# Regression analysis in aerostatic weighing and weighing series

**Chander, Hima**

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**Vrije Universiteit Amsterdam**
**Faculty of Sciences**
**De Boelelaan 1081a**
**1081 HV Amsterdam**

**Nederlands Meetinstituut**
**Department of Mass and Related Quantities**
**Thijsseweg 11**
**2629 JA Delft**

## Preface

The final phase of the study Business Mathematics and Informatics (BMI) at the Vrije Universiteit Amsterdam consists of an internship. This master thesis covers the work done during my internship at the Department Mass and Related Quantities at the Nederlands Meetinstituut. The section Mass is dealing with the improvement of calibration methods for mass measurement.

Projects are hardly performed alone; therefore I would like to thank several people for their support and help during my internship.
First I would like to thank Dr. Hugo Ent, the manager of the department of Mass and Related Quantities, Drs. Inge van Andel, the leader of this project, and Dr. Adriaan M.H. van der Veen for giving me the opportunity to perform my internship within the group. Thank you for your support and encouragement. Your energy and efficient way of working inspired me to get the best out of myself. I would also like to thank Dr. G.J. Franx and Prof. Dr. A.C.M. Ran, my supervisors, and Dr. S. Bhulai, the second reader, from the Vrije Universiteit. Thank you for your time and guidance.

Furthermore I would like to thank all my colleagues, in particular Jos Verbeek, Jan Westerhoud and Gerard van Winden for the great time and for their patience while answering all my questions.

Hima Chander
September 2006

## Summary

This work consists of two subjects, the determination of the volume by aerostatic weighing and finding the best weighing scheme for the weighing series.

The first part of this work addresses the joint determination of the mass and volume of weights by means of aerostatic weighing. Metrology institutes use special weight sets for the calibration of weights with various nominal masses. All weights and calibrated weighing equipments used in daily practice are metrologically traceable to the international mass standard, the 'Grand K', which is stored at the Bureau des Poids et Mesures (BIPM) in France. The 'Grand K' is a small cylinder, made of platinum-iridium of which is agreed that it is exactly 1 kg. For mass calibration, NMi VSL has a platinum-iridium copy of the International mass standard, known as PtIr53. Because platinum-iridium is sensitive to erosion and above all has a higher density than the stainless steel weights used in the industry, mass calibrations are usually done with mass standards made of stainless steel. However for the calibration of these stainless steel mass standards the PtIr53 must be used and because of the difference in density, the air buoyancy leads to an apparent mass difference of approximately 100 mg. This effect can be accounted for if the air density at the time of weighing and the volume of the weight are known.

The volume determination of weights can be done by once-only hydrostatic weighing or by aerostatic weighing. During hydrostatic weighing the weight is immersed in water. There is need for an alternative method to determine the volume, as not all artefacts can be immersed in water. Furthermore, even for weights that can be immersed, there are negative effects, such as, e.g., the surface effects of water on the artefact's surface (adsorption) and the long time that the artefact needs to stabilise and equilibrate with the humidity from air,. Aerostatic weighing might be such an alternative method.

The principle of aerostatic weighing is that the apparent mass difference between two artefacts is recorded as a function of the air density. In practice, there is another variable that may influence the measurement, namely the temperature. The temperature not only influences the air density, but also the volumes (through cubic expansion) of the artefacts, so that this second order effect needs to be taken into account too. By plotting the apparent mass as a function of the air density and fitting a straight line through the data, the mass and volume differences can be determined . An algorithm has been developed and implemented to perform this regression. In order to propagate the uncertainty associated with the input variables (mass difference and air density), generalised distance regression is used, which weighs the points in the dataset on the basis of the uncertainty associated with the input quantities. The regression method has been augmented to take care of effects of the ambient temperature on the volume of the artefacts.

The first results from aerostatic weighing suggest that the range of the air density, which can be influenced during weighing, should be expanded for a better regression.

The second part of this work concerns finding the best weighing scheme in weighing series. Weighing using a substitution method based on the principle of de Borda is commonly used in mass calibration. Mass calibration is done by comparing an unknown weight with a reference mass standard by alternatively placing them on a balance. This is called Borda weighing. Usually, an assembly of weight(s) is calibrated against a (single) calibrated artefact. This calibration is realised by using a weighing scheme, i.e., different combinations of weights that are compared among one another. Such a weighing scheme can be designed in numerous ways. In practice, it is often seen that there is a long-standing tradition of using a particular scheme. In this work, the weighing scheme used in the Netherlands for primary calibration is subjected to a rigorous mathematical optimisation, to determine the weighing scheme that produces the most accurate calibration of the weights under measurement.

The optimisation is carried out by first modelling the uncertainty structure of the mass differences experimentally obtained in each Borda sequence. The structure of the resulting covariance matrix is the basis for determining the mass difference in each of the Borda sequences forming the weighing scheme. Several constraints have been put in the optimisation to exclude undesired solutions, such as practically unfeasible weighing schemes. For practical reasons, the number of Borda sequences has been limited to 14 and the number of repeated weighings in a sequence has been restricted to 30. Two different loss functions have been defined to allow judging the various weighing schemes. One is based on the absolute variances of the calibrated weights, whereas the second is based on the relative variances.

Although the modelling of the data structure is much more transparent than the currently used method of uncertainty evaluation, the uncertainties estimated with the new model seem to be too small in view of the results. Two important uncertainty components are likely to be responsible for this discrepancy: the effects of convection and centre of gravity. It is not known to what extent these effects lead to correlations in the dataset; these correlations however appear to be very important in the uncertainty structure. This problem could not be resolved in due course of this work, so that the optimum weighing scheme could not be determined.

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# 1 Introduction

Nederlands Meetinstituut (NMi) is a company active in measurement, calibration, testing and certification.
The main activities of NMi are:

- Guardian of the metrological infrastructure in the Netherlands (NMi VSL)
- Testing and certification institute (NMi Certin)
- Market Surveillance (NMi Verispect)

NMi van Swinden Laboratory (NMi VSL) is the Dutch national standard institute. It keeps and maintains the present Dutch measurement standards and develops new measurement standards and reference materials.

The section Mass of the department Mass and Related Quantities is dealing with the improvement of calibration methods for mass measurement. Mass measurements play an important role in trade, industry, laboratory and process control. In many instances the accuracy of these measurements is essential with regard to safety, health and cost. Furthermore, several other frequently measured quantities like pressure, force, viscosity and density are derived from mass. This has led to an increasing demand for accurate measurement techniques and traceability in mass.

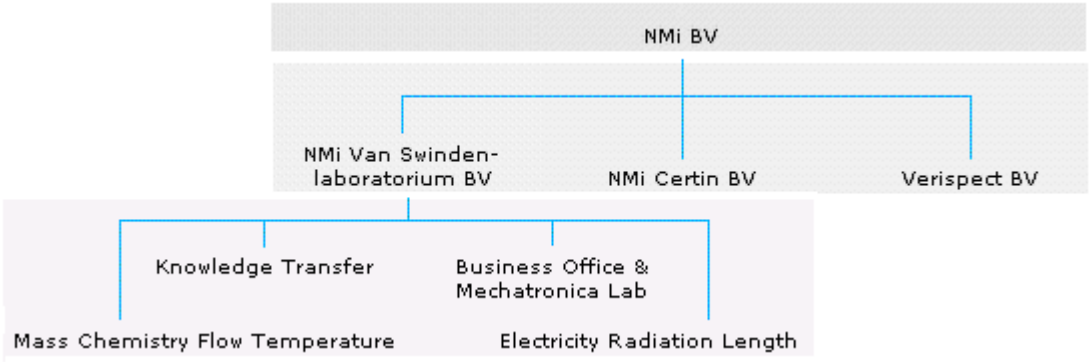


Figure 1: Organisation chart of NMi BV

The Department of Mass had two projects asking for a mathematical solution for a measurement problem. The two problems are related to each other. The first one concerns aerostatic weighing and the second the determination of the optimal weighing schemes.

Usually hydrostatic weighing is used to determine the volume of weights. For many other objects this method is not possible and therefore geometrical measurement or density data from the manufacturer is used to compute the volume. This determination is often not very accurate. Other disadvantages of hydrostatic weighing include the surface effects of water on the artefact's surface (adsorption) and the long time that the artefact needs to stabilise and equilibrate with the humidity from air. Considering the importance of the volume for the determination of the mass, there is need for an alternative method to determine the volume.

Aerostatic weighing might be such an alternative method. During aerostatic weighing objects are not submerged in water, but in air of different densities. By measuring the apparent mass differences, the volume can be calculated. Aerostatic weighing can be used in weighing schemes; this is not done yet, as the method needs first to be fully validated. The work presented here is a key element in the validation of aerostatic weighing.

For the calibration of weights with various nominal masses, metrology institutes use special weight sets. For instance the decade from 1000 g to 100 g is 'covered' by six weights: 1000 g, 500 g, 2 x 200 g and 2 x 100 g. In order to be able to distinguish between weights with the same nominal mass, a small dot is used to mark one of them. So one can speak of 100 g and 100 g•.

The mass of each individual weight of the set can be determined by direct comparison with a mass standard of identical nominal mass or by using a weighing scheme. At the highest level of metrology only the national mass standard made of platinum-iridium is available. This mass standard has a nominal value of 1000 g and cannot be used for the determination of e.g. the mass of a 200 g weight by using direct comparison. So at this level weighing schemes must be used.

A weighing scheme is an overdetermined system of weighing equations. The scheme consists of several mass comparisons carried out with certain combinations of weights. In this scheme the mass standard with known mass also participates. With a very accurate balance the mass differences of the weighing equations are measured. The best weighing series has to be found.

This work is subdivided into two parts: volume determination with aerostatic weighing (chapter 3) and the evaluation of weighing schemes (chapter 4). The background of the statistics used, and some concepts from mass metrology are the subject of chapter 2. Finally, in chapter 5 the conclusions are given. The report is concluded by the reference section, list of symbols, list of matrices and all appendices. They contain the CIPM-81/91 equation, the mass difference, hydrostatic weighing, matrix factorisations, the Gauss-Jordan elimination and the results of the weighing series. All the datasets for aerostatic weighing and weighing schemes are available on the accompanying CD.

# 2 Calibration, uncertainty and traceability

## 2.1 Calibration

The calibration of unknown weights is usually achieved by direct comparison against a reference standard of the same nominal value. Where necessary, the use of a group of reference standards, which total the nominal value of the unknown weight, is acceptable. To be able to perform mass calibrations of the highest accuracy, NMi VSL maintains many high-level mass reference standards, among which the national mass standard of the Netherlands, the platinum-iridium kilogram nr. 53. With these mass standards and several very sensitive balances, NMi VSL can calibrate mass standards with accuracy class E1 to M1. To determinate whether a weight belongs to a certain accuracy class, the density of the weight (depends on material), the surface, the magnetic properties, the shape of the weight (marks on the weight) and the maximum deviation from the nominal mass are of importance. Class E1 is the highest accuracy class and therefore the above mentioned properties must meet the strictest requirements.

For the highest level of mass calibrations, simply taking the value displayed by the balance is not accurate enough. These calibrations are done by determining the mass difference between a weight and an appropriate mass standard. This can be done by direct comparison or, in case of a set of weights, by a weighing scheme. The unknown mass of the weight can thus be calculated from the well known mass of the standard taking into account the effects of air buoyancy, the altitude-dependency of the gravitational force, convection, electrical and magnetic force. For example: if 500 g, 200 g, 200 g•, 100 g and 100 g• have to be calibrated against a 1 kg weight, this can be done by a scheme of equations in which two assemblies of weights with the same nominal mass are compared.

## 2.2 Uncertainty

The calibration of a weight must be accompanied by an estimate of the uncertainty of the calibration if the weight is to be used as the basis for a valid mass measurement. The calibration uncertainty will include contributions arising from the calibration of the mass standards used, the performance of the balance, the variability of the weighing process and the deviations of air and the density of the weights from the conventional values. In some cases these contributions may be insignificant – nevertheless they must be demonstrated.

Many improvements have been made to decrease the measurement uncertainty further by using automatic weighing devices (AWDs) and an airtight container to keep the air buoyancy nearly constant during the measurements.

Table 1: The NMi uses the following four automatic weighing devices:

| ***Balance*** | ***Decade*** |
|---|---|
| *AWD* 1 | 1 – 10 kg |
| *HK* 1000 | 100 g – 1000 g |
| *AWD* 2 | 1 – 100 g (1 – 10 g, 10 – 100 g) |
| *AWD* 3 | 0,1 mg – 1000 mg (0,1 mg – 1 mg, 1 mg – 10 mg, 10 mg – 100 mg, 100 mg – 1000 mg) |

### *2.2.1 Uncertainty propagation*

Many measurements are done indirectly, that is, several (input) quantities are measured and the measurand, the quantity to be measured, is subsequently calculated using a measurement model. Such a model is often explicit, that is, of the form

$$y = f(x_1, x_2, \ldots, x_n)$$

If the uncertainty associated with the $n$ input quantities $x_i$ are known, the uncertainty associated with $y$ can be expressed as follows using the uncertainty propagation formula

$$u^2(y) = \sum_i c_i^2 u^2(x_i) + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} c_i c_j u(x_i, x_j),$$

where

$$c_i = \frac{\partial f}{\partial x_i}$$

is called the *sensitivity coefficient*. The sensitivity coefficient is the partial derivative of the measurement model $f$ with respect to one of the input quantities $x_i$. It expresses the sensitivity of the uncertainty in $y$ for the uncertainty in $x_i$.

The uncertainty propagation formula does not make any assumptions concerning existing dependencies between the input quantities $x_i$. In fact, the second double summation contains the terms in the expression for the standard uncertainty of $y$ that are due to covariances between any pair of $x_i$, $x_j$. If two variables are independent, then their covariance is zero. If *all* input quantities are mutually independent, then the uncertainty propagation formula may be written as

$$u^2(y) = \sum_i c_i^2 u^2(x_i)$$

The uncertainty propagation formula can be written in matrix form as follows:

$$u^2(y) = \mathbf{c} V_x \mathbf{c}^{\mathbf{T}}$$

where $\mathbf{c}^{\mathbf{T}}$ denotes the transpose of the row vector $\mathbf{c}$ and the covariance matrix is denoted by $\mathbf{V_x}$.

## 2.3 Traceability

All weights and calibrated weighing equipment used in daily practice are traceable to the international mass standard, the ‘Grand K’, which is stored at the Bureau des Poids et Mesures (BIPM) in France. The 'Grand K' is a small cylinder, made of platinum-iridium of which is agreed that it is precisely 1 kg. Hereby mass is the last quantity with a tangible object as primary standard.

For mass calibration, the NMi VSL has a platinum-iridium copy of the International mass standard. This Dutch mass standard, the PtIr53, is sent regularly to the BIPM for calibration versus the international mass standard. Because platinum-iridium is sensitive to erosion and above all has a higher density than the steel weights used in industry, mass calibrations are done with mass standards made of stainless steel. The mass standards made of stainless steel of the NMi VSL are calibrated regularly versus the PtIr53 and are divided in reference and working standards. The working standards are used for calibrations for the industry and the working standards are calibrated with the reference standards each one or two years.

The traceability chain for mass starts at the International mass standard ("Grand K"). Via the Dutch PtIr53, the reference/working standards of NMi VSL and the standards in various RvA accredited laboratories, the traceability chain ends at the weights and weighing equipment used by industry, shops, test laboratories and at home. At each calibration however, the uncertainties of the used mass standard, the measurement and the environment factors must be taken into account, so the uncertainties increase at each step down the chain.

