MODELLING SUBDIVISION IN MASS METROLOGY

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Abstract:
Subdivision is a crucial technique in mass metrology because it allows the determination of the mass of weights of various nominal values and the realisation of the mass scale.

This technique is usually based on complicated mathematics. The current models are generally sufficient for many practical aims but far from the best performance.

Project 19RPT02, "Improvement of the realisation of the mass scale" (EMPIR Call 2019 – Research Potential), has been, among others, investigating an improved model for the calculations.

Keywords: mass scale; weights; kilogram; multiples and submultiples; subdivision; OIML R 111

1. INTRODUCTION

Subdivision (multiplication) [1] is the main method to realise the mass scale. It involves using at least one reference mass standard to determine the masses of weights across the required range of mass values.

As in [2][3] was pointed out the improvement of the subdivision method would be beneficial for many National Metrology Institutes (NMI). This improvement needs a solid base, especially aiming at small uncertainties. The method to be developed shall be capable of handling correlations, because ignoring them could lead to underestimating the uncertainties.

In this article, we show the model for this work. The actual outcome will be presented in a separate article.

2. EXISTING METHODS

Different combinations of weights of equal total nominal mass are compared in these weighings. The subdivision method is initially for calibrating sets with the highest accuracy.

If only one reference weight is used with this method, the number of weighing equations should be equal to the number of unknown weights; the values of the test weights can be easily calculated.

In reality, the number of weighing equations is always larger than the minimum required ones to avoid propagating errors. The redundancy gives greater confidence in the results and provides smaller uncertainties.

The usual way is to perform a least-squares analysis that requires complicated software to evaluate the set of redundant data.

The project studied several least-squares techniques from the simplest case, the ordinary least squares methods (OLS); and the weighted least squares method (WLS) which provides better results and generalised least squares (GLS) which can handle more than one mass standard.

The methods described above usually include only the weights and the weighing results. Weighing results are the corrected apparent mass differences. They are corrected for the buoyance (air densities and the volumes of the weights), the thermal expansion of the weights, the height difference of the gravity centres of the weights and the linearity and the position errors of the mass comparators. When corrections are applied to the apparent mass differences, they should be included in the least-squares calculations. In doing so the correlations among the input quantities can be introduced.

Considering the correlations among the input parameters, the simpler methods (OLS, WLS) do not suffice; more complicated methods are required. One of them is the generalised least squares algorithm.

The entire list of considered and analysed methods is: Ordinary Least Squares, Weighted Least Squares, Generalised Least Squares, Total Least Squares, Maximum Likelihood Estimation, Maximum a Posteriori Probability and Least Square Adjustment. Additionally, Iteratively Re-weighted Least Squares method was analysed.

3. CONSIDERATION FOR THE IMPROVED METHOD

The first task is to identify the possible correlations. The following list is in estimated order of the importance of the correlation source.

- The mass standards used are definitely correlated. These correlations can be very significant if the mass standards have large nominal values and have the same traceability.
- Air density measurements are correlated using the same instrument or instruments calibrated in the same laboratories (e.g. two thermometers calibrated against the same standard).
- Weights thermal expansions are correlated because of the used thermometer and possibly by estimating the coefficient (usually not measured).
- Heights of the weights are usually correlated, but they can be safely neglected due to the small overall contribution to the uncertainty.
- Position error of the balance can be strongly correlated. It shall be carefully investigated in each case. An example is a balance used at the same nominal value for several measurements.
- Linearity of the balance is strongly correlated if the same balance is used for several measurements.
- The drift of the mass standards can be correlated. The reasons are the common traceability (same calibration history of the mass standards) and the possible similar storage, and use conditions.

4. THE DEVELOPED METHOD

The project recognised the Weighted Least Squares method as suitable for simple cases.

