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DISSEMINATION OF THE KILOGRAM AT METAS: EXTENDED METHOD OF LAGRANGE MULTIPLIERS FOR AIR BUOYANCY CORRECTION

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Abstract: We present the current mathematical procedures at METAS for disseminating the kilogram. We compare the classical method for solving a linear system of equations of mass comparisons to the Lagrange multiplier method. In addition, we have studied the influence of redundancy in mass comparisons and found that the combined standard uncertainty can be reduced when using a redundant design matrix.

Keywords: Kilogram, dissemination, Lagrange multipliers, centre of gravity correction.

1. INTRODUCTION

Today, the entire mass scale is traceable to the International Prototype of the Kilogram or, in future, to the upcoming new definition of the kilogram realized by Watt balance [1], [2], [3], [4], [5] and Avogadro experiments [6], [7], [8]. However, the dissemination of the unit is and will be realized by direct mass comparison between a reference and a sample. The sample may be a combination of submultiples having in total the same nominal mass as the reference. Various calculation methods and weighing designs for the calibration of decimal multiples and submultiples are used today by national metrology and designated institutes. The method of Lagrange multipliers is very popular as it is redundant and enables one to separate type A and type B uncertainties, although there are other methods. In the Lagrange multiplier method presented by Kochsiek et *al*. [9] corrections for air buoyancy and centre of gravity are not taken into account. In our model, the Lagrange multiplier method is used with air buoyancy corrections, which allows a more precise determination of the mass. We verified our extended Lagrange multiplier method by comparing its results to the results obtained by a classical non-redundant system of equations. Finally, we established the linear system of equations needed for comparing PtIr against stainless steel (1 kg vs 1 kg and 2x500 g vs 1 kg) where the corrections for both air buoyancy and centre of gravity of all masses are imperative.

2. METHOD OF LAGRANGE MULTIPLIERS

The current best practice for determining the masses of multiples and submultiples is to write the system of equations

$$A\vec{\beta} = \vec{y} - \vec{e} \tag{1}$$

where $A = [a_{ij}]$ is the n by p design matrix with $a_{ij} \in \{-1,0,1\}$, $\vec{\beta}$ is the column vector with p unknowns, $\vec{y} = [y_i]$ is the weighing difference and $\vec{e} = [e_i]$ is the error of the weighing difference [10]. We can derive the normal equations

$$A^T A\vec{\beta} = A^T\vec{y} \tag{2}$$

where $A^T\vec{e} = 0$ when $[e_i]$ are random and uncorrelated. The best estimates for the masses are then obtained by

$$\langle\vec{\beta}\rangle = L_s\vec{y} \tag{3}$$

$$L_s = (A^T A)^{-1}A^T \tag{4}$$

where L_s is the solution matrix. Since the measured values $\vec{y}$ represent differences between two masses, the determinant of $(A^T A)$ is zero and the inversion is not possible without considering constraints. Thus, the reference mass m_R can serve as a constraint and, e.g., be included in the mass vector $\vec{\beta} = [m_R\ m_1 \dots m_n]'$. As a consequence, $(A^T A)$ is no longer square and remains non-invertible. The symmetry can be re-established by adding the Lagrange-multiplier λ as a formal parameter to the vector $\vec{\beta} = [m_R\ m_1 \dots m_n\ \lambda]'$. Further adjustments can be found in [9]. The great advantage of the Lagrange multiplier method is that the system of equations can be redundant, i.e. the number of mass comparisons can be larger than the number of weights whose masses are to be determined. But in Kochsiek's calculations the effect of air buoyancy is neglected.