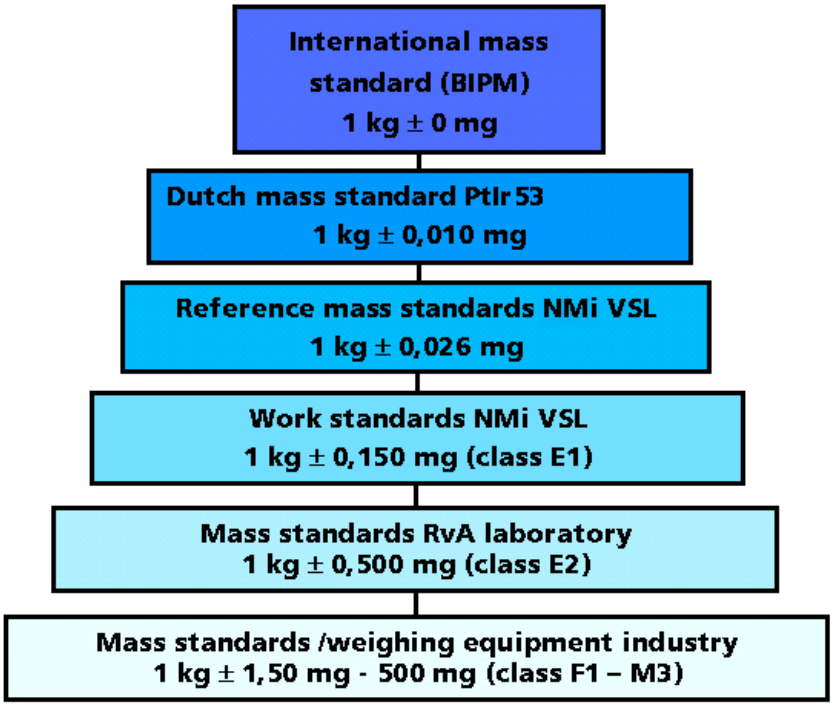


Figure 2: Traceability chain

# 3 Aerostatic weighing

## 3.1 Problem description

In very accurate calibration of mass standards, as well as the weighing of voluminous objects, the air buoyancy plays an important role. Especially at the second step of the traceability chain (see figure 2), at which the platinum-iridium kilogram is compared to a stainless steel kilogram, because due to the great difference in density, there is a great difference in volume. The density of the platinum-iridium kilogram is much greater than that of the stainless steel kilogram. In this case, the air buoyancy leads to an apparent mass difference of approximately 100 mg. This effect can be calculated with the air density and the volume of the weight[1]

For the calculation of the air density the CIPM-81/91 equation (Appendix A) is used. The uncertainty associated with the model is approx. $10^{-4}$ relative. In absolute terms, the uncertainty associated with the air density $\rho$ is given by

$$u(\rho) = 10^{-4} \cdot \rho .$$

To prevent a significant increase in the uncertainty due to air buoyancy, the uncertainty associated with the volume of a stainless steel weight should be less than $2 \cdot 10^{-5}$ relative.

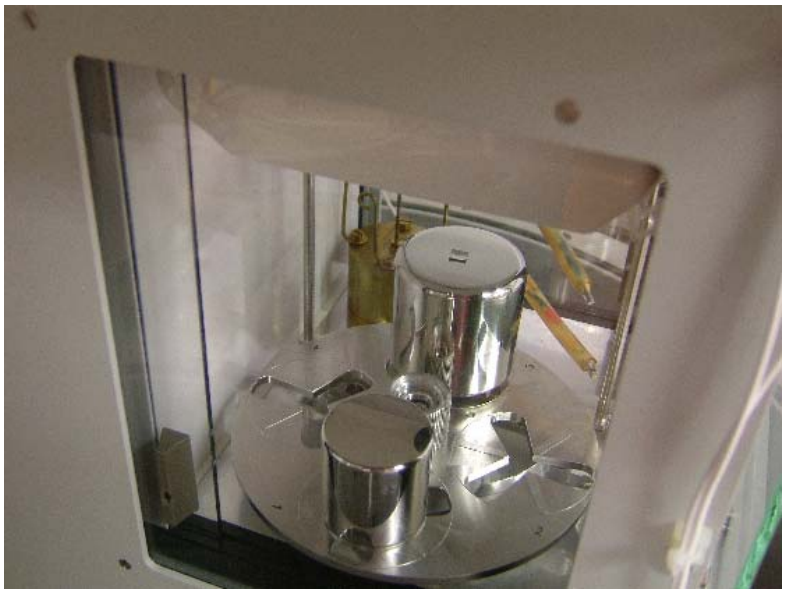

Figure 3: Comparison of a stainless steel work standard with the PtIr53

To determine the volume of weights, hydrostatic weighing is commonly used (see Appendix C). Weighing, using the results of such a hydrostatic weighing, will hereafter be referenced as the "traditional method". For many other objects this method is not possible and therefore geometrical measurement or density data from the manufacturer is used to compute the volume. This method is often not very accurate. Other disadvantages of hydrostatic weighing include the surface effects of water on the artefact's surface (adsorption) and the long time that the artefact needs to stabilise and equilibrate with the humidity from air. Furthermore not all artefacts can be immersed in water. An example of such an artefact, an adjustable weight, can be seen in Figure 4. Considering the importance of the volume for the determination of the mass, there is need for an alternative method to determine the volume.

Figure 4: Adjustable weight (example of an artefact that cannot be immersed in water)

Aerostatic weighing might be such an alternative method. It has a great advantage over hydrostatic

[1] Law of Archimedes: the buoyancy force on an object is equal to the weight of the volume of material that is displaced

weighing in that aerostatic weighing allows calibrating weights that cannot be immersed in water. Aerostatic weighing can be practised on all artefacts. The principle of aerostatic weighing is that the apparent mass difference between two artefacts is recorded as a function of the air density. In practice, there is another variable that may influence the measurement, namely the temperature. The temperature not only influences the air density, but also the volumes of the artefacts, so that it needs be taken into account.


Figure 5: airtight container

The goal is to use the existing arrangement of the airtight container for aerostatic weighing. The existing airtight container is equipped with a means to control the temperature using a thermostat bath and a pressure regulator. The air density hereby varies +/- 10% by changing the pressure / temperature in the airtight container, after which the volume of the object can be calculated from the apparent mass differences. For the mass measurements a Mettler HK1000 MC comparator is used, the most accurate balance in the range of 100 to 1000 g. To determine the air density, the environmental conditions are measured using existing equipment. The method offers good possibilities to meet the uncertainty demand for accurate measurements, without the disadvantages of the current methods.

## 3.2 Modelling

The true mass $\tilde{m}_T$ of a test weight can be related to its apparent mass $m_T$, its volume at 20°C $V_T$ and its cubic expansion coefficient $\gamma_T$ as follows:

$$\tilde{m}_T = m_T + \rho V_T + \gamma_T V_T \rho (t - 20), \quad (1)$$

where $\rho$ is the air density and $t$ is the temperature. The second term in the model accounts for air buoyancy, whereas the third accounts for the temperature effect on the weight's volume.

Likewise, the true mass of the reference weight $\tilde{m}_R$ can be expressed in terms of its true mass $m_R$ and volume $V_R$:

$$\tilde{m}_R = m_R + \rho V_R + \gamma_R V_R \rho (t - 20), \quad (2)$$

where the subscript "R" is used to indicate that the variables now refer to the reference weight.

Subtraction of (2) from (1) leads then to

$$\tilde{m}_T - \tilde{m}_R = m_T - m_R + (V_T - V_R)\rho + (\gamma_T V_T - \gamma_R V_R)\rho (t - 20) \quad (3)$$

The only two variables unknown are $V_T$ and $\tilde{m}_T$. Hence, the regression problem should provide values and uncertainties for these two parameters. By defining

$$\Delta t = (t - 20) \quad (4)$$

the model equation can be improved in behaviour during fitting, as otherwise the fitting problem may become close to singular for measurements close to $t$ = 20°C (reference temperature). It is often the case that when going from an implicit expression to an explicit expression there is a preferred choice

(depending on the particular circumstances) and that some choices are excluded because the equations become singular in some way. Sometimes an implicit form is preferable even when an explicit form can be deduced from it because the former has better numerical stability [1].

Considering that the apparent masses $m_T$ and $m_R$ are recorded as a function of the air density, and defining

$$\Delta m_j = m_T - m_R ,$$

and

$$\Delta \tilde{m}_T = \tilde{m}_T - \tilde{m}_R ,$$

equation (3) can be written as

$$\Delta \tilde{m}_T = \Delta m_j + (V_T - V_R)\rho_j + (\gamma_T V_T - \gamma_R V_R)\rho_j (t_j - 20) \qquad (5)$$

The regression has now $\Delta \tilde{m}_T = \tilde{m}_T - \tilde{m}_R$ instead of $\tilde{m}_T$ as regression parameter.

The input variables in the regression analysis are: the air density $\rho_j$, the temperature $t_j$ and the mass difference $\Delta m_j$. The output quantities are $V_T$–$V_R$ and $\Delta \tilde{m}_T$.

The air density is calculated from the environmental conditions (air pressure, temperature, humidity and $CO_2$ mole fraction) using the 1981/1991 equation (Appendix A).

The second input parameter for the regression analysis is the temperature. This is due to the fact that the volume of an object depends on the temperature.

$$V_t = V_{20^\circ C}.(1 + \gamma(t - 20))$$

where $V_t$ is the volume of the object at temperature $t$, $V_{20^\circ C}$ is the volume at 20°C and $\gamma$ the cubic thermal expansion coefficient.

The temperature is determined by measuring the resistance of two NTC (negative temperature coefficient) thermistors with a Prema multimeter. The thermistors are encased in aluminium and the wiring is protected by plastic tube. Coloured dots provide identification. One thermistor is positioned near the top of the weight under test and the other near the bottom of the weight (see the arrows in Figure 6). The average temperature of both thermistors is used as input for the regression analysis, but also used to calculate the air density which is also used as input for the regression analysis.

Figure 6: set-up of two thermistors

This means that temperature and air density are correlated. Because both thermistors are calibrated together against the same temperature standard and the same multimeter measures their resistance, there will also be a correlation between the temperatures thus measured.

The last input variable for the regression is the mass difference between mass standard and test weight determined by Borda-weighing (see Appendix B).

Equation (5) may be rewritten as

$$\Delta m_j = \Delta \tilde{m}_T + \{(V_R - V_T) + (\gamma_R V_R - \gamma_T V_T)\Delta t_j\}\rho_j . \qquad (6)$$

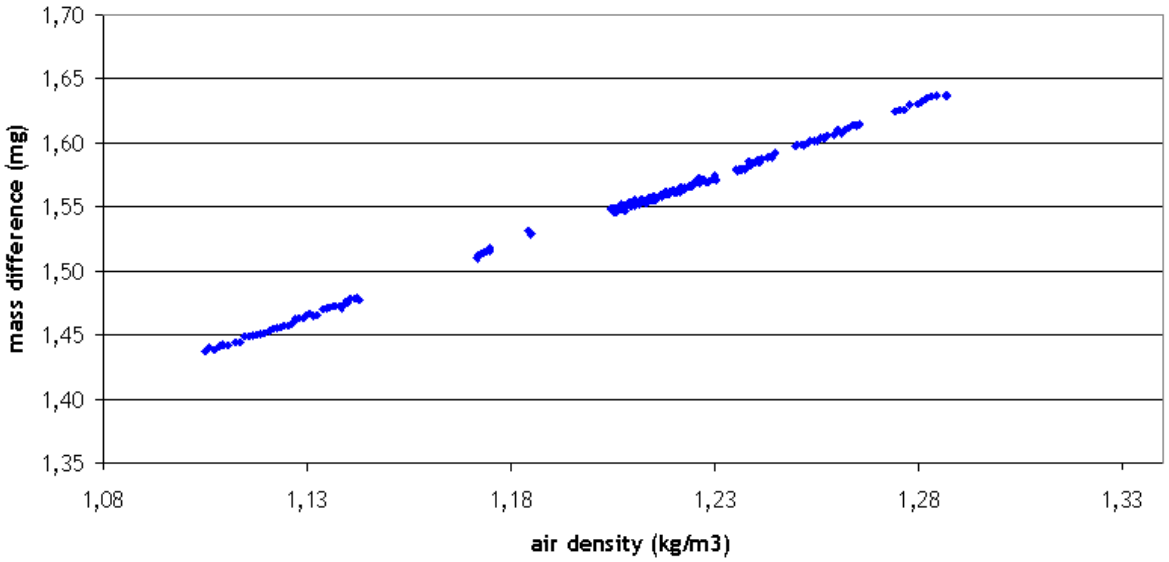


Figure 7: Mass difference vs air density

In Figure 7 the measured mass is plotted as function of the air density. It is almost a straight line, so there is a linear relation between the mass difference and the air density.

The calibration results are to be expressed at 20°C. Measurements at temperatures (slightly) differing from this reference temperature should not only address changes in air density, but also in the volume of the weights. Options for addressing the temperature-effect are a multivariate regression or adjusting the apparent mass of the artefact for volume change. Because the temperature-effect is very small, the second option is chosen.

The algorithm now runs as follows. First assume that

$\Delta t_j = 0$ for all $j$

Then equation (6) can be written as

$\Delta m_j = \Delta \tilde{m}_T + (V_R - V_T)\rho_j$.

Generalised Distance Regression (GDR) is used to estimate the value for

$\Delta V = (V_R - V_T)$.

Because $V_R$ is known, $V_T$ can be calculated as follows:

$V_T = V_R - \Delta V$.

Use this value of $V_T$ to calculate the correction term $\delta_j$ given by

$\delta_j = \left((\gamma_R V_R - \gamma_T V_T)\Delta t_j\right)$ for each $j$.

Equation (6) can now be written as

$$\Delta m_j = \Delta \tilde{m}_T + \{(V_R - V_T) + \delta_j\}\rho_j \qquad (7)$$

Equation (7) can be written as

$$\left(\Delta m_j - \delta_j \rho_j\right) = \left(V_R - V_T\right)\rho_j + \Delta\tilde{m}_T \qquad (8)$$

The left–hand side of (8) is considered as the new measured value. Equation (8) is used to obtain a new value for $\left(V_R - V_T\right)$ using GDR.

## 3.3 Solving the regression problem

The equation $\Delta m_j = \Delta V.\rho_j + \Delta\tilde{m}_T$ has to be solved and is of the form: $y_j = ax_j + b$

All variables have uncertainty. To propagate the uncertainty we do a weighted fit (regression).
We can solve the equation above with GDR.

$\Delta m_j = \Delta V.\rho_j + \Delta\tilde{m}_T$ can also be written as $\Delta m_j = a_1.\rho_j + a_0$, where $a_0$ and $a_1$ are the regression coefficients.

In matrix-form it becomes: $\Delta\overline{m} = X.\overline{a}$, where $\overline{a} = \begin{bmatrix} \Delta\tilde{m}_T \\ \Delta V \end{bmatrix}$

$$\begin{bmatrix} \Delta m_1 \\ \vdots \\ \Delta m_n \end{bmatrix} = \begin{bmatrix} 1 & \rho_1 \\ \vdots & \vdots \\ 1 & \rho_n \end{bmatrix} \begin{bmatrix} \Delta\tilde{m}_T \\ \Delta V \end{bmatrix} \text{ or equivalently } \mathbf{y} = C\mathbf{a}$$

The Ordinary Least Squares (OLS) method is used to calculate the start values for $\overline{a}$.

### *3.3.1 Ordinary Least Squares*

The flowchart of OLS is shown in Figure 9.

We have the function $y = \varphi(x;\mathbf{a})$, (9)

where $\varphi(x;\mathbf{a}) = \sum_{j=1}^{m} a_j \varphi_j(x)$, $y$ denotes the dependent variable, $x$ denotes the independent variable.

The functions $\varphi_j$ are for polynomials of the type $\varphi_j(x) = x^{j-1}$.

The objective of any regression method is to find the set parameters **a** that minimises the residuals **f**. The difference $y_i - \hat{y}_i$ is called a *residual*. Introduce

$$c_i = \begin{bmatrix} \varphi_1(x_i) \\ \varphi_2(x_i) \\ \ldots \\ \varphi_m(x_i) \end{bmatrix} \qquad (10)$$

then the predicted value $\hat{y}_i$ is given by the vector product $\hat{y}_i = \mathbf{c_i^T a}$.

Different approaches for minimising the residuals can be used, here the *least squares* minimisation is used. In *least squares*, the sum of the squared residuals is minimised. Hence, the least squares minimisation problem can be formulated as follows:

$$\min \sum_{i=1}^{n} \left( y_i - \mathbf{c_i}^{\mathrm{T}} \mathbf{a} \right)^2 . \tag{11}$$

The vector of residuals **f** can be defined as

$$\mathbf{f} = \begin{bmatrix} y_1 - \hat{y}_1 \\ y_2 - \hat{y}_2 \\ \cdots \\ y_n - \hat{y}_n \end{bmatrix} .$$

The sum of squared residuals is equivalent to the vector product $\mathbf{f}^{\mathrm{T}}\mathbf{f}$, which is equivalent to $\|\mathbf{f}\|_2^2$, the 2–norm of **f**. Hence, the minimisation problem as defined in (11) can be written as

$$\min \sum_{i=1}^{n} \|\mathbf{y} - C\mathbf{a}\|_2^2 . \tag{12}$$

Given the function $F(\mathbf{a})$,

$$F(\mathbf{a}) = \mathbf{f}^{\mathrm{T}}\mathbf{f}$$

at the solution $\hat{\mathbf{a}}$, the partial derivatives with respect to $a_j$ are zero, i.e.,

$$\frac{\partial F(\mathbf{a})}{a_j} = 0 . \tag{13}$$

The partial derivatives with respect to $a_j$ of the regression function are the elements of the vector $\mathbf{c_i}$. Hence, each row of the matrix $C$ contains the partial derivates of $\varphi$ with respect to $a_j$ for a given value of $x_i$. From the condition (13) the normal equations can be derived, which in matrix form read as $C^T C\mathbf{a} = C^T \mathbf{y}$.

Multiplication on both sides with the matrix product $\left(C^T C\right)^{-1}$ gives an expression for **a**

$$\mathbf{a} = \left(C^T C\right)^{-1} C^T \mathbf{y}$$

but this expression is hardly usable as a basis for developing a numerically stable method for obtaining the solution vector $\hat{\mathbf{a}}$.

