276 945 36 | 3.000 692 025 62 |

and the variances of  $B$  coincident with the scenario, are almost coincident.

In the WLS scenario, the variances of errors in  $D$  are independently and uniformly in the interval  $[0.01, 0.51]$  for  $B$ , whereas those of  $A$  are chosen equal to zero. Figure 1(b) shows the behaviour of the EWLS solution, obtained by choosing all the variances coincident with those of the scenario, and the behaviour of the WLS solution. The two curves are completely superposed, as expected.

The last scenario is TLS: here  $\sigma_{ij} = 0.1$  for all  $i$  and  $j$ . Results are shown in figure 1(c), where the EWLS solution coincides with the TLS one, as expected. Table 2 shows the true value  $X_0$  in the first column, the starting point (WLS) in the second column and the EWLS solution, coincident with the TLS solution, in the last column in the case  $m = 1000$  for the TLS.

Simulation results confirm the consistency of the EWLS estimator, as in [12, 14]. Moreover, for WLS and TLS set-ups, EWLS coincides with the corresponding estimators, which are known to be consistent. As a consequence, the EWLS is a generalization of these well-known methods.

### 7. Linear transformations in colorimetry

In colorimetry, when we wish to define colour coordinates with respect to some arbitrary visual systems with  $N$  photosensors, we assume that the spectral responsivity of the visual photosensor is known up to a linear transformation. If  $T$  is an  $N \times N_\lambda$  matrix whose entries are the sensitivities of each sensor at each sample wavelength, we can compute the response of these sensors to any colour stimulus, defined by the  $N_\lambda$  vector  $w$  whose entries are the spectral characteristics of the stimulus, as  $t = Tw$ , where  $t$  is the vector containing the response of each sensor type to the stimulus. Then we can use  $t$  as the device colour coordinates of  $w$ .

Suppose now that we have two different visual systems and we wish to transform between the colour coordinates of each. Let  $N_s$  be the number of source sensors, with sensitivities specified by  $T_s$ . Similarly let  $N_d$  be the number of destination sensors, with sensitivities specified by  $T_d$ . For any  $w$ , the source device colour coordinates are given by  $t_s = T_s w$  and the destination device colour coordinates are given by  $t_d = T_d w$ . To transform between  $t_s$  and  $t_d$  without direct knowledge of  $w$ , we have to find a  $N_d \times N_s$  matrix  $M$  such that  $T_d = MT_s$ . Then it is easy to show that the matrix  $M$  may be used to compute the destination device colour coordinates from the source device colour coordinates through  $t_d = Mt_s$ . When a linear transformation between  $T_d$  and  $T_s$  exists, it can be found by standard regression techniques. When there is no exact linear transformation, it is not in general possible to transform between the two sets of coordinates. The reason for this is that a pair of lights that have the same colour coordinates for the

source device and different colour coordinates for the source device will always exist. The transformation will therefore be incorrect for at least one member of this pair. When no exact linear transformation exists, it is still possible to make an approximated transformation  $M$  in a LS sense. This transformation is then applied to the source colour coordinates as if it were exact.

A typical example is trying to compute the CIE 1931 XYZ tristimulus values of a colour stimulus from the RGB response of a colour camera. For any colour stimulus, the corresponding camera response  $r, g, b$  can be represented by a  $1 \times 3$  vector and their corresponding XYZ tristimulus values can be represented by a  $1 \times 3$  vector. If only  $r, g, b$  values are used, the transformation between RGB and XYZ is a simple linear transform.

Now, let us consider two different colorimetric devices and try to calibrate one with respect to the other. Let subscript R denote the reference device and D the device under test, and let  $M$  be the number of sensors in both devices. Let us suppose to have  $N > M$  test colours as input to both devices. The output signals from the devices will be denoted by  $\Gamma_R \equiv \{\Gamma_{Ri,n}\}$  and  $\Gamma_D \equiv \{\Gamma_{Di,n}\}$ , respectively, with  $i = 1, 2, \dots, M$  and  $n = 1, 2, \dots, N$ . Taking into account that both  $\Gamma_D$  and  $\Gamma_R$  are affected by errors  $\tilde{\Gamma}_D$  and  $\tilde{\Gamma}_R$  with zero averages and different variances, we have more generally

$$\begin{aligned} \Gamma_{Ri,n} &\rightarrow \Gamma_{Ri,n} + \tilde{\Gamma}_{Ri,n} & i = 1, 2, \dots, M & \quad n = 1, 2, \dots, N, \\ \Gamma_{Di,n} &\rightarrow \Gamma_{Di,n} + \tilde{\Gamma}_{Di,n} & i = 1, 2, \dots, M & \quad n = 1, 2, \dots, N. \end{aligned}$$