For more demanding cases the project recommends the Gauss Markov approach with the augmented design concept based on publication [4]. The essential point is that the constraints are viewed as data with expected values and uncertainties. Even if this data was not obtained from the current calibration, it still could be included in the calculations. This is a vital aspect in case multiply standards are used. It allows modifying the prior knowledge (change of the standard due to drift, surface changes, etc.). The improved implementation is based on the following equation using matrix notation:

$$Y = X\beta \tag{1}$$

$$Y = \Delta w + \{(1 - 20\alpha)I + \alpha T\}\rho X V - \nabla g D M \tag{2}$$

where:

- Y is the vector of measurand estimate
- β is the vector of the required parameters
- α is the vector of the weights' coefficients of thermal expansion
- X is the design matrix
- Δw is the vector of the weighing indications
- $\rho = \mathrm{diag}\{\rho_\mathrm{a}\}$ matrix, where ρ_a is the air density vector
- V is the vector of the volumes of the standards at 20 °C
- I is an identity matrix
- $T = \mathrm{diag}\{t\}$ matrix, where t is the (air) temperature, assuming the weights temperatures are the same
- ∇g is a constant, the relative gradient of the gravitation acceleration at the weights
- $D = \mathrm{diag}\{d\}$ matrix, where d is the vector of the centre of gravities differences between the mass groups
- M is the vector of the nominal masses for each comparison

The covariance is calculated as:

$$\mathrm{cov}[Y] = \Psi_Y \tag{3}$$

$$\Psi_Y = \Psi_{\nabla W} + \mathrm{diag}\{XV\}\Psi_\rho \mathrm{diag}\{XV\} + \rho X \Psi_V X^T \rho^T \tag{4}$$

where Ψ_Y is the covariance of the measure and estimate

With the constraint used as prior information, the values of the mass standards:

$$R = A^T\beta. \tag{5}$$

where R is the vector of the masses of the mass standards and A^T is the design matrix of constraints

The covariance of R is given by:

$$\mathrm{cov}[R] = \Psi_R \tag{6}$$

Augmenting the design, it results:

$$Z = \begin{bmatrix} Y \\ R \end{bmatrix} \text{and } Z = W\beta \tag{7}$$

or:

$$\begin{bmatrix} Y \\ R \end{bmatrix} = \begin{bmatrix} X \\ A^T \end{bmatrix}\beta \tag{8}$$

The covariance of the augmented design:

$$\Psi_Z = \begin{bmatrix} \Psi_Y & 0 \\ 0 & \Psi_R \end{bmatrix} \tag{9}$$

The result is the Best Linear Unbiased Estimator (BLUE) and is estimated as:

$$\hat{\beta} = (W^T \Psi_Z^{-1} W)^{-1} W^T \Psi_Z^{-1} Z \tag{10}$$

and:

$$\Psi_{\hat{\beta}} = (W^T \Psi_Z^{-1} W)^{-1} \tag{11}$$

Note: $W^T W$ is not singular since the values of the mass standards are introduced as variables (no

Lagrange multiplicator is needed). This solves the Gauss-Markov Minimum Variance:

$$\hat{\beta} = \left[(X^T \Psi_Y^{-1} X) + A\,\Psi_R^{-1} A^T\right]^{-1} \left[(X^T \Psi_Y^{-1} Y) + A\,\Psi_R^{-1} R\right] \tag{12}$$

Note: It would be probably a mistake to treat the constraint information deterministically to find a solution and then treat stochastically to find the correct final covariance matrix. It would be inconsistent and probably inaccurate.

Since the constraint is the mass value resulting from a calibration, it can be logically handled as stochastic. The constraint can be introduced in the design as a parameter.

5. INVESTIGATION OF EXISTING WEIGHING DESIGNS

Apart from the mathematical method, the weighing design is the critical aspect of the subdivision. The project explored new areas of it.

The project analysed the known published weighing designs for sets containing weights with nominal values of 5, 2, 2* and 1, as one of the most typical sets for a decade (nominal values 10 to 1). This investigation includes the OIML, the PTB [5], some of the designs from the EURAMET 1210 project [6] the two improved “PTB” designs from [7] and for demonstration purposes the introductory design from [8].

The used measurements in these designs are in Table 1. The weights are used as standard (S), check weights (C) or test weights (T). For this analysis we considered as seen in Table 1, that there are only four weights to calibrate (test weights), even if in the publications it was stated otherwise. This is necessary to compare the designs.