For applications where the associated uncertainty of measurement plays a role, the approach outlined needs augmenting. Firstly, it needs to be considered that the input vectors **x** and **y** are accompanied by associated uncertainty matrices $U_x$ and $U_y$. In OLS, only the uncertainties associated with **y** are considered .

If the $y_i$ are mutually independent, then the covariance matrix $U_y$ contains on the diagonal the variances $u^2(y_i)$. The weights $w_i$ assigned to the points are the reciproques of the standard uncertainties. The minimisation problem now becomes

$$\min \sum_{i=1}^{n} w_i^2 \left( y_i - \mathbf{c_i}^{\mathrm{T}} \mathbf{a} \right)^2 \tag{14}$$

with $w_i = 1/u(y_i)$. The vector **y** and matrix $C$ are affected by these weights. Algorithms used for unweighted regression can also be used for weighted regression by applying them to $\widetilde{y}_i = w_i y_i$ and $\widetilde{C}_{ij} = w_i C_{ij}$.

More generally, when the vector **y** has a joint multivariate distribution that can be characterised by covariance matrix *V*, then the minimisation problem can be stated as

$$\min_{\mathbf{a}} (\mathbf{y} - C\mathbf{a})^T V^{-1} (\mathbf{y} - C\mathbf{a}) \tag{15}$$

which leads, when solved, to a *Gauss-Markov* estimator **a**.

The weighted vector $\tilde{\mathbf{y}}$ and matrix $\tilde{C}$ can be calculated as follows. If *V* has a Cholesky decomposition (see Appendix D) $V = LL^T$, where *L* is lower triangular. Then put

$$\tilde{\mathbf{y}} = L^{-1}\mathbf{y} \tag{16}$$

and

$$\tilde{C} = L^{-1}C\,. \tag{17}$$

Rather than inverting *L*, the equation

$$L\tilde{\mathbf{y}} = \mathbf{y}$$

is solved instead by means of, e.g., back substitution. The formation of $\tilde{C}$ can be done in a similar way. The minimisation problem can now be stated as

$$\min_{\mathbf{a}} (\tilde{\mathbf{y}} - \tilde{C}\mathbf{a})^T (\tilde{\mathbf{y}} - \tilde{C}\mathbf{a})$$

which is nothing else than solving the overdetermined system of equations

$$\tilde{\mathbf{y}} = \tilde{C}\mathbf{a}\,. \tag{18}$$

From a couple of algorithms, two algorithms for solving this system of equations have been implemented: QR–factorisation and singular value decomposition (SVD), see Appendix D. Both algorithms rely on the orthogonal decomposition of the matrix $\tilde{C}$. These two algorithms have been chosen because they are numerically very stable in comparison to the other algorithms like Gauss-Jordan elimination and LU decomposition.

When using QR, $\tilde{C}$ can be decomposed as

$$\tilde{C} = \tilde{Q}\begin{bmatrix} \tilde{R} \\ 0 \end{bmatrix},$$

where $\tilde{Q}$ is an $n \times n$ orthogonal matrix and $\tilde{R}$ is an $m \times m$ upper triangular matrix. Using the fact that $\|\tilde{Q}^T\mathbf{x}\| = \|\mathbf{x}\|$, one gets

$$\|\tilde{\mathbf{y}} - \tilde{C}\mathbf{a}\| = \|\tilde{Q}^T\tilde{\mathbf{y}} - \tilde{Q}^T\tilde{C}\mathbf{a}\| = \left\| \begin{bmatrix} \tilde{\mathbf{q}}_1 \\ \tilde{\mathbf{q}}_2 \end{bmatrix} - \begin{bmatrix} \tilde{R} \\ 0 \end{bmatrix}\mathbf{a} \right\|,$$

where $\tilde{\mathbf{q}}_1$ are the first *n* and $\tilde{\mathbf{q}}_2$ are the second $m - n$ elements of $\tilde{Q}^T\tilde{\mathbf{y}}$. The minimisation problem is solved if **a** solves the upper triangular system

$$\tilde{R}\mathbf{a} = \tilde{\mathbf{q}}_1\,.$$

The covariance matrix associated with **a** is given by

$$V_a = \sigma^2 (UU^T),$$

where $U$ solves the upper triangular system

$\widetilde{R}U = I$,

where $I$ is the identity matrix.

The second approach for solving the regression problem also starts with the formation of $\widetilde{\mathbf{y}}$ and $\widetilde{C}$, followed by singular value decomposition of $\widetilde{C}$ to solve the overdetermined system $\widetilde{C}\mathbf{a} = \widetilde{\mathbf{y}}$. The SVD of matrix $\widetilde{C}$ is given by

$$\begin{pmatrix} \\ \widetilde{C} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \mathbf{U} \\ \\ \end{pmatrix} \begin{pmatrix} W_1 & & \\ & \ddots & \\ & & W_m \end{pmatrix} \begin{pmatrix} \\ \mathbf{V^T} \\ \\ \end{pmatrix},$$

where $\mathbf{U}$ is an $n \times m$ column orthogonal matrix, the matrix $\mathbf{W}$ is an $m \times m$ diagonal matrix containing the singular values, and $\mathbf{V}$ is an $m \times m$ orthogonal matrix.

Given

$\widetilde{C} = \mathbf{U}\mathbf{W}\mathbf{V}^{\mathbf{T}}$

the inverse of $\widetilde{C}$ can be expressed as

$\widetilde{C}^{-1} = \mathbf{V}\left[\mathrm{diag}\left(1/W_j\right)\right]\mathbf{U}^{\mathbf{T}}$

and hence, given the system

$$\begin{pmatrix} \\ \widetilde{C} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{a} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ y \\ \\ \end{pmatrix}$$

the solution $\mathbf{a}$ can be expressed as follows

$$\begin{pmatrix} \\ \mathbf{a} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \mathbf{V} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{diag}\left(1/w_j\right) \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{U^T} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{y} \\ \\ \end{pmatrix}.$$

The covariance matrix $\mathbf{V_a}$ associated with the solution parameters $\mathbf{a}$ is given by $V_a = \sigma^2\left(\widetilde{C}^T\widetilde{C}\right)^{-1}$

The matrix product on the right-hand side can be expressed in terms of the matrices generated by SVD as follows

$\left(\widetilde{C}^T\widetilde{C}\right)^{-1} = \mathbf{V}\mathbf{W}^{-2}\mathbf{V}^{\mathbf{T}}$.

A value for $\sigma^2$ can be obtained from

$\hat{\sigma}^2 = \dfrac{\|\mathbf{f}\|_2^2}{n-m}$,

where **f** is the vector of residuals, defined as
$\mathbf{f} = \tilde{\mathbf{y}} - \tilde{C}\mathbf{a}$.

Data points are fitted to a best fit line, which is the line that minimizes the sum of the square residuals. For OLS the residual is the vertical distance from each data point.

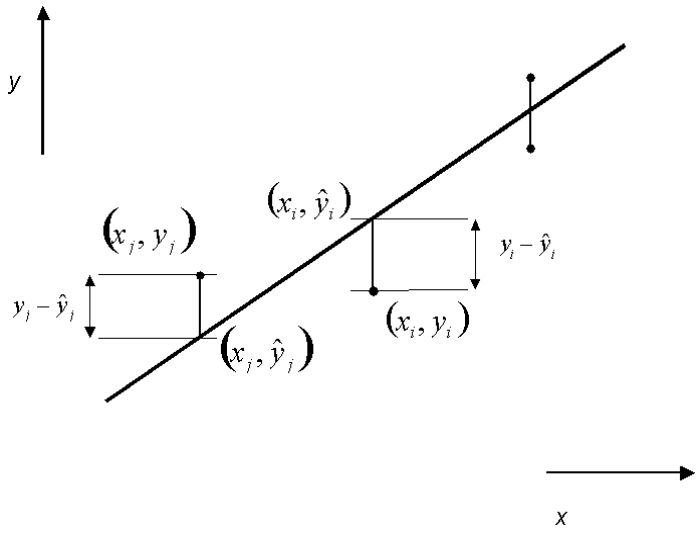


Figure 8: Residuals OLS

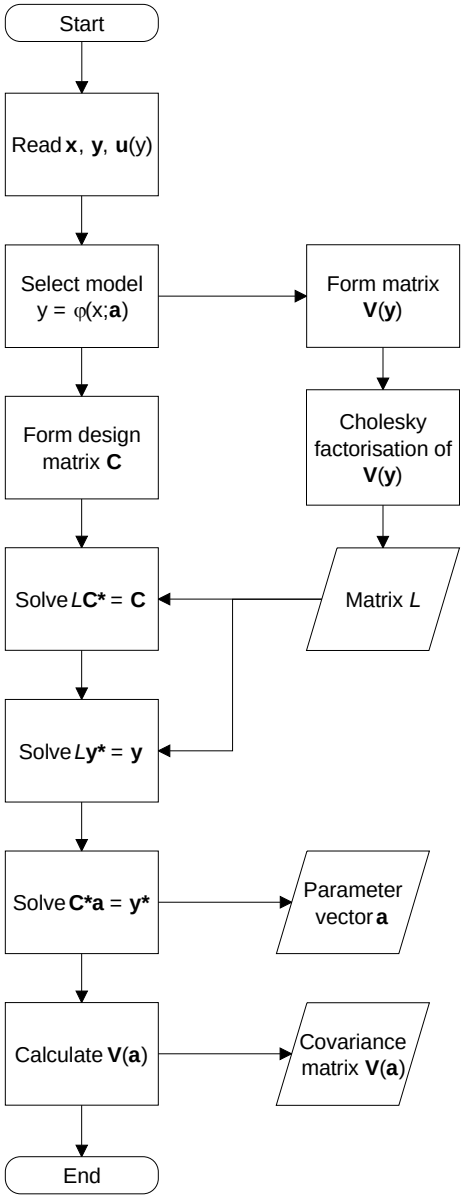


Figure 9: Flowchart of OLS

### *3.3.2 Generalised Distance regression*

The flowchart of GDR is shown in Figure 11.

Given the regression model

$$y = \varphi(x;\mathbf{a}) \tag{19}$$

a predicted value for $y$ can be related to a predicted value of $x$ as follows $\hat{y} = \varphi(\hat{x};\mathbf{a})$.

The minimisation problem in Generalised Distance Regression can be expressed as

$$\min_{\mathbf{a},\hat{\mathbf{x}}} \begin{bmatrix} \varphi(\hat{\mathbf{x}};\mathbf{a}) - \mathbf{y} \\ \hat{\mathbf{x}} - \mathbf{x} \end{bmatrix}^{\mathrm{T}} U_t^{-1} \begin{bmatrix} \varphi(\hat{\mathbf{x}};\mathbf{a}) - \mathbf{y} \\ \hat{\mathbf{x}} - \mathbf{x} \end{bmatrix}, \tag{20}$$

where the uncertainty matrix $U_t$ is given by

$$U_t = \begin{bmatrix} U_x & U_{xy} \\ U_{xy}^T & U_y \end{bmatrix}.$$

In those cases, where there is no dependence between **x** and **y**, this expression reduces to

$$U_t = \begin{bmatrix} U_x & 0 \\ 0 & U_y \end{bmatrix}.$$

The vector of residuals is defined as

$$\mathbf{f}(\hat{\mathbf{x}};\mathbf{a}) = \begin{bmatrix} \varphi(\hat{\mathbf{x}};\mathbf{a}) - \mathbf{y} \\ \hat{\mathbf{x}} - \mathbf{x} \end{bmatrix}.$$

The solution of the minimisation problem can be rephrased as follows. The covariance matrix can be factorised using a Cholesky factorisation $U_t = LL^T$, followed by solving the lower triangular systems

$L\tilde{\mathbf{f}} = \mathbf{f}$ and $L\tilde{J} = J$, where $J$ is the Jacobian matrix.

The Jacobian matrix is given by

$$J = \begin{bmatrix} \frac{\partial\varphi}{\partial\hat{x}}(\hat{x}_1;\mathbf{a}) & 0 & 0 & 0 & \frac{\partial\varphi}{\partial a_1}(\hat{x}_1;\mathbf{a}) & \dots & \frac{\partial\varphi}{\partial a_m}(\hat{x}_1;\mathbf{a}) \\ 0 & \frac{\partial\varphi}{\partial\hat{x}}(\hat{x}_2;\mathbf{a}) & 0 & 0 & \frac{\partial\varphi}{\partial a_1}(\hat{x}_2;\mathbf{a}) & \dots & \frac{\partial\varphi}{\partial a_m}(\hat{x}_2;\mathbf{a}) \\ 0 & 0 & \dots & 0 & \dots & \dots & \dots \\ 0 & 0 & 0 & \frac{\partial\varphi}{\partial\hat{x}}(\hat{x}_n;\mathbf{a}) & \frac{\partial\varphi}{\partial a_1}(\hat{x}_n;\mathbf{a}) & \dots & \frac{\partial\varphi}{\partial a_m}(\hat{x}_n;\mathbf{a}) \\ 1 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 1 & 0 & \dots & 0 \end{bmatrix}$$

which can be written in shorthand as

$$J = \begin{bmatrix} J_x & J_a \\ I & \mathbf{0} \end{bmatrix},$$

where $J_x$ is the diagonal matrix with elements

$$J_x(i,i) = \frac{\partial\varphi}{\partial\hat{x}_i}(\hat{x}_i;\mathbf{a})$$

and $J_a$ is the $n \times m$ matrix with elements

$$J_a(i,j) = \frac{\partial\varphi}{\partial a_j}(\hat{x}_j;\mathbf{a}).$$

$I$ is the $n \times n$ identity matrix and $\mathbf{0}$ is the $n \times m$ null matrix.
The regression problem (15) can now be stated as

$$\min_{\mathbf{a},\hat{\mathbf{x}}} \tilde{\mathbf{f}}^{\mathbf{T}}(\hat{\mathbf{x}};\mathbf{a})\tilde{\mathbf{f}}(\hat{\mathbf{x}};\mathbf{a}). \qquad (21)$$

The regression problem must be solved iteratively. A suitable algorithm for this minimisation is the Gauss-Newton minimisation, which requires to solve at each iteration, in the least squares sense the system

$$\tilde{J}\mathbf{p} = -\tilde{\mathbf{f}}$$

which is equivalent to minimising

$$\min_{\mathbf{p}} \left\| \tilde{J}\mathbf{p} + \tilde{\mathbf{f}} \right\|_2 .$$

The solution of this set of equations is either done by means of QR–decomposition or by SVD. If using QR, the first step is to decompose the Jacobian

$$\tilde{J} = \tilde{Q}\begin{bmatrix} \tilde{R} \\ 0 \end{bmatrix}$$

followed by solving the upper triangular system

$$\tilde{R}\mathbf{p} = \hat{\mathbf{f}}_1 ,$$

where $\hat{\mathbf{f}}_1$ is the first $n + m$ elements of $Q^T\tilde{\mathbf{f}}$ .

If using SVD, the first step is to decompose the Jacobian

$$\begin{pmatrix} \\ \tilde{J} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \mathbf{U} \\ \\ \end{pmatrix} \begin{pmatrix} W_1 & & \\ & \ddots & \\ & & W_m \end{pmatrix} \begin{pmatrix} \\ \mathbf{V^T} \\ \\ \end{pmatrix}$$

Given

$$\tilde{J} = \mathbf{U}\mathbf{W}\mathbf{V}^{\mathbf{T}}$$

the inverse of $\tilde{J}$ can be expressed as

$$\tilde{J}^{-1} = \mathbf{V}\left[\mathrm{diag}\left(1/W_j\right)\right]\mathbf{U}^{\mathbf{T}}$$

and hence, given the system

$$\begin{pmatrix} \\ \tilde{J} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ p \\ \\ \end{pmatrix} = \begin{pmatrix} \\ -\tilde{f} \\ \\ \end{pmatrix}$$

the solution **a** can be expressed as follows

$$\begin{pmatrix} \\ \mathrm{p} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \mathbf{V} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{diag}\left(1/w_j\right) \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{U}^{\mathbf{T}} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ -\tilde{f} \\ \\ \end{pmatrix} .$$

The update vector **p** can be used to update the solution vector

$$\hat{\zeta} = \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{a}} \end{bmatrix}$$

This update is as follows

$$\hat{\zeta}_{new} = \hat{\zeta}_{new} + \alpha \mathbf{p}$$

where $\alpha$ is the step size. In classical Gauss-Newton, $\alpha = 1$, and this choice works usually well for regression problems.

The step size is by default in accordance to the classical Gauss-Newton minimisation. If the proposed step leads to an increase in the object function **f**, then the following step size is used

$$\alpha = \frac{\sqrt{1+6r}-1}{3r}$$

where

$$r = \frac{\|\mathbf{f}(\zeta + \mathbf{p})\|_2^2}{\|\mathbf{f}(\zeta)\|_2^2}.$$

GDR is weighted Orthogonal Distance Regression (ODR). For ODR the residual is the perpendicular distance from the best fit line.