To calibrate the device D, we determine a linear transformation  $C$  such that

$$\Gamma_D \cdot C = \Gamma_R. \tag{15}$$

The conventional WLS techniques cannot be applied to solve the overdetermined system of linear equations (15), as they assume that i.d. errors affect only the known terms  $\Gamma_R$ . So, we apply the LS formulation with element-wise weighing, EWLS, to solve the problem in an appropriate way. In the following, we focus on the particular case of tristimulus colorimeters.

### 8. The EWLS calibration method for tristimulus colorimeters

Traditionally, for the calibration of a tristimulus head, the CIE illuminant A is recommended, as it is characterized by a spectral power distribution and chromaticity coordinates  $\{x_A, y_A, z_A\} = \{0.44758, 0.40745, 0.14497\}$  known *a priori*. The CIE-A illuminant is realized experimentally by a CIE-A source, i.e. an incandescent source operating at a given current intensity.

When a tristimulus head with  $M = 3$  channels, called  $x, y, z$ , is illuminated with the CIE-A source, the output photocurrents  $V_{xA}, V_{yA}, V_{zA}$  are measured and, when multiplied by the appropriate calibration factors  $c_x, c_y, c_z$ , give the tristimulus values  $X_A, Y_A, Z_A$ . As a consequence, the values to be assigned to the calibration factors are found from the solution of the exact equation system defined by

$$\gamma_D \cdot c = \gamma_R,$$

with

$$\gamma_D = \begin{bmatrix} V_x & 0 & 0 \\ 0 & V_y & 0 \\ 0 & 0 & V_z \end{bmatrix},$$

$$c = \begin{bmatrix} c_x \\ c_y \\ c_z \end{bmatrix}$$

and

$$\gamma_R = \begin{bmatrix} X_A \\ Y_A \\ Z_A \end{bmatrix} = \begin{bmatrix} x_A \\ y_A \\ z_A \end{bmatrix} \cdot \frac{Q_A}{y_A},$$

where  $Q_A$  is the luminance in candela per square metre of the CIE-A source. In other words, calibration factors are simply given by  $c = \gamma_D^{-1} \cdot \gamma_R$ . If the device under test is only to be used for measurements on tungsten based sources then the traditional method for calibration gives good results. If this is not the case, you can get odd results.

To overcome these drawbacks, the EWLS method allows one to make use of  $i = 1, \dots, N > M$  test colours and solve the overdetermined equation system (15) in a EWLS environment, where

$$\Gamma_D = \begin{bmatrix} \dots & \dots & \dots \\ V_{xi} & V_{yi} & V_{zi} \\ \dots & \dots & \dots \end{bmatrix}, \quad C = \begin{bmatrix} c_{xx} & c_{xy} & c_{xz} \\ c_{yx} & c_{yy} & c_{yz} \\ c_{zx} & c_{zy} & c_{zz} \end{bmatrix},$$

$$\Gamma_R = \begin{bmatrix} \dots & \dots & \dots \\ X_i & Y_i & Z_i \\ \dots & \dots & \dots \end{bmatrix},$$

and covariance matrices are taken into account appropriately.

With the formalisms of section 2, EWLS considers the linear model described by the linear algebraic system of equations  $\Gamma_D C = \Gamma_R$ . Here  $G := [\Gamma_D \quad \Gamma_R]$  contains the *measured data* and  $C$  is the *parameter* matrix to be estimated. With fewer parameters than equations and with noisy data the model equations cannot be exactly satisfied; the residual matrix  $R = \Gamma_D C - \Gamma_R$  is considered and an approximate solution for  $X$  is sought. Solving the EWLS problem consists in finding the optimal values of the problem variables  $C$  and  $\Delta G = [\Delta \Gamma_D \quad \Delta \Gamma_R]$  minimizing the cost function