Extended method of Lagrange multipliers Based on the system of weighing equations we have included the air buoyancy corrections in the design matrix. For illustration and without loss of generality, we choose the following example: $m_R = 1$, $m_1 = 0.5$, $m_2 = m_3 = 0.2$ and $m_4 = m_5 = 0.1$ in milligram for the nominal masses and, for the subsequent verification, we choose the following non-redundant (r=0) system of equations including the terms for air buoyancy corrections

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} m_1 + m_2 + m_3 - m_R \\ -m_1 + m_2 + m_3 + m_4 \\ -m_2 + m_3 \\ -m_2 + m_4 + m_5 \\ m_4 - m_5 \end{bmatrix} - \begin{bmatrix} \rho_{air,1}\left(\frac{m_1}{\rho_1} + \frac{m_2}{\rho_2} + \frac{m_3}{\rho_3} - \frac{m_R}{\rho_R}\right) \\ \rho_{air,2}\left(-\frac{m_1}{\rho_1} + \frac{m_2}{\rho_2} + \frac{m_3}{\rho_3} + \frac{m_4}{\rho_4}\right) \\ \rho_{air,3}\left(-\frac{m_2}{\rho_2} + \frac{m_3}{\rho_3}\right) \\ \rho_{air,4}\left(-\frac{m_2}{\rho_2} + \frac{m_4}{\rho_4} + \frac{m_5}{\rho_5}\right) \\ \rho_{air,5}\left(\frac{m_4}{\rho_4} - \frac{m_5}{\rho_5}\right) \end{bmatrix} \quad (5)$$

Note that the reference mass m_R is part of the vector $\vec{\beta}$. The system of equations can be expressed in short form as

$$\vec{y} = A \cdot \vec{\beta} - L \cdot A \cdot R^{-1} \cdot \vec{\beta} = X \cdot \vec{\beta} \quad (6)$$

with $X = A - L \cdot A \cdot R^{-1}$ where L and R are the diagonal matrices of air densities and material densities, respectively, and A is the design matrix.

$$L = \begin{bmatrix} \rho_{air,1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \rho_{air,n} \end{bmatrix} \quad (7)$$

$$R^{-1} = \begin{bmatrix} \rho_R^{-1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \rho_n^{-1} \end{bmatrix} \quad (8)$$

$$A = \begin{bmatrix} -1 & 1 & 1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 1 & 1 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix} \quad (9)$$

The solution matrix Ls from equation (4) now becomes $L_s = (X^T X)^{-1} X^T$ and the system of equations is solved according to the Lagrange multiplier method described by Kochsiek et *al*. [9].

3. METHOD OF CLASSICAL APPROACH

We rewrite the system of equations and treat the reference mass m_R separately.

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} m_1 + m_2 + m_3 \\ -m_1 + m_2 + m_3 + m_4 \\ -m_2 + m_3 \\ -m_2 + m_4 + m_5 \\ m_4 - m_5 \end{bmatrix} - \begin{bmatrix} \rho_{air,1}\left(\frac{m_1}{\rho_1} + \frac{m_2}{\rho_2} + \frac{m_3}{\rho_3}\right) \\ \rho_{air,2}\left(-\frac{m_1}{\rho_1} + \frac{m_2}{\rho_2} + \frac{m_3}{\rho_3} + \frac{m_4}{\rho_4}\right) \\ \rho_{air,3}\left(-\frac{m_2}{\rho_2} + \frac{m_3}{\rho_3}\right) \\ \rho_{air,4}\left(-\frac{m_2}{\rho_2} + \frac{m_4}{\rho_4} + \frac{m_5}{\rho_5}\right) \\ \rho_{air,5}\left(\frac{m_4}{\rho_4} - \frac{m_5}{\rho_5}\right) \end{bmatrix} - \begin{bmatrix} m_R - \rho_{air,1} \cdot \frac{m_R}{\rho_R} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (10)$$

The system can be expressed in short form as

$$\vec{y} = A \cdot \vec{m} - L \cdot A \cdot R^{-1} \cdot \vec{m} - \left(m_R \cdot \vec{r} - L \cdot \vec{r} \cdot \frac{m_R}{\rho_R}\right) \quad (11)$$

with $\vec{m} = [m_1 \dots m_5]$ and $\vec{r} = [1\ 0\ 0\ 0\ 0]'$. The solution of equation (10) is

$$\vec{m} = X^{-1}\left[\vec{y} + \left(m_R \cdot \vec{r} - L \cdot \vec{r} \cdot \frac{m_R}{\rho_R}\right)\right] \quad (12)$$

provided that the inverse of X exists, i.e. X must be square and not singular. In other words, the number of equations, and hence the number of mass comparisons, must be equal to the number of masses (weights) to be determined. Thus, this system cannot be redundant.