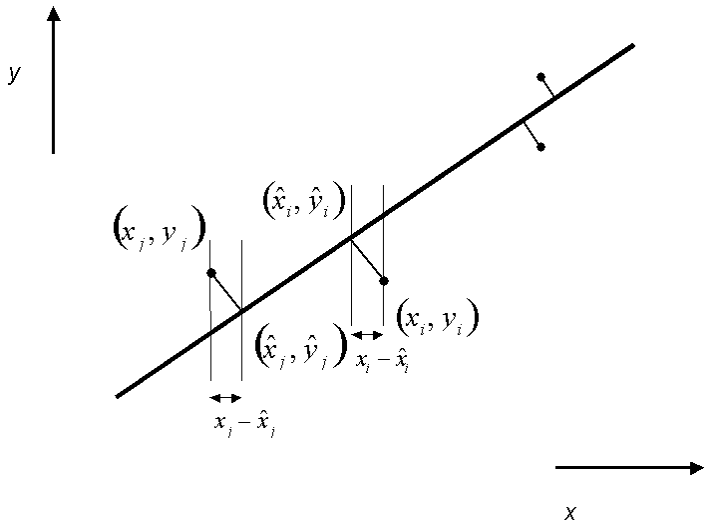


Figure 10: Residuals ODR

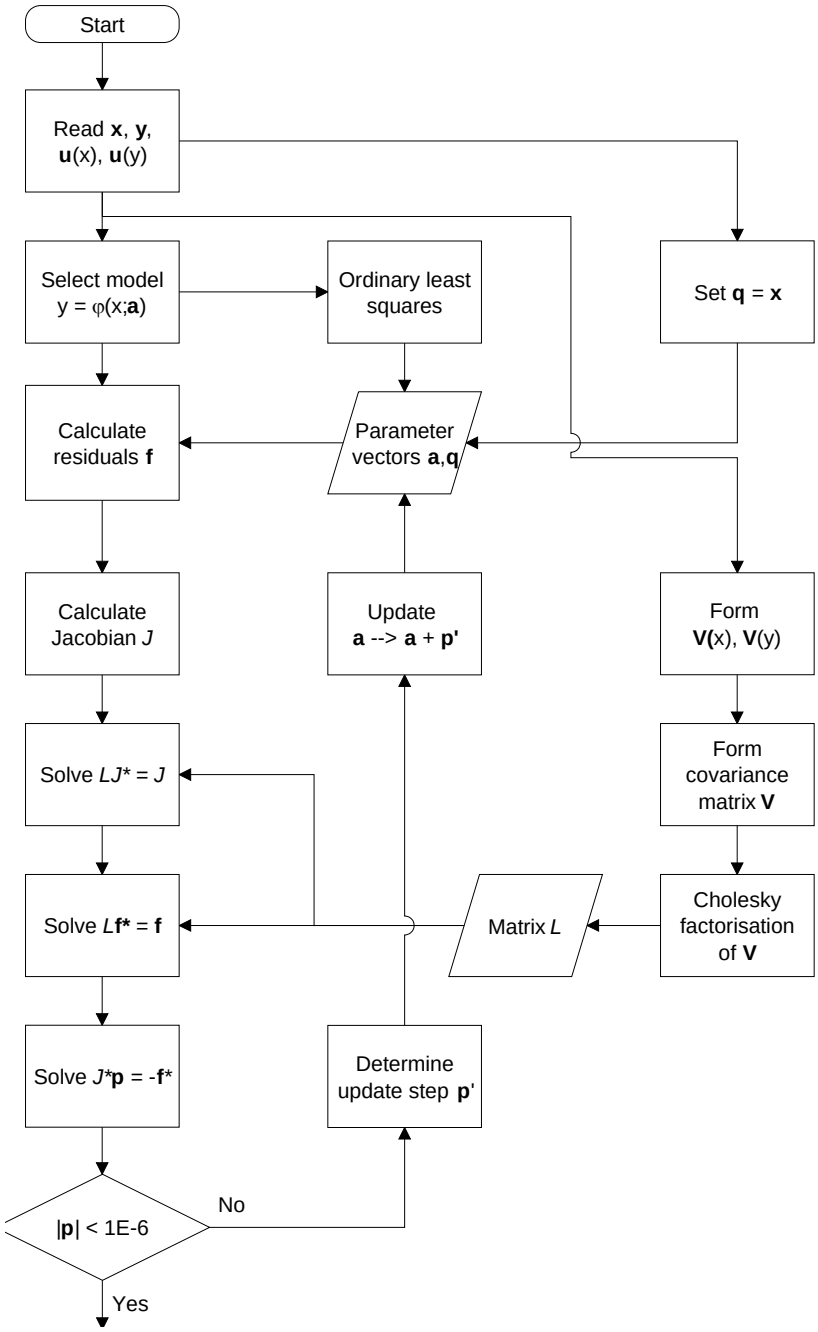


Figure 11: Flowchart of GDR

## 3.4 Gauss-Newton algorithm

Non-linear least squares problems are generally solved using some variant of the Gauss-Newton algorithm, which will be briefly described below.

Given $m$ non-linear functions $f_i(a)$ of parameters $a$, we wish to minimise

$$F(a) = \sum_{i=1}^{m} f_i^2(a) = f^T f \ ,$$

where $f = \begin{bmatrix} f_1(a) \\ \vdots \\ f_m(a) \end{bmatrix}$,

with respect to parameters $a = (a_1, ..., a_n)^T$ where $m \geq n$.

If $J$ is the associated Jacobian matrix defined at an estimate $a$ of the solution parameters by $J_{ij} = \frac{\partial f_i}{\partial a_j}$,

then an updated estimate is given by $a + p$, where $p$ (known as the *Gauss-Newton step*) solves the matrix equation $Jp = -f$ in the least squares sense. This is a linear least squares problem and can be solved using an orthogonal factorisation approach.

In practice, the update step is often of the form $a = a + t\,p$ where the step length parameter $t$ is chosen to ensure there is a sufficient decrease in the value of the objective function $F(a)$ at each iteration [2].

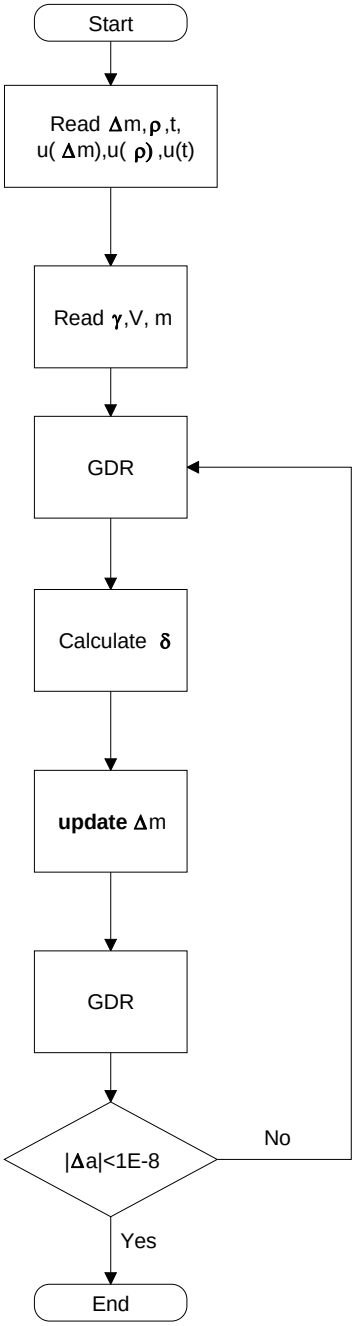


Figure 12: Flowchart of algorithm

## 3.5 Results

The uncertainty of the mass difference does not contain the effect of the convection because the uncertainty in the mass difference would become too big to do a good fit. This might cause the fitting problem to be " ill conditioned". In other words, small changes in (one of) the coefficients of the solution, in this case the mass difference, can have drastic effects on the results, which makes iterating the solution to a small residual difficult. Because the uncertainty contribution of the convection is independent of air density and temperature, the uncertainty of it can be added later.

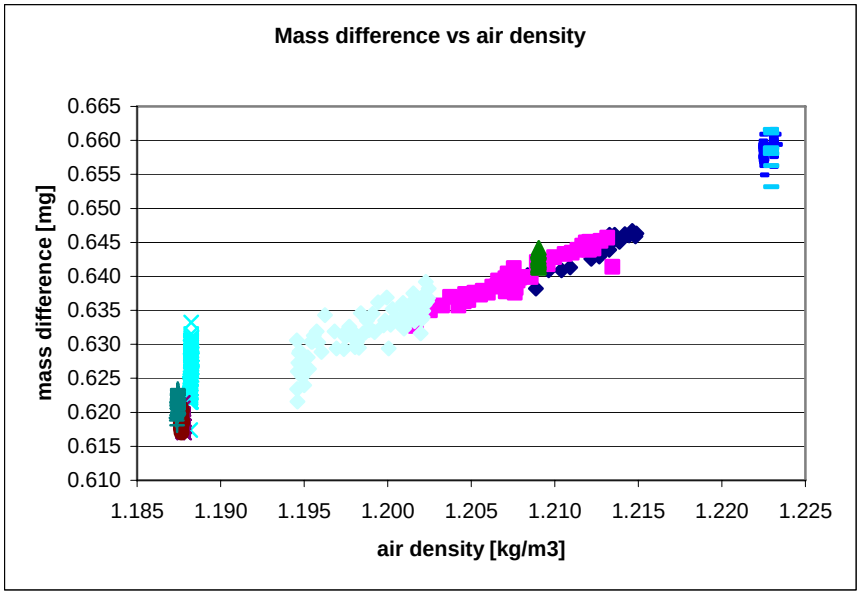


Figure 13: Measured mass difference plotted as function of the air density (Test2_v2)

In Figure 13 the mass difference is plotted as a function of the air density .There is a great dispersion in the measured mass differences, possibly due to convection or instability of the balance. This dispersion is covered by the uncertainty in the mass difference when the convection is taken along. Each measurement series has its own colour, so it is easy to see which series gives the most information. In this measurement period the airtight container is regularly opened and the temperature is adjusted. Each time that the container is opened the (air) pressure changes and because of this the air density changes.
The file Test2_v2 is composed with the results of a number of long measurements-runs. The data of Test2_v2 can be found on the accompanying CD. In Test2_v2, the 1S4-1000g is used as reference weight and the 4S4-1000g as weight under test. In the uncertainty of the mass difference, the uncertainty of convection is included. The runs in this file cover a small range of the air density.

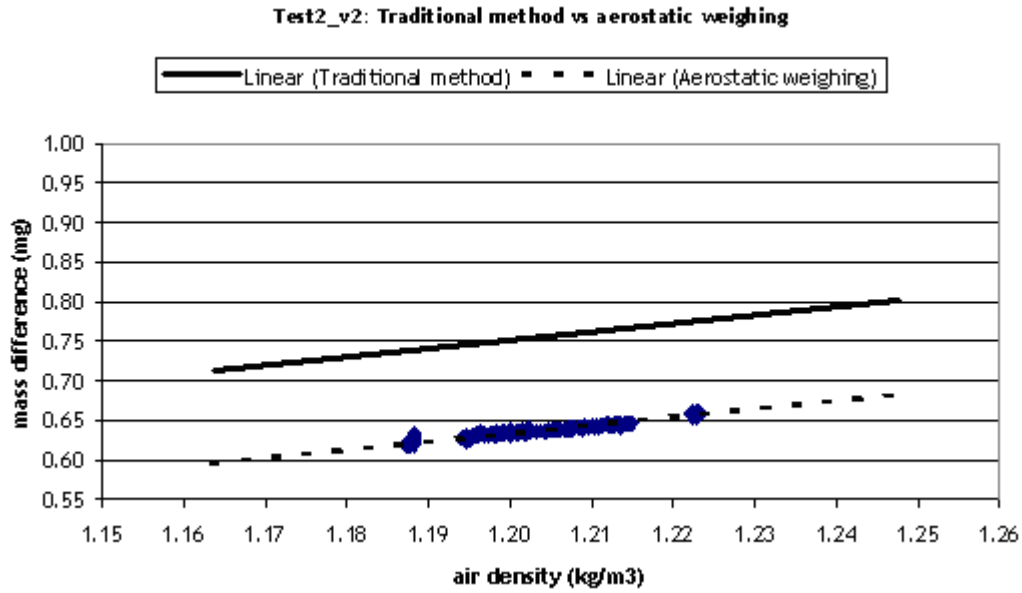


Figure 14: Mass difference fitted as function of the air density, where the 1S4-1000g is used as reference mass piece and the 4S4-1000g as weight under test

In Figure 14 it can be seen that the line constructed from the values obtained by the traditional method lies above the regression line of aerostatic weighing. This means that the mass difference $\Delta\tilde{m}$ obtained by the traditional method (0,712 mg) is greater than that obtained by aerostatic weighing (0,596 mg). The difference between the traditional method and aerostatic weighing is 0,116 mg. At present we can not explain this difference.

The uncertainty of the convection can be expressed as

$$u(\delta m_{conv}) = \frac{0{,}05}{\sqrt{3}}.$$

The uncertainty of the convection can be added to the uncertainty of the mass.

$$u(mass) = \sqrt{u(\Delta\tilde{m})^2 + u(\delta m_{conv})^2}\ .$$

In the tables below, $u(\delta m_{conv})$ is included in the $u(mass)$.

Table 2: Values obtained by the traditional method

| *Weight* | *Mass [mg]* | *u(mass) [mg]* | *Volume [cm$^3$]* | *u(volume) [cm$^3$]* |
|---|---|---|---|---|
| Reference weight (1S3) | 1,047 | 0,1095 | 126,235 | 0,0063 |
| Test weight (2S3) | 0,519 | 0,0465 | 125,169 | 0,0104 |
| Difference | -0,528 | 0,119 | 1,066 | 0,0122 |

Table 3: Values obtained by aerostatic weighing (Test2_v2)

| *Weight* | *Mass [mg]* | *u(mass) [mg]* | *Volume [cm$^3$]* | *u(volume) [cm$^3$]* |
|---|---|---|---|---|
| Reference weight (1S3) | 1,047 | 0,1095 | 126,235 | 0,0063 |
| Test weight (2S3) | 0,462 | 0,1172 | 125,22 | 0,0101 |
| Difference | -0,585 | 0,0419 | 1,015 | 0,0079 |

Table 4: Mass difference and difference in volume obtained by the traditional method and aerostatic weighing

| *Weighing method* | *Mass difference [mg]* | *u(mass difference) [mg]* | *Volume difference [cm$^3$]* | *u(volume difference) [cm$^3$]* |
|---|---|---|---|---|
| Traditional method | -0,528 | 0,119 | 1,066 | 0,0122 |
| Aerostatic weighing | -0,585 | 0,0419 | 1,015 | 0,0079 |

The standardized error is often used to determine the equivalence of measurements:

$$En = \left| \frac{(value\ traditional\ method - value\ aerostatic\ weighing)}{2 \cdot \sqrt{(u(traditional\ method)^2 + u(aerostatic\ weighing)^2)}} \right|$$

$$En(\Delta\tilde{m}_T) = \left| \frac{(-0{,}528 + 0{,}585)}{2 \cdot \sqrt{((0{,}119)^2 + (0{,}0419)^2)}} \right| = \left| \frac{0{,}057}{0{,}252} \right| = 0{,}23 \cdot$$

$$En(\Delta V) = \left| \frac{(1{,}066 - 1{,}015)}{2 \cdot \sqrt{((0{,}0122)^2 + (0{,}0079)^2)}} \right| = \left| \frac{0{,}051}{0{,}03} \right| = 1{,}7 \cdot$$

If $En < 1$ than the difference is acceptable. The *En* value for the difference in true mass is acceptable, but the *En* value for the difference in volume is not acceptable.

When the value of the difference in true mass is known, the value of the true mass of the test weight can be calculated:

$\tilde{m}_T = \tilde{m}_R + \Delta\tilde{m}_T$

= 1,047 mg – 0,585 mg
= 0,462 mg

with uncertainty $\sqrt{((0{,}1095)^2 + (0{,}0419)^2)} = 0{,}1172$ mg.

When the value of the difference in volume is known than the volume of the test weight can be calculated:

$V_T = V_R - \Delta V$

= 126,235 cm$^3$ – 1,015 cm$^3$
= 125,220 cm$^3$

with uncertainty $\sqrt{((0{,}0063)^2 + (0{,}0079)^2)} = 0{,}0101$ cm$^3$.