$$\min_{C, \Delta G} \sum_{i=1}^m \Delta g_i^T [V_i^g]^{-1} \Delta g_i$$

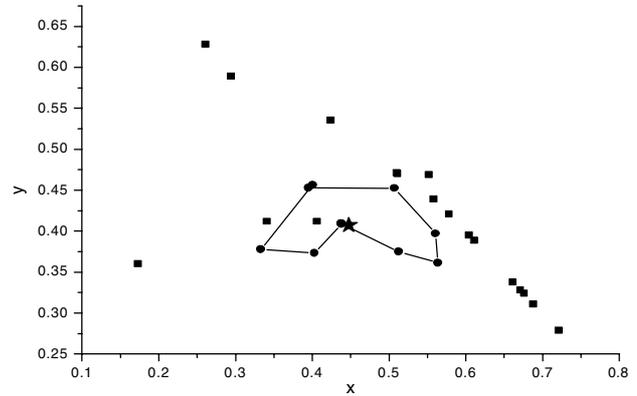
subject to

$$(G + \Delta G) \begin{bmatrix} C \\ -I \end{bmatrix} = 0,$$

where  $\Delta G$  is the correction on measured data to compensate for the measurement error  $\tilde{G}$ , random matrices defined as  $\tilde{G} = [\tilde{\Gamma}_D \quad \tilde{\Gamma}_R]$ , with zero mean and independent rows  $\tilde{g}_i$  with known covariance matrices  $V_i^g$ .

### 9. Experimental results

To test the capabilities of the proposed method for accurate calibrations, the tristimulus colorimeter described in [15] has been calibrated according to the method proposed here and results have been compared with the results obtained by the traditional method for calibration.



**Figure 2.** Chromaticity coordinates  $(x, y)$  of the CIE-A source (star) used by the classical method, the colour stimuli (squares) used by the EWLS method and colour tiles (circles, solid line) used to test the EWLS solution with respect to the classical solution.

To perform the test, a CIE-A source has been realized by means of a luminance standard source, characterized by a double-sphere arrangement to achieve a better uniformity over the exit aperture, and a distribution temperature of  $(2856 \pm 20)$  K.

According to the traditional method, the  $M = 3$  tristimulus heads have been illuminated with the CIE-A source, the output photocurrents  $V_{xA}, V_{yA}, V_{zA}$  were measured and the following calibration vector has been obtained:

$$c = \begin{bmatrix} c_x = 0.127\ 15 \\ c_y = 0.043\ 93 \\ c_z = 0.163\ 60 \end{bmatrix}. \quad (16)$$

Then, according to the EWLS method, the CIE-A source has been filtered in turn by  $N = 19$  Schott glasses to get red, orange, yellow, green and blue colour stimuli. Their chromaticity coordinates are represented by squares in figure 2, where the star represents the chromaticity coordinates of CIE-A. Their distribution around the CIE-A point in figure 2 suggests that important improvements should be expected for stimuli in the blue region, whereas almost no improvement will be expected in the green region.

The tristimulus values of these colour stimuli were first measured by the reference spectroradiometer and the related uncertainties evaluated according to [16]. Then the output photocurrents of the colorimeter under test were recorded and uncertainties evaluated in the same manner. By solving the EWLS problem, we obtained the calibration matrix below:

$$C = \begin{bmatrix} c_{xx} = 0.120\ 35 & c_{xy} = 0.001\ 15 & c_{xz} = 0.013\ 46 \\ c_{yx} = 0.002\ 69 & c_{yy} = 0.042\ 72 & c_{yz} = 0.003\ 29 \\ c_{zx} = -0.005\ 85 & c_{zy} = 0.002\ 98 & c_{zz} = 0.154\ 65 \end{bmatrix}$$

Note how the diagonal elements of the  $3 \times 3$  matrix  $C$  are similar to the elements of the  $1 \times 3$  vector  $c$ .

Finally, the following ceramic colour standards: white, pale grey, mid-grey, difference grey, deep grey, deep pink, red, orange, cyan, green, yellow and deep blue, were illuminated by an incandescent light source with a distribution temperature of 2890 K. Their resulting chromaticity coordinates, as measured by the reference spectroradiometer, are represented in figure 2 by circles connected by solid lines. As you can understand

**Table 3.** Reference tristimulus values,  $X_{ref}$ ,  $Y_{ref}$ ,  $Z_{ref}$ , tristimulus values  $X_c$ ,  $Y_c$ ,  $Z_c$ , obtained by the traditional method, and tristimulus values  $X_C$ ,  $Y_C$ ,  $Z_C$ , obtained by the EWLS method. Data are reported tile by tile.