4. COMPARISON OF METHODS

We now compare the results obtained by our extended method of Lagrange multipliers to the results obtained by the classical approach. As input data we take the values $\vec{y}$ = [-0.09853, -0.00095, -0.00095, 0.00178, -0.00373] mg, $\rho_{air,i}$=1.13296 kg/m^3, ρ_i= 2400 kg/m^3, ρ_R=8000 kg/m^3, m_R = (1+0.000565) mg. The calculated mass deviation from the nominal value is exactly the same for both methods (Table 1). The uncertainty contributions u_A (air buoyancy) and u_N (reference standard) as well as the combined standard uncertainty u_c are very similar for both methods; differences in the sub-nanogram region may be neglected (Table 2).

Table 1: Mass deviation calculated by classical and Lagrange multiplier methods using a non-redundant design matrix (*r*=0).

	Mass deviation (ng)	
	classical	Lagrange (*r*=0)
m_1	564.998	564.998
m_2	1391.000	1391.000
m_3	947.000	947.000
m_4	-4.000	-4.000
m_5	-502.000	-502.000

Table 2: Uncertainty contributions u_A, u_N and combined standard uncertainty u_c obtained by classical and Lagrange method (r=0).

	u_A (ng)		u_N (ng)		u_c (ng)	
	classical	Lagrange	classical	Lagrange	classical	Lagrange
m_1	11.150	11.150	82.650	82.638	83.399	83.387
m_2	5.958	5.958	33.060	33.055	33.593	33.588
m_3	6.527	6.528	33.060	33.055	33.698	33.694
m_4	5.625	5.626	16.530	16.528	17.461	17.459
m_5	6.375	6.376	16.530	16.528	17.717	17.715

The results show the consistency between the two calculation methods. In the next section we are going to investigate the influence of redundancy on mass determination and uncertainty.

5. INFLUENCE OF REDUNDANCY

One advantage of the Lagrange multiplier method is that the system of equations may contain more equations, i.e. more mass comparisons than there are masses to be determined. In this way, the design matrix becomes redundant and the accuracy of mass determination is improved. We extended the design matrix A from equation (9) by adding r additional rows of mass comparisons where $r \in \{1,2,3,4\}$

$$A_{add} = \begin{bmatrix} 0 & -1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 0 & 1 \end{bmatrix} \quad (13)$$

The design matrix A then becomes redundant A_{red} (here r=4)

$$A_{red} = \begin{bmatrix} A \\ A_{add} \end{bmatrix} = \begin{bmatrix} -1 & 1 & 1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 1 & 1 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & -1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 0 & 1 \end{bmatrix} \quad (14)$$

The influence of adding an additional equation (mass comparison) on the measurement uncertainty, u_A, has been investigated and the results are compared to those of the classical method and Lagrange multiplier method without redundancy (r = 0). The investigation showed that the larger the redundancy the smaller the uncertainty of the weighing process u_A (Table 3, Figure 1).

Table 3: Influence on the standard uncertainty of the weighing process u_A when adding additional mass comparisons to the system of equations. r = 0 represents a non-redundant (A) and r > 0 represents a redundant (A_{red}) design matrix where r is the number of added mass comparisons.

	u_A (ng)					
	classical	Lagr. r=0	Lagr. r=1	Lagr. r=2	Lagr. r=3	Lagr. r=4
m_1	11.150	11.150	9.779	9.625	4.361	2.947
m_2	5.958	5.958	5.315	4.822	3.212	3.151
m_3	6.527	6.528	5.936	4.758	3.045	2.980
m_4	5.625	5.626	5.431	4.694	3.824	3.121
m_5	6.375	6.376	5.029	4.228	4.021	2.827