After an initial selection, the ten designs, listed with reference to their publications in Table 2, were investigated more comprehensively. The measurements in each design are also listed in Table 2. The additional check weights of nominal values 5 or 10 are marked with X. Design 2 also has an additional check weight of nominal value 2.

Table 1: Used measurements

Nom.	**10**	**10**	**5**	**5**	**2**	**2**	**2**	**1**	**1**
Use	S	C	T	C	T	T	C	T	C
1	-1	1							
2	-1		1	1					
3	-1		1		1	1		1	
4	-1		1		1	1			1
5	-1			1	1	1		1	
6				1	1	1			1
7		-1	1	1					
8		-1	1		1	1		1	
9		-1	1		1	1			1
10		-1		1	1	1		1	
11		-1		1	1	1			1
12			-1	1					
13			-1		1	1		1	
14			-1		1	1			1
15				-1	1	1		1	
16				-1	1	1			1
17					-1	1			
18					-1			1	1
19						-1		1	1
20								-1	1
21					-1	1		1	-1
22					1	-1		-1	1
23		-1	1		1		1		1
24				-1		1	1	1	
25						-1	1		
26							-1	1	1
27	-1			1	1	1			1
28					-1	1		-1	1

Table 2: Measurements in the different designs

Design	Measurements	+5	+10
Com [8]	3, 14, 17, 19, 18, 13, 20		
OIML [1]	3, 4, 13, 14, 18, 18, 19, 19, 21, 21, 22, 22		
PTB [5]	1, 2, 7, 12, 13, 16, 17, 18, 19, 20	X	X
1 [6]	1, 2, 5, 7, 11, 12, 14, 16, 17, 18, 19, 20	X	X
2 [6]	1, 2, 5, 7, 12, 13, 14, 17, 18, 19, 20, 20, 23, 24, 25, 26	X	X
3 [6]	3, 8, 11, 13, 16, 18, 19, 20, 27	X	X
4 [6]	1, 2, 7, 12, 13, 14, 15, 16, 17, 18, 19, 20	X	X
5 [6]	3, 4, 13, 14, 17, 18, 19, 20, 22, 28		
I [7]	1, 3, 4, 4, 8, 13, 16, 18, 19, 20	X	X
II [7]	1, 4, 5, 5, 9, 14, 15, 18, 19, 20	X	X

The base for this simulation was a weighted design with ideal measurements. The mass differences were set to the values calculated from the hypothetical values of the weights used in these measurements. The standard uncertainty of each measurement was 2 % of the Maximum Permissible Error of class E_1 (MPE). The results obtained were identical to the hypothetical values of the weights.

The properties and the results of this base calculation are in Table 3.

Description of the data provided in Table 3:

- *n* weights: number of weights used
- *n* measurements: number of the direct comparisons
- min weight use: minimum of each weight usage. (Weight usage means how many times the weight was placed in the balance.)
- max weight use: maximum of each weight usage.
- total weight usage: sum of all weight usage
- average of weight use: total weigh usage divided by the number of measurements
- *n* check weights: number of used check weights
- U (k = 2): is the calculated uncertainty of the smallest weight in the decade without the uncertainty component from the used standard and expressed in percent of the Maximum Permissible Error of class E_1

Apart from the fact that some designs have additional check weights (see Table 2) the numbers of measurements are also varying from 7 to 16. It has a correlation with the calculated uncertainty (see Figure 1). Generally, more measurements provide smaller uncertainties, but it is varying, so it gives a possibility for optimisation.

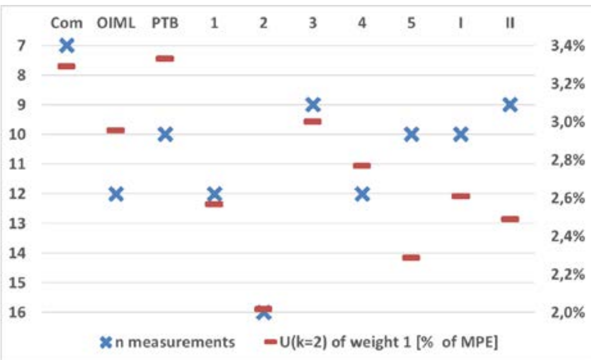

Figure 1: Number of measurements (left axis) and the obtained relative uncertainty (right axis)