| Colour    | $X_{ref}$ | $Y_{ref}$ | $Z_{ref}$ | $X_c$ | $Y_c$ | $Z_c$ | $X_C$ | $Y_C$ | $Z_C$ |
|-----------|-----------|-----------|-----------|-------|-------|-------|-------|-------|-------|
| White     | 198.0     | 184.6     | 69.1      | 198.0 | 184.6 | 69.1  | 197.9 | 185.0 | 68.7  |
| Blue      | 16.2      | 15.1      | 9.0       | 17.5  | 16.4  | 10.2  | 17.8  | 16.5  | 9.9   |
| Cyan      | 40.3      | 45.6      | 35.0      | 38.3  | 45.3  | 35.9  | 40.4  | 45.6  | 35.3  |
| Green     | 45.3      | 52.0      | 17.4      | 46.5  | 52.2  | 17.4  | 46.8  | 52.0  | 17.8  |
| Yellow    | 165.7     | 147.9     | 13.2      | 170.0 | 147.8 | 11.7  | 165.7 | 147.6 | 13.3  |
| Orange    | 140.3     | 99.4      | 10.6      | 144.0 | 99.8  | 11.3  | 139.8 | 100.3 | 10.8  |
| Red       | 73.1      | 46.9      | 9.7       | 76.4  | 45.0  | 10.7  | 74.3  | 45.6  | 9.7   |
| Pink      | 54.5      | 39.9      | 12.0      | 56.7  | 39.6  | 12.9  | 55.8  | 39.9  | 12.3  |
| Mid-grey  | 67.9      | 63.5      | 23.8      | 67.7  | 63.4  | 24.3  | 67.7  | 63.5  | 24.2  |
| Pale grey | 147.1     | 137.3     | 51.2      | 145.5 | 136.2 | 51.1  | 145.5 | 136.6 | 50.8  |

**Table 4.** Reference values,  $X_{ref}$ ,  $Y_{ref}$ ,  $Z_{ref}$ , values  $Y_c$ ,  $x_c$ ,  $y_c$  by the traditional method, and values  $Y_C$ ,  $x_C$ ,  $y_C$  by the EWLS method. Data are reported tile by tile.

| Colour    | $Y_{ref}$ | $x_{ref}$ | $y_{ref}$ | $Y_c$ | $x_c$  | $y_c$  | $Y_C$ | $x_C$  | $y_C$  |
|-----------|-----------|-----------|-----------|-------|--------|--------|-------|--------|--------|
| White     | 184.6     | 0.4383    | 0.4087    | 184.6 | 0.4383 | 0.4087 | 185.0 | 0.4382 | 0.4094 |
| Blue      | 15.1      | 0.4027    | 0.3732    | 16.4  | 0.3963 | 0.3729 | 16.5  | 0.4020 | 0.3738 |
| Cyan      | 45.6      | 0.3331    | 0.3778    | 45.3  | 0.3203 | 0.3791 | 45.6  | 0.3330 | 0.3762 |
| Dif green | 53.0      | 0.4005    | 0.4564    | 53.2  | 0.4065 | 0.4529 | 53.0  | 0.4062 | 0.4496 |
| Green     | 52.0      | 0.3950    | 0.4530    | 52.2  | 0.4007 | 0.4497 | 52.0  | 0.4011 | 0.4467 |
| Yellow    | 147.9     | 0.5070    | 0.4525    | 147.8 | 0.5159 | 0.4486 | 147.6 | 0.5076 | 0.4518 |
| Orange    | 99.4      | 0.5605    | 0.3970    | 99.8  | 0.5643 | 0.3914 | 100.3 | 0.5578 | 0.3998 |
| Red       | 46.9      | 0.5636    | 0.3614    | 45.0  | 0.5779 | 0.3409 | 45.6  | 0.5734 | 0.3519 |
| Pink      | 39.9      | 0.5126    | 0.3749    | 39.6  | 0.5192 | 0.3626 | 39.9  | 0.5160 | 0.3700 |
| Mid-grey  | 63.5      | 0.4377    | 0.4092    | 63.4  | 0.4355 | 0.4082 | 63.5  | 0.4356 | 0.4091 |
| Pale grey | 137.3     | 0.4382    | 0.4092    | 136.2 | 0.4373 | 0.4093 | 136.6 | 0.4372 | 0.4100 |

from figure 2, this test is not really challenging for the classical method, as circles, connected by the solid line and representing the reference chromaticity of the ceramic tiles used for the test, encircle the star which represents the illuminant CIE-A.

