Estimation technique of the mass of drifting mass standards

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Abstract. This article presents a novel estimation technique for the drift and stability of the mass standards using generalised least squares method with augmented design taking into account the correlations among the measurements over a longer time period. The suggested approach provides numerous advantages over the traditional ones, such as smaller uncertainties and more robust estimate.

1. Introduction
The kilogram, the unit of mass is currently defined as being equal to the mass of the International Prototype of the Kilogram (IPK). Some national metrology institutes own copy of the international prototype kilogram (national prototype). The IPK as well as the copies are made of platinum iridium alloy to provide good stability. Due to the high price and the high density of the prototypes they are not suitable for daily calibrations of stainless steel standards.

The national measurement institutes calibrate their stainless steel standards against their national prototype which is calibrated against a working copy of the International Bureau of Weights and Measures (BIPM) traceable to the IPK. Even if this situation will be changed due to the new definition, the good and known stability of the group of stainless steel mass standards remains crucial [1].

2. General considerations
The practicalities lead to some limitations:
- the national prototype cannot be too often calibrated at BIPM;
- the use of the national prototype shall be limited in order to maintain good stability therefore
  - calibration of stainless steel standards against it cannot be made frequently;
  - not all the stainless steel standards can be calibrated directly against it

It results a numerous comparisons among the stainless steel standards and very few using the national prototype.

2.1. Mathematical model of the weighing
The well known method is the so called substitution weighing in air. The mass of the test weights \( m_t \) is measured by comparison with a known mass standard \( m_r \) measuring the actual mass difference \( \Delta m_{t-r} \): \n
\[
m_t = m_r + \Delta m_{t-r} + \sum_{i}^{n} c_i
\]  

(1)

To calculate the correct value numerous corrections \( c_i \) have to be applied.
3. Traditional estimation of the mass and drift of the mass standards

3.1. Basic calculation of the linear drift of the mass of a single standard against the national prototype

Assume that a stainless steel mass standard was calibrated against the national prototype several times during a long period. The calibration history is shown in Figure 1.

The mass standard was safely handled and not cleaned during this period, therefore it can be assumed that the change is small due to wear and change in the amount of contamination absorbed on the surface. The measured mass of the standard can be expressed as

\[ m_i = m_0 + dt + \delta m_i \quad (2) \]

Due to the varying uncertainties of the measurements weighted linear regression was used.

3.2. Calculation of the linear drift of the mass of a mass standard using the results of the calibration campaigns

A calibration campaign is the procedure when a group of stainless standards are compared against each other and a small selection of them against the national prototype. This method has the advantage of providing calibration result for all the member of the group with small uncertainty while the usage of the national prototype is limited. The used calculation method was a traditional weighted least squares with Lagrange multiplier method [2]. The mass values of the selected standard calculated during each campaign were used as input of a weighted linear regression.

The results using the data of the campaigns (Figure 2) are better than the direct comparison against the national prototype (Figure 1).
4. New model for the estimation of the mass and drift of the mass standards

The above described methods are not effective as they are not using all the available measurement results and they are not handling the possible correlation among the measurement results. An improved method was introduced to include all the measurement results between the campaigns.

4.1. Modelling the comparison of two drifting mass standards

Two mass standards \((m_k\text{ and } m_l)\) with an unknown drift \((d_k\text{ and } d_l)\) are compared in a certain time \((t_i)\). Both are modelled according to equation (2) and the mass difference \((\Delta m_i)\) can be expressed as:

\[
\Delta m_i = m_{ki} - m_{li} = m_k + d_k t_i - (m_l + d_l t_i) + \delta m_i
\]

The uncertainties of the comparisons are very different. Comparisons of stainless steel weights with stainless steel ones having small uncertainties (typical 2–4 \(\mu g\); \(k=2\)) while the stainless steel with national prototype having much larger uncertainties (typical 22–40 \(\mu g\); \(k=2\)) during the studied period. The difference is due to the uncertainty of the buoyance caused by the large volume difference.

4.2. Generalized least squares

The generalized linear least-squares estimation can be used to estimate the mass of the weights in a specific time. The parameters \((\hat{\beta}, m_i, \text{and } d_i)\) are estimated as:

\[
\hat{\beta} = \hat{\mathbf{C}} \mathbf{X}^T \hat{\Phi}^{-1} \mathbf{Y}
\]

Where the \(g \times h\) (\(g\) is the number of measurements; \(h\) is the number of the parameters) matrix \(\mathbf{X}\) represents the design of the measurements. Each row of \(\mathbf{X}\) represents one measurement: the used weights and the time of the measurement while the associated measured mass differences \((\Delta m_i)\) are in the corresponding row of vector \(\mathbf{Y}\). The first two rows of \(\mathbf{X}\) and \(\mathbf{Y}\) were filled with the calibration results of the national prototype. This is the so called augmented design approach [3].

The uncertainty matrix \(\hat{\mathbf{C}}\) is given as:

\[
\hat{\mathbf{C}} = \left(\mathbf{X}^T \hat{\Phi}^{-1} \mathbf{X}\right)^{-1}
\]

The matrix \(\hat{\Phi}\) is a symmetric \(g \times g\) matrix. The diagonal elements of \(\hat{\Phi}\) are given by the quadratic sum of estimated uncertainty of measurement result \((u(\Delta m_i))\). The off-diagonal of \(\hat{\Phi}\) represents the covariance between measurements.

3 types of covariance were assumed:

- Covariance between the calibration results of the national prototype;
- Covariance among the measurements in the “same time”. Same time defines all the measurements made during a calibration campaign (usually in a month). Correlation is assumed being higher, since the instruments were used with the same calibration status.
- Covariance among the measurements in “different times”. All measurements belong to different calibration campaigns. Correlation is assumed being smaller with the elapsed time between the campaigns.

The correlations were estimated as 0.1; 0.3 and 0.1.

The expanded uncertainty of any predicted values are estimated as: [4]

\[
U(m_i) = k(\sigma^2 + x_0^T \hat{\mathbf{C}} x_0)^{1/2}
\]

\(x_0\) vector can represent a comparison of two weights in a definite time. In case \(x_0\) vector contains only a single weight and a specific time, it gives the estimate of the uncertainty of the mass of the weight (red lines in figure 3).
Figure 3. Measured mass differences from the estimated differences of a mass standard against any other one (blue). Error bars represent the expanded uncertainties ($k=2$) of the measured mass differences while the red lines the uncertainty of the estimated mass. Values are in microgram. Note: larger error bars indicate measurements against the national prototype.

The major advantages of this method over the traditional approaches are: using all available measurement data; taking into account the correlation and providing the smallest uncertainty of the weights. It is in this example (44% of the one directly against the national prototype and 71% of the one using the campaign data).

5. Discussion and conclusion
The result using the new model (Figure 3) shows a certain inconsistency due to the small uncertainties of the single mass comparisons with good reproducibility. This phenomenon is often referred to as the stability of the weights. Some possible causes are described in [1]. There are approaches how to handle it [5, 6].
This study shows that a more sophisticated approach provides better results regarding the estimate of the stability and drift of the mass standards than the classical methods used in mass metrology.

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