Table 5: True mass and volume of test weight obtained by the traditional method and aerostatic weighing (Test2_v2)

| *Weighing method* | *True mass of test weight [mg]* | *u(mass of test weight) [mg]* | *Volume of test weight [cm$^3$]* | *u(volume of test weight ) [cm$^3$]* |
|---|---|---|---|---|
| Traditional method | 0,519 | 0,0465 | 125,169 | 0,0104 |
| Aerostatic weighing | 0,462 | 0,1172 | 125,22 | 0,0101 |

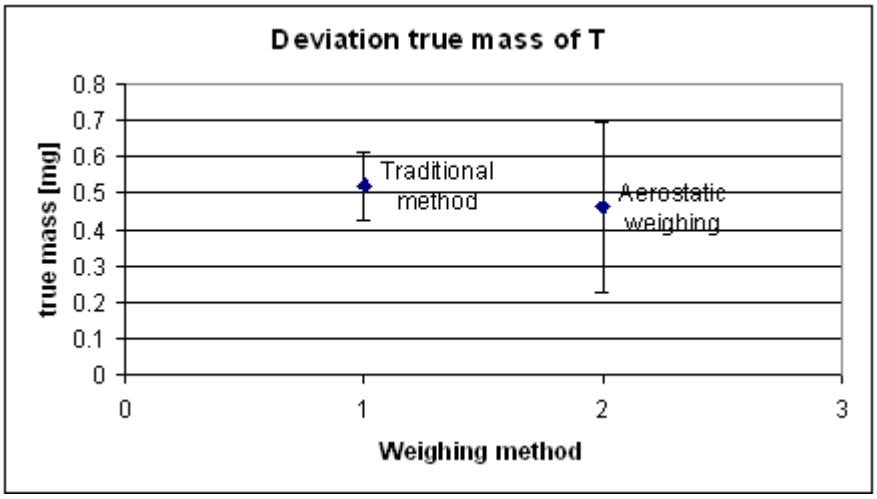


Figure 15: Deviation of the true mass of T (Test2_v2)

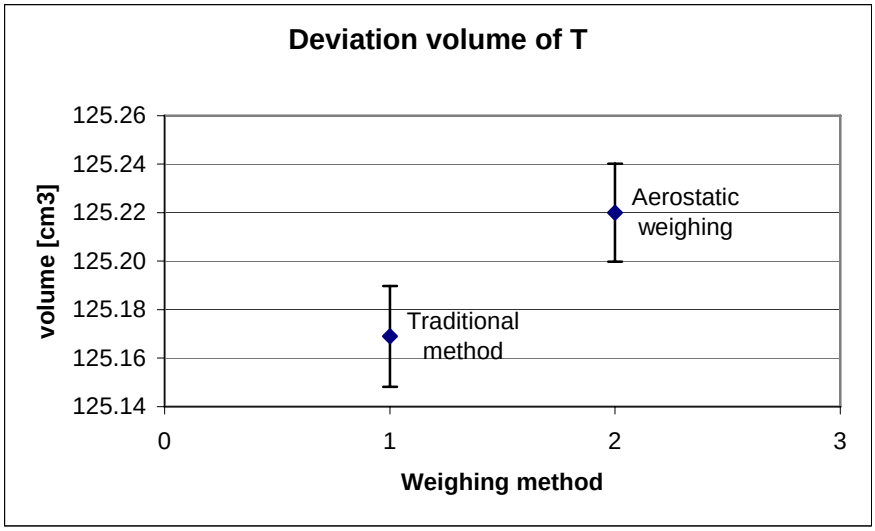


Figure 16: Deviation of the volume of T (Test2_v2)

In Figure 15 it can be seen that the true mass of T obtained by aerostatic weighing falls within the confidence interval of the true mass of T obtained by the traditional method and that uncertainty obtained by aerostatic weighing lies totally in the confidence interval of the true mass of T obtained by the traditional method. In Figure 16 it can be seen that the volume of T obtained by aerostatic weighing and its uncertainty are not within the confidence interval of T obtained by the traditional method.

The basic measures of the goodness of fit are the *coefficient of determination* and the *residual*. The *coefficient of determination* $r^2$ is the fraction of the *y*-variable that is explained by the variation of the *x*-variable; it ranges from 0 to 1.*Residuals* are defined as the difference between the *observed* values of the dependent variable and the values that are *predicted* by the model.

Here the residuals are used to measure the goodness of fit. To calculate fit parameters for a linear model, the sum of the squares of the residuals are minimised to produce a good fit. This is called a least-squares fit.
You can gain insight into the "goodness" of a fit by examining a plot of the residuals: if the residual plot has a pattern, this indicates that the model does not properly fit the data.

The fit is good if the following conditions hold:

- x-residuals: $\left|\hat{x} - x\right| < k.u(x)$
- y-residuals: $\left|\hat{y} - y\right| < k.u(y)$

where usually $k$ =2 is taken, corresponding with a normal or t-distribution and 95% level of confidence.

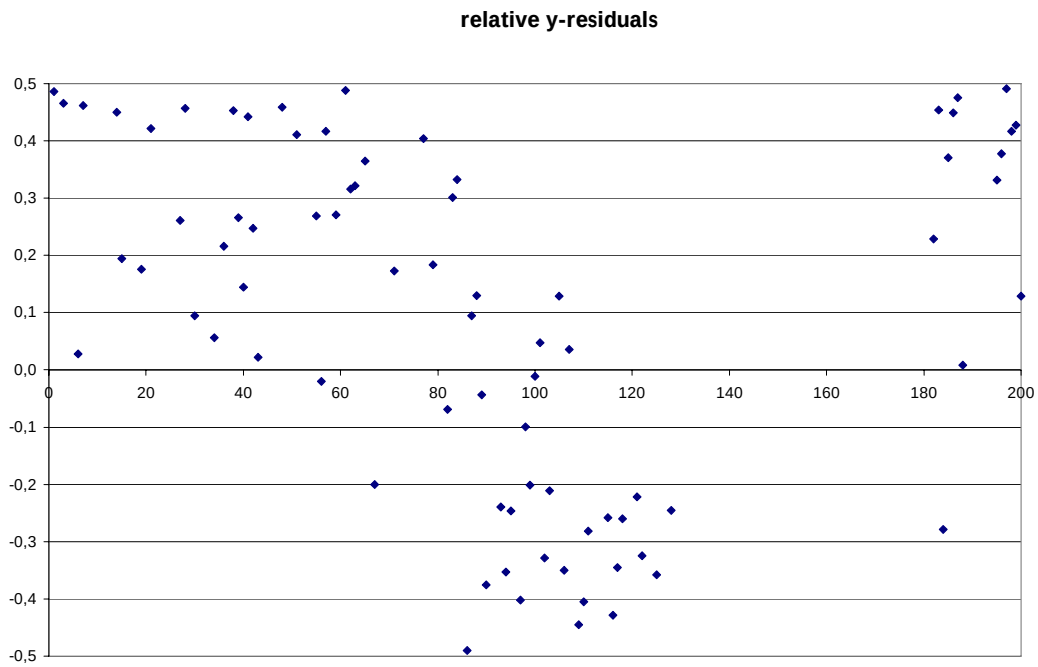


Figure 17: Graph of the relative y-residuals of Test2_v2

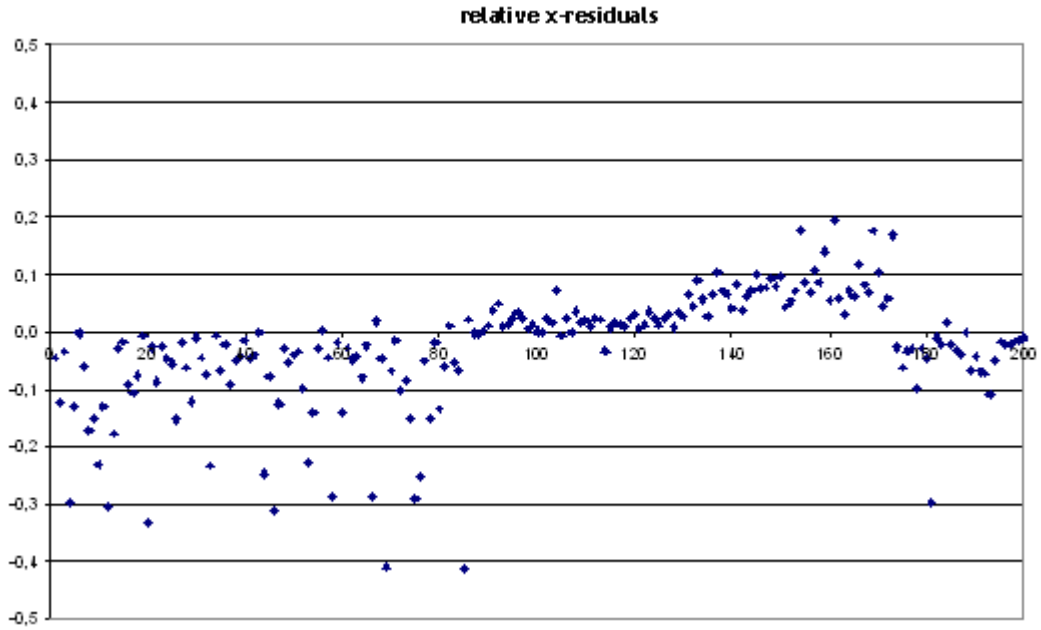


Figure 18: Graph of the relative x-residuals of Test2_v2

In Figure 17 it can be seen that the relative y-residuals lie between $[-0.5, 0.5]$ and in Figure 18 it can be seen that the relative x-residuals lie between $[-0.5, 0.2]$. In the graph of the relative y-residuals it can be seen that the residuals are scattered around and in the graph of the relative x-residuals the residuals mostly lie between $[-0.1, 0.1]$. This fit can be remarked as a good one, because the relative residuals lie between $[-2.0, 2.0]$.

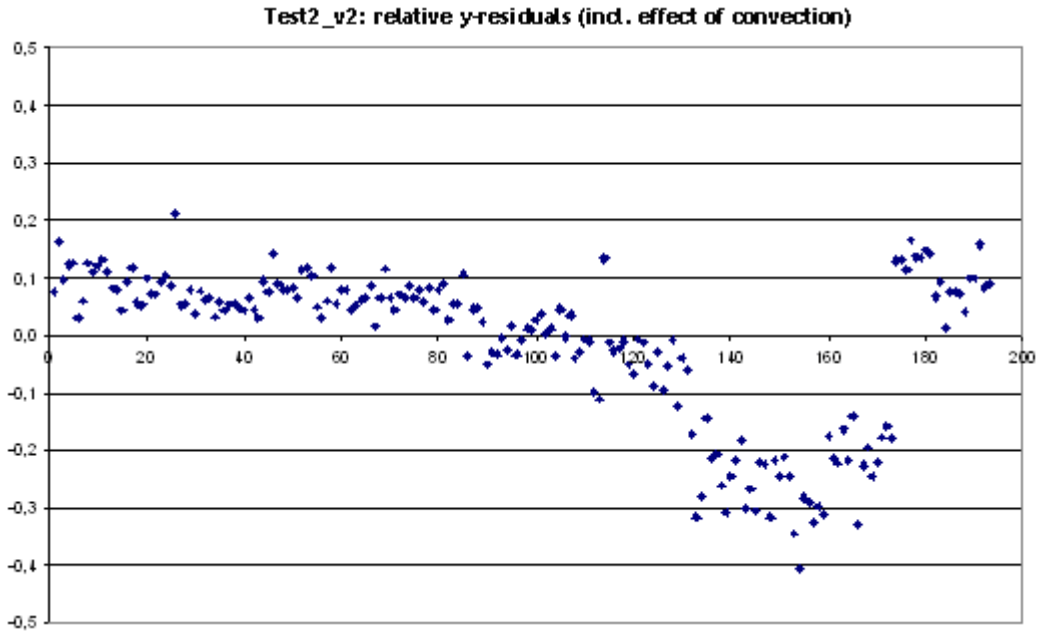


Figure 19: Graph of y-residuals (incl. effect of convection) of Test2_v2

In Figure 19 it can be seen that the relative y-residuals inclusive the effect of convection lie between $[-0.4, 0.2]$. The y- residuals without the effect of convection (Figure 17) mostly lie between $[-0.5, 0.5]$.This indicates that the convection plays an important role.

Apart from the Test2_v2 data, also another dataset has been obtained from measurements. The data of this Test3_v1 can be found on the accompanying CD. In Test3_v1, the 1S3-1000g is used as reference weight and the 2S3-1000g as weight under test. In the uncertainty of the mass difference, the uncertainty of the convection is included. The runs at this file cover a bigger range of the air density. At the beginning the airtight container was closed and the air pressure within was increased. The temperature was kept at 20 $^{o}$C but due to a small leak, the air pressure slowly decreased at a nearly constant and very slow rate. As long as the leaking is slow, the thermostat bath can keep the temperature constant and the air density of each group is almost constant. In the ideal situation, after each two groups a little bit air would be let out, wait for stabilization and then there can be measured again.
But this is not possible yet.

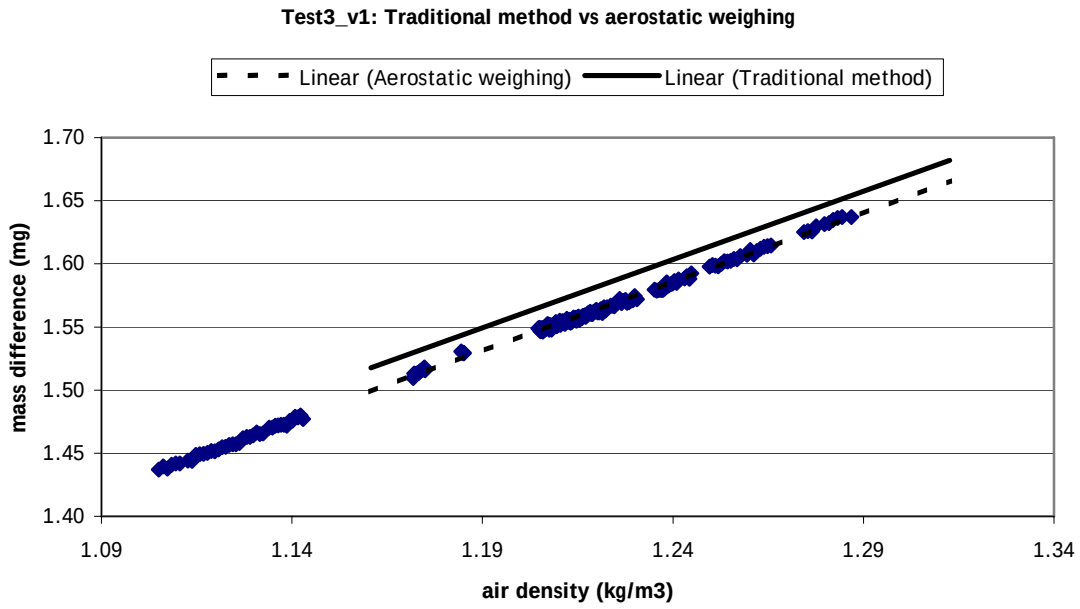


Figure 20: Mass difference fitted as function of the air density, where the 1S3-1000g is used as reference mass piece and the 2S3-1000g as weight under test

Figure 20 once again shows that the line constructed out of the values obtained by the traditional method lies above the regression line of aerostatic weighing. The mass difference obtained by the traditional method is 1,518 mg and the mass difference obtained by aerostatic weighing is 1,499 mg. The difference between the traditional method and aerostatic weighing is 0,019 mg. The difference is less than for Test2_v2 but we still can not explain this difference.

Table 6: Values obtained by the traditional method

| *Weight* | *Mass [mg]* | *u(mass) [mg]* | *Volume [$cm^3$]* | *u(volume) [$cm^3$]* |
|---|---|---|---|---|
| Reference weight (1S3) | -0,018 | 0,013 | 126,250 | 0,006 |
| Test weight (2S3) | 0,245 | 0,047 | 125,169 | 0,010 |
| Difference | 0,263 | 0,0488 | 1,081 | 0,0117 |

Table 7: Values obtained by aerostatic weighing (Test3_v1)

| *Weight* | *Mass [mg]* | *u(mass) [mg]* | *Volume [$cm^3$]* | *u(volume) [$cm^3$]* |
|---|---|---|---|---|
| Reference weight (1S3) | -0,018 | 0,013 | 126,250 | 0,006 |
| Test weight (2S3) | 0,203 | 0,0431 | 125,149 | 0,0074 |
| Difference | 0,221 | 0,0411 | 1,101 | 0,0043 |

Table 8: Mass difference and difference in volume obtained by the traditional method and aerostatic weighing

| *Weighing method* | *Mass difference [mg]* | *u(mass difference) [mg]* | *Volume difference [$cm^3$]* | *u(volume difference) [$cm^3$]* |
|---|---|---|---|---|
| Traditional method | 0,263 | 0,0488 | 1,081 | 0,0117 |
| Aerostatic weighing | 0,221 | 0,0411 | 1,101 | 0,0043 |

$$En(\Delta\tilde{m}_T) = \left| \frac{(0{,}263 - 0{,}221)}{2 \cdot \sqrt{((0{,}0488)^2 + (0{,}0411)^2)}} \right| = \left| \frac{0{,}042}{0{,}128} \right| = 0{,}33 \cdot$$

$$En(\Delta V) = \left| \frac{(1{,}081 - 1{,}101)}{2 \cdot \sqrt{((0{,}0117)^2 + (0{,}0043)^2)}} \right| = \left| \frac{-0{,}02}{0{,}024} \right| = 0{,}83 \cdot$$

The *En* values for the difference is true mass and the difference in volume indicate that the observed differences between the two methods are smaller than the associated uncertainties.