Table 3: Properties of the investigated designs

	Com	OIML	PTB	1	2	3	4	5	I	II
Number of weights	6	6	8	8	8	8	8	6	8	8
Number of measurements	7	12	10	12	16	9	12	10	10	10
Minimum weight use	1	2	2	3	3	2	2	2	1	2
Maximum weight use	5	10	4	6	6	7	6	8	7	7
Total weight use	23	46	28	38	49	36	36	36	38	38
Average weight use	3.29	3.83	2.80	3.17	3.06	4.00	2.58	3.60	3.80	3.80
Number check weights	1	1	3	3	3	3	3	1	3	3
U (k = 2) / %	3.3	3.0	3.3	2.6	2.0	3.0	2.8	2.3	2.6	2.5

The number of minimum weights used also shows that some of the designs cannot be robust. Therefore, a test was carried out to test the robustness, “the ability to withstand or overcome adverse conditions”.

Each weighing result (as input to the design) was increased with a value equal to 10 % of the MPE. The results were evaluated, and any bigger than 2 % deterioration in the calibration results from the error free values were considered wrong. There are two important methods to detect the possible error: the (more than 2 %) deterioration of the values of the check weights and the residual analysis. If the residual changed at least 5 %, we considered that the change showed the discrepancy.

Iteratively reweighing as in [9] was applied to see if it would improve results.

The results are summarised in Table 4. Description of the data provided in Table 4.

- Failure to detect error: “Yes” means that (overall) at least one error was not detected.
- Failure check weight: “Yes” means that the check weights at least in one case did not detect the error.
- Failure residual: The number of cases when the residual analysis did not detect the error.
- “Number of undetected errors with IRLS” shows that after applying iterative reweighing how many measurements remans with undetected errors.
- “Number of improved measurements with IRLS” shows how many cases were possible to compensate for the input error with iterative reweighing.
- “Good result with IRLS”: “Yes” indicates if, in all cases after applying iterative reweighing the results were not changed by more than 2 % (error-free results).

This investigation shows that more than half of the (published and probably used) designs are unable to detect in all cases the error in a single measurement. This is a high risk considering the quality of the calibration results. This is definitely having higher importance than the achieved lower uncertainties.

Using IRLS is generally recommended, even if in case of some designs does not able to improve the results.

Design 2 with the highest (16) measurements and the 4 check weights was not able to detect all the errors. On the other hand, using IRLS this design was the only one, which could provide in all cases good (“error-free”) results.

Table 4: Results from the investigation of the designs

	Com	**OIML**	**PTB**	**1**	**2**	**3**	**4**	**5**	**I**	**II**
Number measurements	7	12	10	12	16	9	12	10	10	10
Failure to detect error	Yes	Yes	Yes	Yes	Yes	No	Yes	No	No	No
Failure check weight	2	1	1	1	1	No	1	1	No	No
Failure residual	6	4	10	7	5	9	7	3	7	7
Number of undetected errors with IRLS	2	1	1	1	0	0	1	0	0	0
Number of improved measurements with IRLS	0	8	0	6	16	0	5	3	3	3
Good result with IRLS	No	No	No	No	Yes	No	No	No	No	No

6. NEXT STEPS

When this paper was written, the project was working on the correct implementation and software.

The project aims to use an improved iteratively re-weighted version of the algorithm. It allows an effective elimination of smaller discrepancies in the measurements. To have a re-weighing effective, a robust weighing design is needed. This method published shall be adapted to allow the correct handling of the correlations. Additionally, estimation of volumes can be introduced [10], even if it is outside the project aims.

A further step is using the developed software to re-evaluate existing weighing designs and find optimal solutions for different needs.

7. CONCLUSIONS

The findings of this project suggest that the best approach is the Generalised Gauss-Markov approach which provides the best estimate for the dissemination of the mass scale. This Generalised Gauss-Markov Method is based on the generalised least squares using a special augmented design with multiply mass standard modelled as stochastic constraints, handling various correlated input quantities.

8. ACKNOWLEDGMENTS

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