Reference tristimulus values  $X_{ref}$ ,  $Y_{ref}$ ,  $Z_{ref}$  are listed, for each tile, in table 3, together with the tristimulus values  $X_c$ ,  $Y_c$ ,  $Z_c$  for each tile, measured by the colorimeter calibrated by the traditional method using the calibration vector  $c$  (16), and the tristimulus values  $X_C$ ,  $Y_C$ ,  $Z_C$  for each tile, obtained by the EWLS method using the calibration matrix  $C$ .

For the sake of comparison, the chromaticity coordinates  $x$ ,  $y$  are also calculated for each tile from the data presented in table 3, and the results are reported in table 4, tile by tile.

As you can see from the values reported in table 4, results obtained by the EWLS method are consistent with those obtained by the traditional method for all tiles and are particularly improved in the blue region. This was expected and is mainly due to the choice of the calibration filters, as shown in figure 1.

### 10. Conclusions

We reviewed a least square problem that is useful in metrology for solving an overdetermined system of equations with row-wise independent and differently sized errors. The defined problem is a constrained optimization problem with the parameter estimate and the noise correction as variables. An iterative algorithm is presented that solves the first order optimality condition by successive approximations with a linear equation. Numerical examples show that the proposed algorithm is more efficient than standard methods in some cases of metrological interest.

The least square approach is proposed for calibrating colorimeters. Experimental results prove that the proposed algorithm is more efficient than the standard method.

### References

- [1] Fuller W A 1989 *Measurement Error Models* (New York: Wiley)
- [2] Golub G H and Reinsch C 1970 Singular value decomposition and least squares solutions *Numer. Math.* **14** 403–20
- [3] Van Huffel S and Vandewalle J 1991 *The Total Least Squares Problem: Computational Aspects and Analysis* (Frontiers in Applied Mathematics) (Philadelphia: SIAM)
- [4] Van Huffel S (ed) 1997 *Recent Advances in Total Least Squares Techniques and Errors-in-Variables Modeling* (Philadelphia: SIAM)
- [5] Van Huffel S and Lemmerling P (ed) 2002 *Total Least Squares and Errors-in-Variables Modeling: Analysis, Algorithms and Applications* (Dordrecht: Kluwer)
- [6] Hodges S D and Moore P G 1972 Data uncertainties and least square regression *Appl. Stat.* **21** 185–95
- [7] Golub G H and Van Loan C F 1980 An analysis of the total least squares problem *SIAM J. Numer. Anal.* **17** 883–93
- [8] Rao D 1997 Unified treatment of LS, TLS and truncated SVD methods using a weighted TLS framework *Recent Advances in Total Least Squares Techniques and Errors-in-Variables Modelling* ed S Van Huffel (SIAM) pp 11–20
- [9] Van Huffel S and Vandewalle J 1989 Analysis and properties of the generalised total least squares problem *SIAM J. Numer. Anal.* **10** 294–315
- [10] De Moor B 1993 Structured total least squares and L2 approximation problems *Linear Algebra Appl.* **188–189** 163–205
- [11] Premoli A and Rastello M L 2002 The parametric quadratic form method for solving total least squares problems

- with element-wise weighting *Total Least Squares and Errors-in-Variables Modelling: Analysis, Algorithms and Applications* ed S Van Huffel and P Lemmerling (Dordrecht: Kluwer) pp 67–76
- [12] Markovsky I, Rastello M L, Premoli A, Kukush A and Van Huffel S 2006 The element-wise weighted total least squares problem *Comput. Stat. Data Anal.* **50** 181–209
- [13] Ichim D, Ciarlini P, Pavese F, Premoli A and Rastello M L 2004 Comparison of LS techniques for the linear approximation of data affected by heteroscedastic errors in both variables with uncertainty estimation *Advanced Mathematical & Computational Tools in Metrology VI* ed P Ciarlini *et al* (Singapore: World Scientific) pp 293–8
- [14] Kukush A and Van Huffel S 2004 Consistency of elementwise-weighted total least squares estimator in a multivariate errors-in-variables model  $AX = B$  *Metrika* **59** 75–97
- [15] Balsamo A, Chimienti A, Desogus S, Grattoni P, Meda A, Nerino R, Pettiti G, Rastello M L and Spertino M 2005 A portable stereovision system for cultural heritage monitoring *Ann. CIRP* **54** 499–502
- [16] CIE TC2-43 2002 *Determination of Measurement Uncertainty in Photometry* 5th draft