The value of the true mass of the test weight can be calculated by:

$\tilde{m}_T = \tilde{m}_R + \Delta\tilde{m}_T$

= 0,018 mg + 0,221 mg
= 0,203 mg

with uncertainty $\sqrt{((0{,}013)^2 + (0{,}0411)^2)} = 0{,}0431$ mg.

The volume of the test weight can be calculated by:

$V_T = V_R - \Delta V$

= 126,250 $cm^3$ – 1,101 $cm^3$
= 125,149 $cm^3$.

with uncertainty $\sqrt{((0{,}006)^2 + (0{,}0043)^2)} = 0{,}0074$ $cm^3$.

Table 9: True mass and volume of test weight obtained by the traditional method and aerostatic weighing (Test3_v1)

| *Weighing method* | *True mass of test weight [mg]* | *u(mass of test weight) [mg]* | *Volume of test weight [$cm^3$]* | *u(volume of test weight ) [$cm^3$]* |
|---|---|---|---|---|
| Traditional method | 0,245 | 0,047 | 125,169 | 0,010 |
| Aerostatic weighing | 0,203 | 0,043 | 125,149 | 0,0074 |

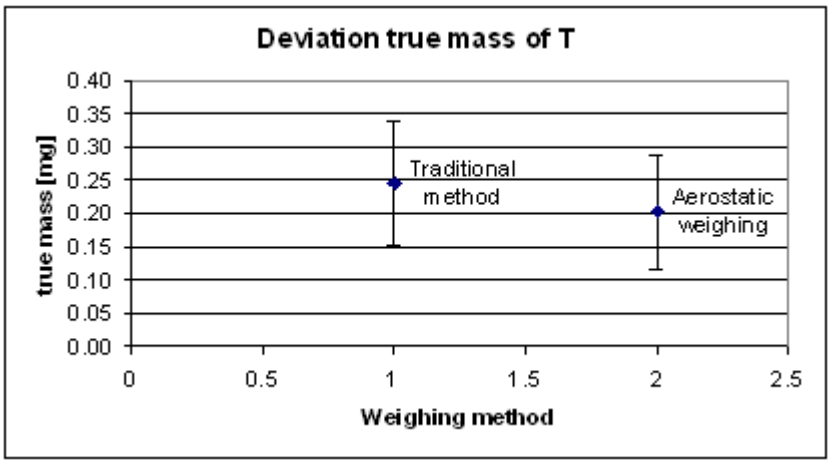


Figure 21: Deviation of the true mass (Test3_v1)

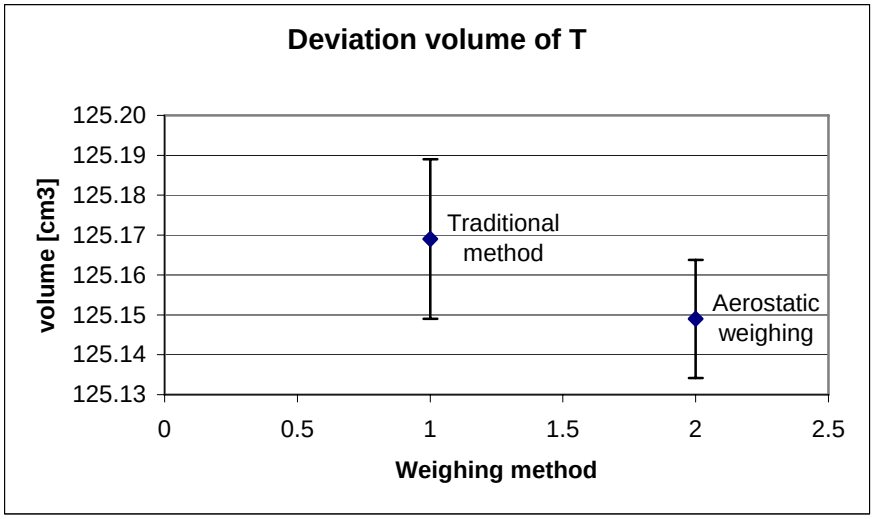


Figure 22: Deviation of the volume of T (Test3_v1)

In Figure 21 it can be seen that the true mass of T obtained by aerostatic weighing lies in the confidence interval of the true mass of T obtained by the traditional method. Likewise, in Figure 22 it can be seen that both volume estimates are consistent with one another (within their respective uncertainties).

There is more evidence needed for demonstrating consistency between the two weighing methods. The mathematical modelling and the algorithms used seem to be appropriate for the purpose of obtaining the differences in true mass and volume from aerostatic weighing data.

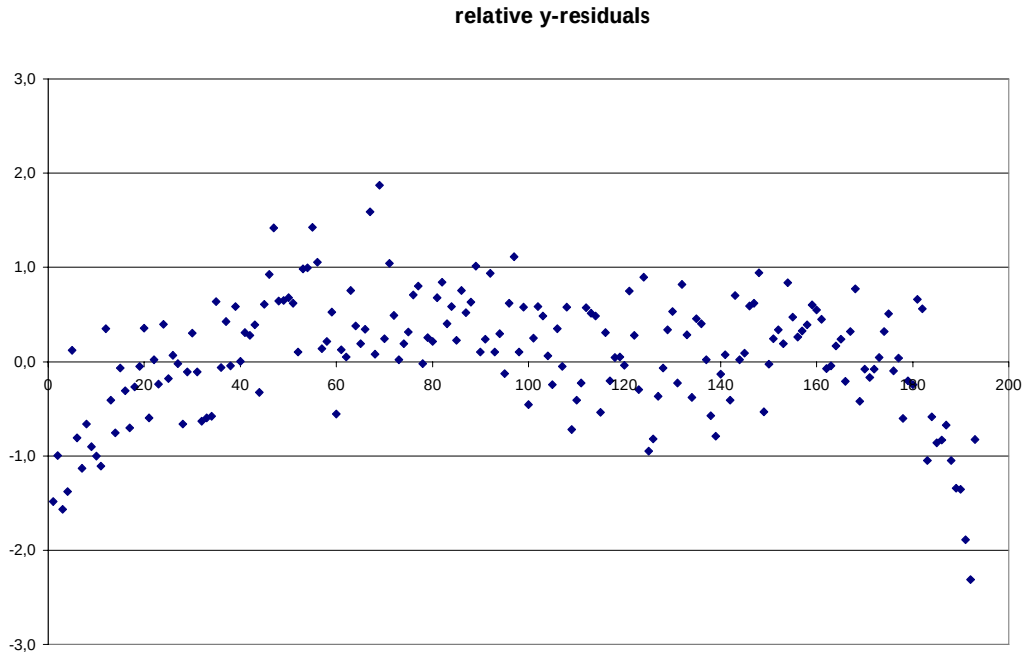


Figure 23: Graph of relative y-residuals of Test3_v1

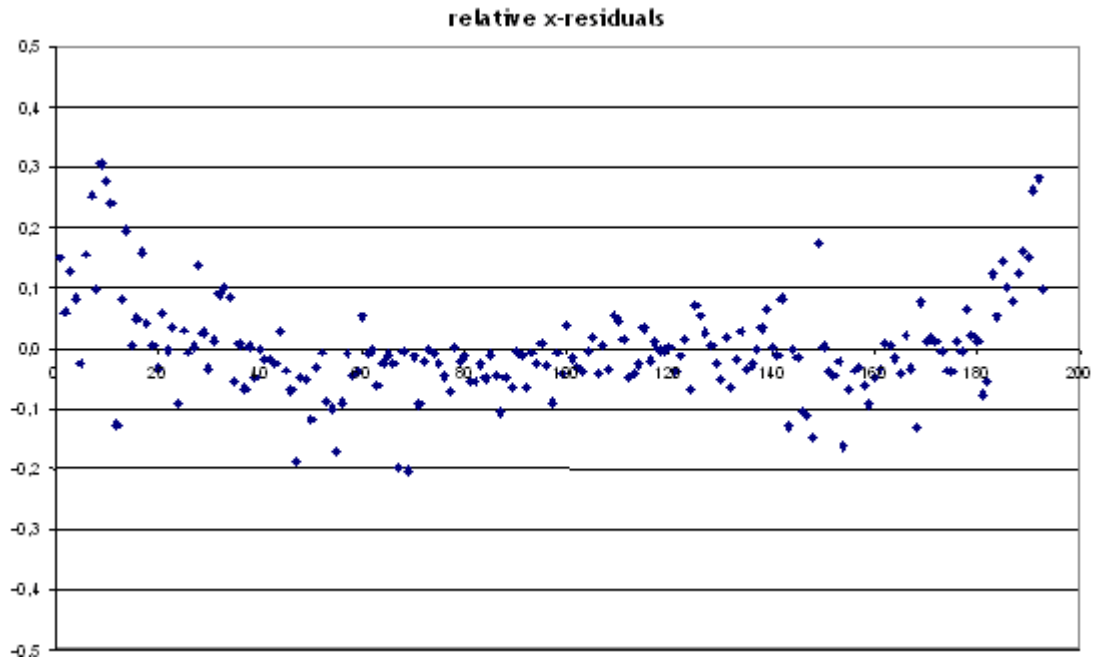


Figure 24: Graph of the relative x-residuals of Test3_v1

In Figure 23 it can be seen that the relative y-residuals lie between $[-2.5, 2.0]$ and in Figure 24 it can be seen that the relative x-residuals lie between $[-0.2, 0.3]$. In the graph of the relative y-residuals it can be seen that the residuals mostly lie around $[-1.0, 1.0]$ and in the graph of the relative x-residuals the residuals mostly lie between $[-0.1, 0.1]$. This fit can also be remarked as a good one.

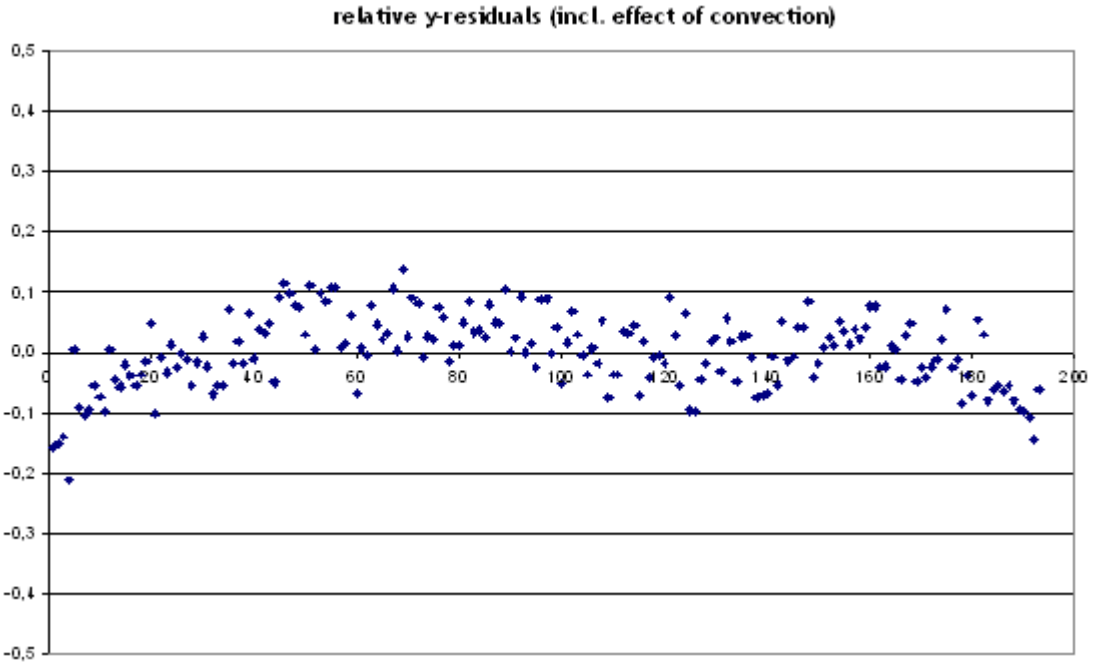


Figure 25: Graph of y-residuals (incl. effect of convection) of Test3_v1

In Figure 25 it can be seen that the relative y-residuals inclusive the effect of convection mostly lie between $[-0.1, 0.1]$. The y- residuals without the effect of convection (Figure 23) mostly lie between $[-1.0,1.0]$.This indicates that the convection plays an important role.

After analyzing both datasets it can be concluded that:

- the accuracy of the regression improves with increasing the air density range
- the algorithm used for obtaining the regression coefficients performs well
- the residual plot of Test3_v1 has a small pattern, this indicates that the model does completely describes the data
- The difference in volume seems to be the most vulnerable part of the comparison of the two weighing methods; more measurements are needed to demonstrate the validity of aerostatic weighing.

# 4 Weighing series

## 4.1 Problem description

For the calibration of weights, NMi VSL uses special weight sets. For practical reasons these sets contain only a limited number of mass standards with specially selected nominal masses. For instance 10 kg, 5 kg, 2 x 2 kg, 2 x 1 kg, 500 g, 2 x 200 g, .... 2 x 1 mg. In order to be able to distinguish between weights with the same nominal mass, a small dot is used to mark one of them. So one can speak of 100 g and 100 g•. Of course the nominal mass of a weight is only an approximate value of the actual mass and during the calibration this actual mass is determined. By convention the calibration result is expressed as the mass difference between actual and nominal mass.

The actual mass of an individual weight can be determined by direct comparison with a mass standard of equal nominal mass. In case no such mass standard is available also a combination of mass standards can be used of which the total mass is equal to the nominal mass of the weight under test. A (combination of) mass standard(s) is called the reference weight. The comparison of test weight and reference weight is done by means of a very accurate electronic balance, because for high classed weights the differences between actual and nominal mass are very small.

Of course, the actual masses of the mass standards must be determined as well. To achieve the smallest uncertainty, these masses must be determined using the Dutch National mass standard, PtIr53[2]. However, this standard has a nominal mass of 1000 g and can not be used for the calibration of e.g. a 200 g weight by means of direct comparison. In this case, so called weighing schemes must be used.

In a weighing scheme several (combinations of) weights are compared with other (combinations of) weights. For example the 1000 g weight is compared with a combination of 500 g, 200 g, 200 g• and 100 g weights. To determine the resulting mass difference more accurately, each individual weighing is performed several times in a sequence which is called a Borda weighing. The mass difference $\Delta m_1$ can be expressed as a mathematical equation :

$$\Delta m_1 = m_{1000} - (m_{500} + m_{200} + m_{200\bullet} + m_{100})$$

For practical reasons the 'reference' and 'test' combination can not both contain the same weight. And by selecting an overdetermined set of equations, the unknown masses $m_{500}$ to $m_{100}$ can be computed from the known mass $m_{1000}$. An example of a weighing scheme is shown in Table 10.

Table 10: Example of a weighing scheme

| Reference combination | Test combination |
|---|---|
| 1000 g | 500 g, 200 g, 200 g•, 100 g |
| 1000 g | 500 g, 200 g, 200 g•, 100 g• |
| 500 g | 200 g, 200 g•, 100 g |
| 200 g | 100 g, 100 g• |
| 200 g +100 g | 200 g•, 100 g• |
| 100 g | 100 g• |

[2] In practice the PtIr53 is used as little as possible to minimise contamination and wear. So in the first step of the dissemination of the mass scale, the PtIr53 is compared to several stainless steel kilograms in a special weighing scheme called a Kohlrausch series for 5 equal nominal masses. From this the actual masses of four stainless steel kilograms is calculated. One of these stainless steel kilograms is subsequently used as reference weight in a weighing series for non-equal nominal masses as described in this project.

It has been shown that the weighing scheme is table 10 is not the most optimal scheme. The aim of this project is to determine the most optimal scheme, that is, the one resulting in the smallest mass uncertainties. To do this three steps must be taken :

- modelling of single weighing result
- determining mass difference of a individual equation
- combining equations to compute the unknown masses.

## 4.2 Modelling of a single weighing result

The mass difference between a reference and test combination is determined from several single weighings. Determination of a weighing result is more than simply writing down the balance indication. The balance indication must be corrected for the effects of the air buoyancy, the centre of gravity, resolution, convection, the drift of the balance and in case of small weights the use of a pad. This can be expressed by :

$$x_i = x_i^* + \Delta x_{buo,i} + \Delta x_{COG,X} + \delta x_{res,i} + \delta x_{conv} + \Delta x_{drift,i} + \Delta x_{pad}$$

where

$x_i$ denotes the corrected mass,

$x_i^*$ the reading (repeatability),

$\Delta x_{buo,i}$ the correction for the air buoyancy,

$\Delta x_{COG,X}$ the correction for the centre of gravity,

$\delta x_{res,i}$ the correction for resolution ,

$\delta x_{conv}$ the correction for convection ,

$\Delta x_{drift,i}$ the correction for the drift of the balance ,

and $\Delta x_{pad}$ is the pad correction in case of small weights[3].

