DISSEMINATION OF THE KILOGRAM AT METAS: Extended Lagrange Multiplier Method

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Abstract

We present the 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 effect of redundancy in mass comparisons and found that the combined standard uncertainty can be reduced when using a redundant design matrix.

Introduction

Today, the entire mass scale is traceable to the International Prototype of the Kilogram or, in future, to the new definition of the kilogram realized by Kibble balance and Avogadro experiments. 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. The method of Lagrange multipliers is very popular as it is redundant and enables one to separate type A and type B uncertainties. In our model, the Lagrange multiplier method is used with air buoyancy corrections, which allows a more precise determination of the mass. Finally, we studied the effect of the centre of gravity when comparing masses of different densities or shapes.

Methods

Lagrange multiplier method

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 to be determined. The current best practice for determining the masses of multiples and sub-multiples is to write the system of equations.

The *system of equation* is

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

We can derive the *normal equation*

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

with the *solution matrix*

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

The *best estimates for the masses* is now

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

- $A = [a_{ij}]$: $n \times p$ design matrix with $a_{ij} \in \{-1,0,1\}$; n number of equations; p number of weights
- $\vec{\beta}$: mass vector with p unknowns
- $\vec{y} = [y_i]$: vector of n weighing differences
- $\vec{e} = [e_i]$: error vector of n weighing differences

Remarks: Since $\vec{y}$ represents differences between two masses, $\det(A^T A) = 0$ and $(A^T A)^{-1}$ is not possible without considering constraints. The reference mass, m_R, is therefore included in the mass vector $\vec{\beta} = (m_R\, m_1 \dots m_n)'$. Consequently, $(A^T A)$ is no longer square and remains non-invertible. Therefore, we have to include the (formal) Lagrange multiplier λ in $\vec{\beta} = (m_R\, m_1 \dots m_n\, \lambda)'$ [Kochsiek 1997].

Extended Lagrange multiplier method

We now **include air buoyancy corrections** and the system of equations can be written as

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

with $X = A - L \cdot A \cdot R^{-1}$

The *solution matrix* is now

$$L_s = (X^T X)^{-1} X^T$$

$$L = \begin{bmatrix} \rho_{air,1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \rho_{air,n} \end{bmatrix} \qquad R^{-1} = \begin{bmatrix} \rho_R^{-1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \rho_n^{-1} \end{bmatrix}$$

$$A = \begin{bmatrix} -1 & 1 & 1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 1 & 1 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}$$

(as an example)

Classical approach

The classical approach is **simple and direct but non-redundant**.

The *system of equations* can be expressed as

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

and the *masses* are given by

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

- m_R: reference mass
- ρ_R: density of reference mass
- L: air density
- R: material density
- A: design matrix
- $\vec{r}$: reference vector (here: $\vec{r} = [1\,0\,0\,0\,0]'$)

Comparison of methods

We compare the results obtained by our extended method of Lagrange multiplier to the results obtained by the classical approach. As input data we take the values

$\vec{y}$ = (98.53, 0.95, 0.95, 1.78, 3.73) µg $\qquad m_R$ = (1+0.000565) mg

$\rho_{air,i}$ =1.13296 kg/m³ $\qquad \rho_i$ = 2400 kg/m³ $\qquad \rho_R$ = 8000 kg/m³

The calculated mass deviation from the nominal value is exactly the same for both methods (Table 1). The uncertainty contributions u_A (Type A), u_N (reference standard) and u_c (combined standard uncertainty) are very similar for both methods (Table 2).

Table 1: Mass deviation calculated by classical approach and by Lagrange multiplier method without redundancy (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 obtained by classical approach and Lagrange multiplier method (r=0).

	u_A (ng)		u_N (ng)		u_c (ng)	
	class.	Lagr.	class.	Lagr.	class.	Lagr.
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 air buoyancy corrections can be included in the Lagrange multiplier method.
- The Lagrange multiplier method and the classical approach for solving a linear system of equations deliver the same results.

Effects

Effect 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 A becomes redundant and the accuracy of mass determination is improved. We extend the design matrix A by adding r additional rows of mass comparisons where $r \in \{1,2,3,4\}$.

$$A_{red} = \begin{bmatrix} A \\ A_{add} \end{bmatrix} = \begin{bmatrix} -1 & 1 & 1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 1 & 1 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & -1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 0 & 1 \end{bmatrix} \begin{matrix} \left.\right\} A \\ \left.\right\} A_{add} \end{matrix}$$

Table 3: Influence on the standard uncertainty of the weighing process, u_A, when adding additional mass comparisons to the system of equations.

	u_A (ng)					
	class.	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

$r = 0$: non-redundant (A) design matrix
$r > 0$: redundant (A_{red}) design matrix

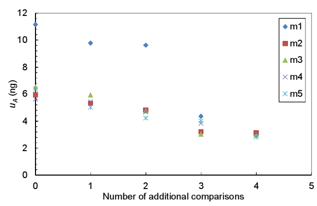

Figure 1: Influence on the standard uncertainty of the weighing process u_A. Data points calculated from a non-redundant ($r = 0$) and redundant ($r > 0$) Lagrange multiplier design matrix.

Effect of centre of gravity

When comparing weights of equal nominal mass but different densities (PtIr: ρ ≈ 21535 kg/m³, stainless steel (SS): ρ ≈ 8000 kg/m³), we have to be aware that the centre of gravity (CG) of these masses is at different heights above a specific reference point. This circumstance has to be taken into account for precise mass determinations.

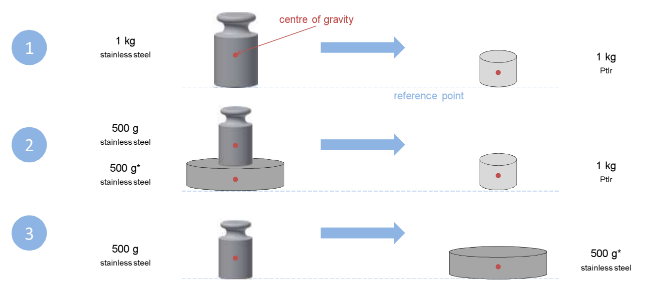

Table 3: Effect of the centre of gravity on the calculated mass value.

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

- The results demonstrate that the standard uncertainty of the weighing process, u_A (Type A), can be reduced by adding additional mass comparisons. Consequently, the combined standard uncertainty, u_c, can be reduced as well.
- For precise mass determination the centre of gravity has to be taken into account when comparing masses of different material densities.

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