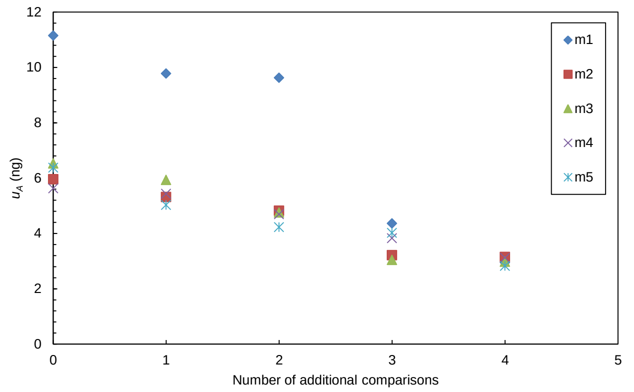

Figure 1: Influence on the standard uncertainty of the weighing process u_A when adding additional mass comparisons to the system of equations. Data points were calculated from a non-redundant (r = 0) and redundant (r > 0) Lagrange multiplier design matrix.

Also the combined standard uncertainty, u_c, is reduced as the number of additional mass comparisons is increased. To show the effect we calculated the ratio between the combined uncertainties without (r = 0) and with (r > 0) redundancy according to the Lagrange multiplier method for the five masses (Figure 2). The results clearly demonstrate that the combined standard uncertainty can be reduced by about 10% when using a redundant design matrix.

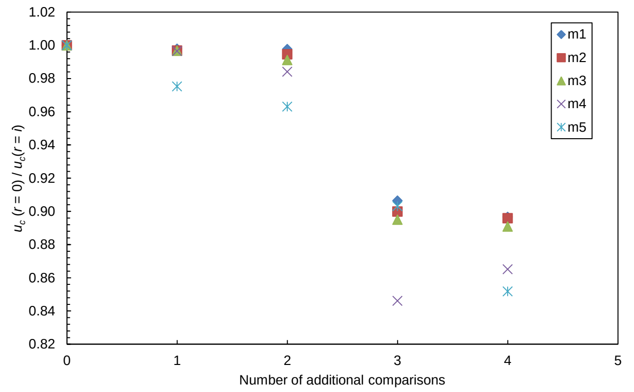

Figure 2: Change of the combined standard uncertainty, u_c, as a function of the number of additional mass comparisons.

6. INFLUENCE OF THE CENTRE OF GRAVITY

For the dissemination of the mass unit, a 1 kg and two 500 g stainless steel working standards are compared to the 1 kg PtIr national prototype. When comparing weights of equal nominal mass but different densities (PtIr: $\rho \approx 21535$ kg/m^3, stainless steel (SS): $\rho \approx 8000$ kg/m^3), the centre of gravity (CG) of these masses is at different heights above a specific reference point, e.g. the floor. This circumstance has to be taken into account for precise mass determinations. As the correction for the centre of gravity is not included in the Lagrange multiplier method by Kochsiek et *al*. [9], we calculated the masses separately by using the classical method based on the three mass comparisons

1. 1 kg (SS) vs. 1 kg (PtIr)
2. 500 g (SS) + 500 g* (SS) vs. 1 kg (PtIr)
3. 500 g (SS) vs. 500 g* (SS)

where 500 g* is an auxiliary weight. We performed the calculations with and without corrections for the centre of gravity and compared the two results to the result obtained by the Lagrange multiplier method. Please note that we cannot present a detailed mathematical derivation of the formulae here. When taking the centre of gravity into account, the calculated mass values for the 1 kg and the two 500 g weights are increased. The results obtained from the Lagrange multiplier method and from the classical method without CG correction are identical, which demonstrates the consistency between these two methods (Table 4).

Table 4: Influence of the centre of gravity on the calculated mass value.

Masses	Deviation from nominal mass (mg)		
	with CG	without CG	Lagrange
1 kg	1.4699	1.4688	1.4688
500 g	0.5669	0.5646	0.5646
500 g*	0.1871	0.1866	0.1866

7. CONCLUSIONS

We have demonstrated that the Lagrange multiplier method can be extended by including air buoyancy corrections in the design matrix. We have verified the results by comparing the results to those of a classical method for solving a linear system of equations (without redundancy). Furthermore, we have demonstrated that redundancy of mass comparisons reduces the combined standard uncertainty by about 10% and we have also shown that for precise mass determinations of a 1 kg and 500 g weight the centre of gravity should be taken into account.

8. REFERENCES

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