These effects and their contribution to the uncertainty will be described in more detail in the following paragraphs.

*Air buoyancy*
Any weighing in air is influenced by air buoyancy. As a balance measures the forceapplied to its scale, the balance display indicates the difference between gravitational mass and air buoyancy. The air buoyancy can be calculated using the Archimedes' Law and if also the expansion is taken into account this results in:

$$\Delta x_{buo,i} = \rho_i . V_X (1 + \gamma_X . \Delta T)$$ [4],

where
ρ is the air density ($\approx 1{,}2\, kg.m^{-3}$),

[3] The letter Δ is used for the corrections that have a non-zero value. Corrections, which usually have value zero but impact the uncertainty are denoted by a δ. This distinction is not strict, and has no impact on how the effects are treated when establishing and uncertainty budget.
[4] For odd cycles, X,I, = Reference, for even cycles, X,I =T (weight under test)

$V_x$ is the volume of the weight,
$\gamma$ is the cubic expansion coefficient and
$\Delta T$ the difference in temperature.

The uncertainty associated with the air buoyancy ($u_{buo}$) can be expressed as:

$$u_{buo} = \sqrt{V_X^2(1+\gamma_X\Delta T)^2 u^2(\rho_i) + \rho_i^2(1+\gamma_X\Delta T)^2 u^2(V_X) + \rho_i^2 V_X^2 \Delta T^2 u^2(\gamma_X) + \rho_i^2 V_X^2 \gamma_X^2 u^2(\Delta T)}\,.$$

Because the weighings are done at 20°C, $\Delta T \approx 0$, a simplification of the model is justified which results in:

$$\Delta x_{buo,i} = \rho_i . V_X$$

The associated uncertainty can now be expressed as:

$$u_{buo} = \sqrt{(\rho_i^2 . u^2(V_X) + V_X^2 . u^2(\rho_i))}\,.$$

*Centre of gravity*

The centre of gravity of the reference weight(s) and the weight(s) under test are usually different. It depends on, e.g., the geometry of the weight(s) used. The correction $\Delta x_{COG,X}$ also depends on the mass of the weight.

By $\Delta g$ we denote the gradient in gravity $(= 3{,}161.10^{-9}\ N.kg^{-1}.mm^{-1})$, by $g$ we denote the gravity $(= 9{,}8124\ N.kg^{-1})$. Then:

$$\Delta x_{COG,X} = \frac{\Delta g \cdot m_X \cdot h_X}{g}$$

where, $m_X$ is the mass of the weight and $h_X$ is the height of the weight.

The uncertainty of the centre of gravity then can be formulated as:

$$u_{COG} = \Delta g . m_{nom} . \frac{u_{h_l}}{g},$$

where $m_{nom}$ is the nominal mass in kg and $u_{h_l}$ is the uncertainty in height.

*Resolution*

Each balance reading has a correction due to the finite resolution of the display of the mass balance. The uncertainty of the resolution is

$$u_{res} = \frac{d}{2},$$

where $d$ is the sensitivity of the last decimal.

Table 11: the sensitivity of the last decimal of each balance.

| *Balance* | *d* |
|---|---|
| *AWD* 1 | 0,1 mg |
| *AWD* 2 | 0,001 mg |
| *HK* 1000 | 0,001 mg |
| *AWD* 3 | 0,0001 mg |

*Convection*
Convection is the airflow induced by small differences in T in the surroundings of the balance. To some extent, such differences can be caused by, e.g., the heat produced by the balance itself.

The uncertainty of convection can be calculated by:

$u_{conv} = F_{conv}.m_{nom}$,

where $F_{conv} = 5.10^{-8}$ for weights of accuracy class E1 and $m_{nom}$ is the nominal mass in grams.


Figure 26: pan of AWD

*Drift of the balance*
The drift of the balance is a gradual trend in the data. By calculating the difference in mass from subsequent weighings of the assemblies R and T, the linear component of the drift is effectively eliminated.

Because some of the weights are very small, e.g. 0,1 mg-1000 mg, a pad is used to put the weight on it. In figure 26 a pan of an AWD can be seen.

It is impossible to put a small weight on it, without it falling off. So a pad has to be used. A pad with a 50 mg weight on it can be seen in figure 27.

*Uncertainty matrix*
The uncertainty matrix $V_x$ can be formed as follows:

$V_x = V_{x^*} + V_{res} + V_{COG} + V_{buo} + V_{conv} + V_{pad}$,

where $V_{res}$, $V_{COG}$, $V_{buo}$, $V_{conv}$, $V_{pad}$ are the uncertainty matrices of the resolution, centre of gravity, air buoyancy, convection and pad respectively.

$V_{x^*} = diag(s^2 I)$

and $s^2$ is the repeatability variance of the reading $x_{i^*}$

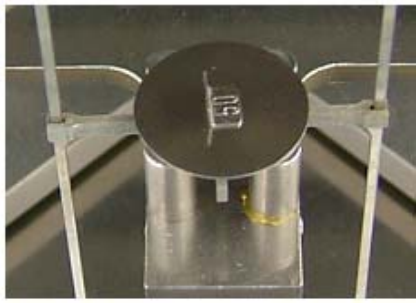
Figure 27: pad with weight of 50 mg

To determine the value of $s^2$ the following assumptions are made:
- time is proportional to index
- drift effects are the same for T and R
- Model function for drift T = model function for drift R, apart from intercept

$x_{R^*} = \varphi(t, \vec{a})\ \ \vec{a} = \begin{bmatrix} a_0 \\ \cdots \\ a_m \end{bmatrix}$, where $a_0$ is the intercept

$x_{T^*} = \varphi(t, \vec{a})\ \ \vec{a} = \begin{bmatrix} a_1 \\ \cdots \\ a_{m+1} \end{bmatrix}$, where $a_{m+1}$ is the intercept

After analyzing the data of the drift in Microsoft Excel it was clear that the data fitted a polynomial of degree 3 the best. So the assumption has been made that $\varphi$ is a polynomial of degree 3.

$x_{R^*} = a[0] + a[1].t + a[2].t^2 + a[3].t^3$

$x_{T^*} = \quad a[1].t + a[2].t^2 + a[3].t^3 + a[4].$

To obtain *a*, apply QR factorisation on $\vec{x} = C.\vec{a}$ and solve this in the least squares sense.

where

$$\vec{a} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} \qquad C = \begin{bmatrix} 1 & t & t^2 & t^3 & 0 \\ 0 & t & t^2 & t^3 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & t & t^2 & t^3 & 0 \end{bmatrix}$$

The residuals $\vec{f}$ can be computed from

$\vec{f} = \vec{x}^* - C.\vec{a}$

The repeatability variance of the reading $x_{i^*}$ is given by $s^2 = \frac{\|f\|_2^2}{[length\ \vec{f} - length\ \vec{a}]}$

Now that $s^2$ is known, the matrix $V_x$ can be formed . $V_x$ is then needed to calculate matrix $V_{\Delta m}$, the uncertainty matrix associated with $\Delta m$, and is given by $V_{\Delta m} = B.V_x.B^T$.

## 4.3 Mass difference in a Borda sequence

The mass difference between two (combinations of) weights is determined by means of a Borda-cycle. During this cycle the reference weight and the test weight are placed alternately on the balance scale. Naturally also combinations can be used as either reference 'weight' R or test 'weight' T. There are several variations for Borda-cycles, e.g. RTTR, TRRT, TRT or RTRTR. NMi VSL used the RTR variant with maximum correlation, because it has been shown that this cycle effectively eliminates the drift of the balance while requiring not too many single weighings.

Differences in mass are calculated by:

$$\Delta m_1 = T_1 - \frac{(R_1 + R_2)}{2}$$

$$\Delta m_2 = \frac{(T_1 + T_2)}{2} - R_2$$

$$\Delta m_3 = T_2 - \frac{(R_2 + R_3)}{2}$$

$$\Delta m_4 = \frac{(T_2 + T_3)}{2} - R_3 \text{, etc..}$$

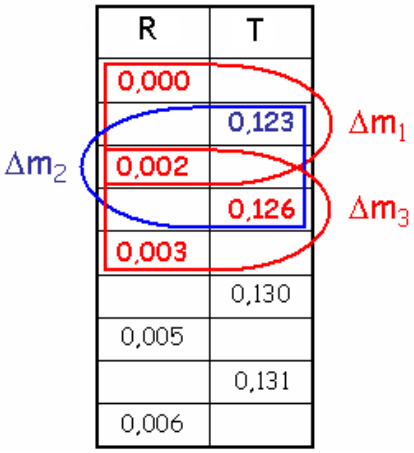

Figure 28: RTR weighing procedure

The process is also shown in Figure 28 and can be comprised in one formula:

$$\Delta m_j = (-1)^{j+1}(x_{j+1} - \tfrac{1}{2}(x_j + x_{j+2})),\ 1 \le j \le k-2$$

Thus from $n$ weightings $n-2$ mass differences can be obtained.

During the measurement the balance generally drifts and this results in gradually changing single weighing results. As long as the drift is the same for reference and test 'weight', this should have little effect in the mass difference provided the computation of the mass difference is such that the drift is effectively eliminated. Generally the balance drift is linear and the RTR cycle described above does eliminate the drift sufficiently.

Due to various effects and uncertainties each single individual weighing deviates a little bit (from the actual value. This means that the individual measured mass differences $\Delta m_j$ deviates a little from the actual mass difference $\Delta\mu_i$. The deviation of the single weighings is denoted as $\varepsilon_i$ and the mass differences obtained by the RTR Borda-cycle can then be written in matrix notation as :

$$\begin{pmatrix} \Delta m_1 \\ \Delta m_2 \\ \vdots \\ \Delta m_j \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \Delta\mu + \begin{pmatrix} -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \dots & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -1 & \frac{1}{2} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \mp\frac{1}{2} & \mp 1 & \mp\frac{1}{2} \end{pmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_k \end{pmatrix}$$

$$\Delta m = \underline{1}\Delta\mu + B_k\varepsilon \qquad (22)$$

To illustrate how to calculate an estimate for $\Delta\mu$, apply Cholesky factorization on $B_k B_k^T$ such that

$$L_k L_k^T = B_k B_k^T =: D_k$$

This is always possible because $D_k$ is symmetric and positive definite. Now multiply Equation (22) by $L_k^{-1}$:

$$L_k^{-1}\Delta m = L_k^{-1}\underline{1}\Delta\mu + L_k^{-1}B_k\varepsilon \qquad (23)$$

Equation (23) corresponds to a standard linear model

$$Y = X\beta + \varepsilon,$$

with $Y = L_k^{-1}\Delta m, X = L_k^{-1}\underline{1}, \beta = \Delta\mu$ . For this model the least squares estimator is given by [5]

$$\hat{\beta} = (X^T X)^{-1} X^T Y,$$

which gives us

$$\Delta\hat{\mu} = \frac{\underline{1}^T D_k^{-1} \Delta m}{\underline{1}^T D_k^{-1} \underline{1}} = \frac{X^T Y}{X^T X}$$

The variance of the least squares estimator is given by

$$Var(\Delta\hat{\mu}) = \frac{Var(x_{i^*})}{\underline{1}^T D_k^{-1} \underline{1}} = \frac{Var(x_{i^*})}{X^T X}$$

## 4.4 Combination of results from a set of Borda sequences

A weighing scheme consists of several equations, each the result of comparing different combinations of weights. An overdetermined set of equations is then used to calculate the unknown masses $\mu_1$, $\mu_2$, $\mu_3$, $\mu_4$ en $\mu_5$ from the mass $\mu_0$ of one known standard which was part of several combinations.

The overdetermined set of equations can be written in matrix notation as shown in the next example. The values of the matrix have to be either –1, 0 or 1. The –1 indicates that a weight is used as reference, a 0 means the weight is not used in the equation and a 1 shows that the weight is used as part of the test combination.

$$\begin{pmatrix} \Delta m_1 \\ \Delta m_2 \\ . \\ . \\ . \\ \Delta m_j \end{pmatrix} = \begin{pmatrix} -1 & 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 0 & 1 \\ 0 & -1 & 1 & 1 & 1 & 0 \\ . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} \mu_0 \\ \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \end{pmatrix}$$

Because the total nominal mass of the 'reference' combination always equals that of the 'test' combination, the entry for $\mu_0$ can be determined by the other series and can therefore be omitted.

$$\begin{pmatrix} \Delta m_1 \\ \Delta m_2 \\ . \\ . \\ \Delta m_j \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ -1 & 1 & 1 & 1 & 0 \\ . & . & . & . & . \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \end{pmatrix}$$

The vector $\Delta\mu$ has the following form:

$$\Delta\mu = \begin{pmatrix} \Delta\mu_1 \\ \Delta\mu_2 \\ \Delta\mu_3 \\ \Delta\mu_4 \\ \Delta\mu_5 \end{pmatrix} = \begin{pmatrix} \mu_1 - 0.5\mu_0 \\ \mu_2 - 0.2\mu_0 \\ \mu_3 - 0.2\mu_0 \\ \mu_4 - 0.1\mu_0 \\ \mu_5 - 0.1\mu_0 \end{pmatrix}$$

Compared to $\mu$, $\Delta\mu$ is small.

Suppose having a combination of weights characterized by a row vector $w = (w_1, ..., w_5)$. Define for convenience $(M_0, M_1, M_2, M_3, M_4, M_5) = (1, 0.5, 0.2, 0.2, 0.1, 0.1)$, so $\mu_i \approx M_i$, for $0 \le i \le 5$.

Define $w_0 = -\sum_{i=1}^{5} M_i w_i$.

Then $w_0$ has to be either –1,0 or 1. This means that there are essentially only ten possible choices of *w*, not taking into account interchanging between the standard set and the test set (this corresponds to taking –*w*). These ten possible combinations are given in the following matrix W:

$$W = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ -1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 0 & 1 \\ 0 & -1 & 1 & -1 & 1 \\ 0 & -1 & 1 & 1 & -1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 & 1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

Two methods have been used to calculate the deviation from the nominal mass and will be described below.

**Method 1:**

If we take k measurements in the RTR-procedure, we see that equation (23) corresponds to:

$$\Delta m = \underline{1}\, w \Delta\mu + B_k \varepsilon \qquad (24)$$

Equation (24) corresponds to a standard linear model

$Y = X\beta + \varepsilon$,

with $Y = \Delta m, X = \underline{1}w, \beta = \Delta\mu$ .

$\Delta\mu$ can be estimated by repeating the RTR-procedure for a suitable set of different combinations.

A choice of different combinations of weights is called a *weighing scheme*.
A weighing scheme can be represented by a matrix *A*, consisting of different rows $A(l)$, which corresponds to rows from matrix *W*. The matrix *A* consist of max. 14 rows. Each row in *A* corresponds to $k = \max.30$ measurements.

Using a block-matrix notation equation (24) becomes:

$$\begin{pmatrix} \Delta\tilde{m}^{(1)} \\ \vdots \\ \Delta\tilde{m}^{(s)} \end{pmatrix} = \begin{pmatrix} \underline{1} & & \\ & \ddots & \\ & & \underline{1} \end{pmatrix} A\, \Delta\mu$$

To illustrate how to calculate an estimate for $\Delta\mu$, apply Cholesky factorization on $V_{\Delta m}$:

$$LL^T = V_{\Delta m}$$

To obtain $\Delta\mu$, apply QR factorisation on $\widetilde{Y} = \widetilde{X}.\Delta\mu$ and solve this in the least squares sense, where

$$\widetilde{Y} = L^{-1}.Y$$

and

$$\widetilde{X} = L^{-1}.X \ ,$$

where

$$Y = \Delta m$$

and

$$X = \underline{1}.A$$

$$\widetilde{X} = \widetilde{Q}\begin{bmatrix}\widetilde{R}\\ 0\end{bmatrix}$$

$V_{\Delta\mu}$, the uncertainty matrix associated with the solution parameters $\Delta\mu$, is given by

$$V_{\Delta\mu} = UU^T \ ,$$

where $U$ is the solution of the upper triangular system

$$\widetilde{R}_0 U = I \ .$$

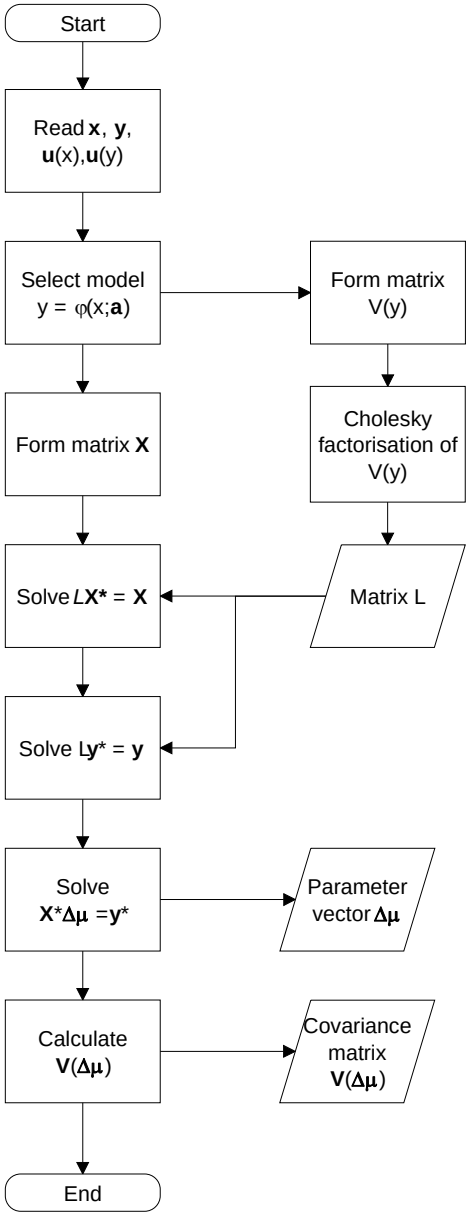


Figure 2929: Flowchart of Method 1

**Method 2:**

Method 2 can be divided in method 2a (Figure 30) and method 2b (Figure 31). Method 2a gives the solution of the system $\widetilde{Y} = \widetilde{X}.a$. The matrix $V_{\Delta m}$ is decomposed to form $LL^T$; $L$ is subsequently used to weigh $X$ and $Y$ and solve the above mentioned system.

To illustrate how to calculate an estimate for $a$, apply Cholesky factorization on $V_{\Delta m}$:

$$LL^T = V_{\Delta m}$$

To obtain $a$, solve $\widetilde{Y} = \widetilde{X}.a$ , where

$\widetilde{Y} = L^{-1}.Y$,

$\widetilde{X} = L^{-1}.X$

and

$a = \frac{\widetilde{X}^T \widetilde{Y}}{\widetilde{X}^T \widetilde{X}}$,

where

$Y = \Delta m$

and

$X = \underline{1}$

$V_a$, the uncertainty matrix associated with the solution parameters $a$, is given by

$V_a = \left(\widetilde{X}^T \widetilde{X}\right)^{-1}$

Method 2b calculates, from the results from each of the weighing series the mass differences of the weights solving the linear system $\widetilde{a} = \widetilde{A}.\Delta\mu$. Where $\widetilde{a}$ is the weighted vector of mass differences obtained from processing series by weighing the weighing results; $\widetilde{A}$ is the weighted matrix of the weighing series (= the weighing scheme). $\Delta\mu$ is the solution vector containing the deviations from nominal mass of the weights. It has the dimension 5: 500 g, 200 g, 200 g·, 100 g, 100 g·.

To illustrate how to calculate an estimate for $\Delta\mu$, apply Cholesky factorization on $V_a$:

$LL^T = V_a$

To obtain $\Delta\mu$, apply QR factorisation on $\widetilde{a} = \widetilde{A}.\Delta\mu$ and solve this in the least squares sense, where

$\widetilde{a} = L^{-1}.a$

and

$\widetilde{A} = L^{-1}.A$,

where

*a* is the parameter obtained by method 2a

and

*A* the matrix of the weighing series

$\widetilde{A} = \widetilde{Q}\begin{bmatrix}\widetilde{R}\\0\end{bmatrix}$

$V_{\Delta\mu}$, the uncertainty matrix associated with the solution parameters $\Delta\mu$, is given by

$V_{\Delta\mu} = UU^T$,

where *U* is the solution of the upper triangular system

$\widetilde{R}_0 U = I$ .

The diagonal of $V_{\Delta\mu}$ gives us the variances of the separate estimators for $\Delta\mu_1,...,\Delta\mu_5$ . The weighing scheme *A* is chosen, such that the variances are minimized in some way. Minimizing the absolute error gives us the following "loss function":

$$L(A) = \sum_{i=1}^{5} V_{\Delta\mu_{ii}}$$

It is wise to minimize the relative error in each weight , so the sum of squares of the relative errors is used as a measure of inaccuracy. Minimizing the relative error gives us the following "loss function":

$$L(A) = \sum_{i=1}^{5} \frac{V_{\Delta\mu_{ii}}}{\Delta\mu_i^2}$$

In the above-mentioned methods the QR factorization is used to solve the system $Y = X.\Delta\mu$ .

To obtain $\Delta\mu$ Singular Value Decomposition can also be applied on $\widetilde{Y} = \widetilde{X}.\Delta\mu$ or $\widetilde{a} = \widetilde{A}.\Delta\mu$ and by solving this in the least squares sense, we get $\widetilde{X} = U.S.V^T$ or $\widetilde{A} = U.S.V^T$

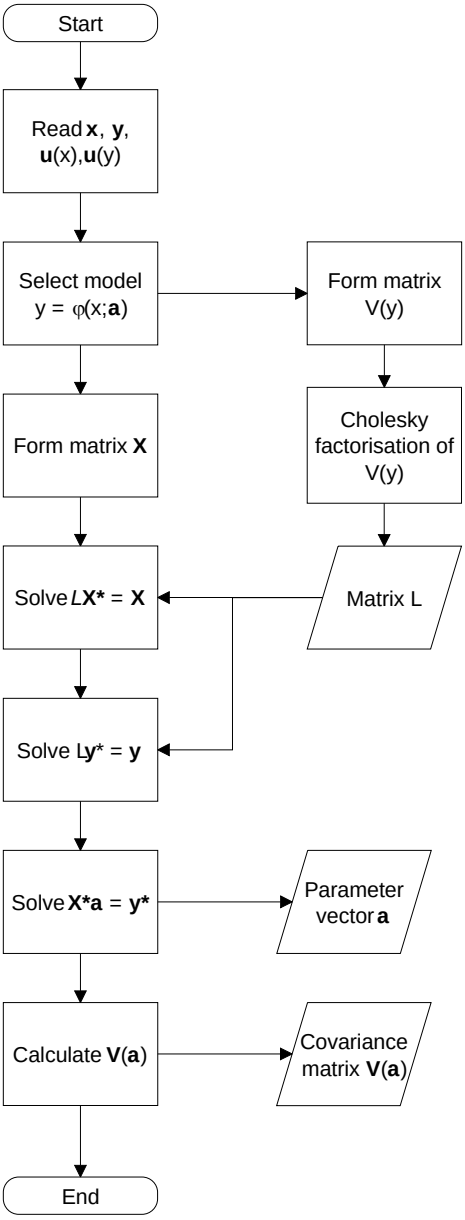


Figure 300: Flowchart of method 2a

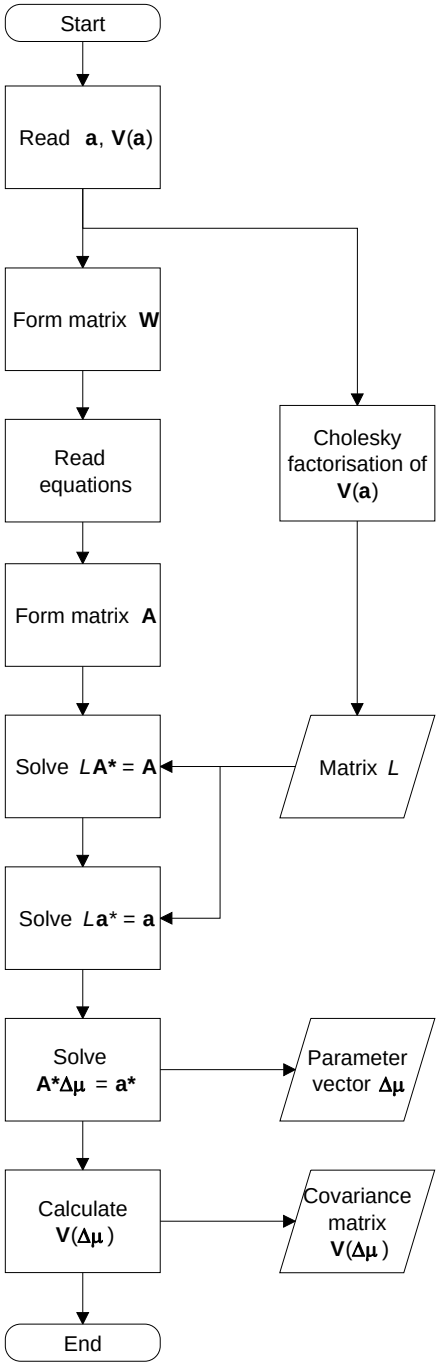


Figure 31: Flowchart of method 2b

## 4.5 Results

Presently NMi uses Gauss-Jordan elimination for the determination of the mass. Gauss-Jordan elimination is a method to find the matrix inverse and is a variation of the Gaussian elimination. Gaussian elimination is used to solve large linear systems numerically. The procedure, which can be found in Appendix E, is numerically unstable unless pivoting (exchanging rows and columns as appropriate) is used. To avoid matrix inverse the Cholesky decomposition is used to decompose the matrix which is numerically very stable, without any pivoting at all. Once the matrix is decomposed, backsubstitution can be used to solve the linear equation.

Both methods (1,2a and 2b) provide the same value for the deviations from the nominal mass of the weights.

Method 1 : $\Delta m = \underline{1} \cdot A \cdot \Delta\mu$

Method 2: $\Delta m = \underline{1} \cdot A \cdot \Delta\mu$

- Method 2a: $\Delta m = \underline{1} \cdot a$
- Method 2b: $a = A \cdot \Delta\mu$

The difference between method 1 and method 2 is that method 1 only give results for the deviations from the nominal mass of the weights ($\Delta\mu$) and method 2 also gives the mass differences obtained from processing series by weighing the weighing results ($\Delta m$).

The datasets of weighing series: BWSData 02-07 (100 mg-1000 mg) and Crosscheck1S3 WS1-WS6 (10 g-100 g) can be found on the accompanying cd. BWS stands for Borda Weighing Scheme.

In the datasets BWSData_02, BWSData_06 and Crosscheck1S3 –WS3 matrix *W* has the following form:

$$W = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ -1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 0 & 1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 & 1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

In these datasets in the matrix *W* the equations 5 and 6 are not used and the equations 1 and 2 are used twice. In the dataset Crosscheck1S3-WS4 the matrix *W* has the following form:

$$W = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ -1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 0 & 1 \\ 0 & -1 & 1 & -1 & 1 \\ 0 & -1 & 1 & 1 & -1 \\ 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 & 1 \end{pmatrix}$$

In this case the matrix *W* does not contain the equations 7 and 10.
In the remaining datasets the original matrix *W*, containing all the equations (once only), is used.

Table 12: deviations from the nominal mass of the weights of 100mg-1000mg from datasets BWSData 02-07

| Test Weight | Delta μ [mg] | | u(delta μ) [mg] | |
|---|---|---|---|---|
| | Gauss-Jordan | Borda weighing | Gauss-Jordan | Borda weighing |
| BWSData-500 mg | -0,008473 | -0,008528 | 0,00027 | 0,000046 |
| | -0,008635 | -0,008695 | 0,00038 | 0,000066 |
| | -0,008431 | -0,008481 | 0,00036 | 0,000058 |
| | -0,008317 | -0,008257 | 0,00039 | 0,000058 |
| | -0,008345 | -0,008334 | 0,00032 | 0,000045 |
| | -0,008402 | -0,008387 | 0,00040 | 0,000056 |
| BWSData-200 mg | -0,011519 | -0,011528 | 0,00035 | 0,000065 |
| | -0,011303 | -0,011322 | 0,00027 | 0,000047 |
| | -0,011361 | -0,011369 | 0,00025 | 0,000038 |
| | -0,011176 | -0,011157 | 0,00026 | 0,000040 |
| | -0,012152 | -0,012156 | 0,00030 | 0,000044 |
| | -0,012160 | -0,012146 | 0,00024 | 0,000040 |
| BWSData-200 mg· | -0,036571 | -0,036610 | 0,00033 | 0,000064 |
| | -0,036175 | -0,036167 | 0,00026 | 0,000044 |
| | -0,036087 | -0,036108 | 0,00025 | 0,000039 |
| | -0,036155 | -0,036150 | 0,00026 | 0,000040 |
| | -0,037109 | -0,037118 | 0,00027 | 0,000041 |
| | -0,037040 | -0,037058 | 0,00024 | 0,000038 |
| BWSData-100 mg | 0,021748 | 0,021769 | 0,00027 | 0,000051 |
| | 0,021752 | 0,021739 | 0,00030 | 0,000049 |
| | 0,021778 | 0,021790 | 0,00028 | 0,000042 |
| | 0,021800 | 0,021851 | 0,00027 | 0,000043 |
| | 0,021701 | 0,021722 | 0,00032 | 0,000049 |
| | 0,021548 | 0,021566 | 0,00030 | 0,000045 |
| BWSData-100 mg· | 0,007272 | 0,007270 | 0,00026 | 0,000050 |
| | 0,006743 | 0,006732 | 0,00029 | 0,000047 |
| | 0,006601 | 0,006589 | 0,00026 | 0,000039 |
| | 0,006691 | 0,006678 | 0,00026 | 0,000042 |
| | 0,006616 | 0,006618 | 0,00033 | 0,000048 |
| | 0,006717 | 0,006714 | 0,00028 | 0,000043 |

Table 13: deviations from the nominal mass of the weights of 10g-100g from datasets Crosscheck1S3 WS1-WS6

| Test Weight | Delta μ [mg] | | u(delta μ) [mg] | |
|---|---|---|---|---|
| | Gauss-Jordan | Borda Weighing | Gauss-Jordan | Borda Weighing |
| Crosscheck1S3-50 g | 0,627600 | 0,627793 | 0,00970 | 0,001183 |
| | 0,627900 | 0,627996 | 0,01000 | 0,001230 |
| | 0,628800 | 0,628264 | 0,00980 | 0,000968 |
| | 0,628100 | 0,628250 | 0,01000 | 0,001292 |
| | 0,628200 | 0,628310 | 0,00980 | 0,001202 |
| | 0,627500 | 0,627648 | 0,00974 | 0,001179 |
| Crosscheck1S3-20 g | 0,369000 | 0,368955 | 0,00410 | 0,000553 |
| | 0,368700 | 0,368902 | 0,00420 | 0,000556 |
| | 0,368800 | 0,368705 | 0,00430 | 0,000591 |
| | 0,368600 | 0,368828 | 0,00450 | 0,000661 |
| | 0,369700 | 0,369783 | 0,00410 | 0,000553 |
| | 0,369500 | 0,369445 | 0,00413 | 0,000544 |
| Crosscheck1S3-20 g· | -0,091300 | -0,091165 | 0,00410 | 0,000581 |
| | -0,091500 | -0,091503 | 0,00420 | 0,000560 |
| | -0,092000 | -0,091961 | 0,00420 | 0,000539 |
| | -0,091600 | -0,091850 | 0,00450 | 0,000663 |
| | -0,091300 | -0,091393 | 0,00410 | 0,000563 |
| | -0,091400 | -0,091295 | 0,00411 | 0,000541 |
| Crosscheck1S3-10 g | 0,142900 | 0,142575 | 0,00260 | 0,000475 |
| | 0,142800 | 0,142945 | 0,00260 | 0,000425 |
| | 0,144600 | 0,144393 | 0,00310 | 0,000683 |
| | 0,144000 | 0,144067 | 0,00300 | 0,000593 |
| | 0,143100 | 0,143045 | 0,00240 | 0,000401 |
| | 0,143600 | 0,143418 | 0,00245 | 0,000395 |
| Crosscheck1S3-10 g· | 0,121300 | 0,121172 | 0,00260 | 0,000473 |
| | 0,120400 | 0,120495 | 0,00260 | 0,000424 |
| | 0,119400 | 0,119635 | 0,00320 | 0,000696 |
| | 0,119800 | 0,120071 | 0,00360 | 0,000611 |
| | 0,120700 | 0,120739 | 0,00250 | 0,000403 |
| | 0,120900 | 0,121188 | 0,00240 | 0,000395 |

The results gained by the datasets can be found in Appendix F. The uncertainty of $\Delta\mu$ determined by Borda weighing is much smaller than the uncertainty determined by Gauss-Jordan. All the values for $\Delta\mu$ determined by Gauss-Jordan lie in the uncertainty of $\Delta\mu$ determined by Borda weighing, this holds for all datasets.

Table 14: Mass differences of the weights 100mg-1000mg

| Dataset | Mass difference [mg] | | u(mass difference) [mg] | |
|---|---|---|---|---|
| | Gauss-Jordan | Borda Weighing | Gauss-Jordan | Borda Weighing |
| BWSData_02: | -0.035148 | -0.035111 | 0.000734 | 0.000193 |
| | -0.03441 | -0.034523 | 0.000373 | 0.000141 |
| | -0.049434 | -0.049493 | 0.000389 | 0.000123 |
| | -0.049416 | -0.049484 | 0.000335 | 0.000112 |
| | -0.018039 | -0.018029 | 0.000235 | 0.000098 |
| | -0.032193 | -0.032204 | 0.000221 | 0.000083 |
| | -0.025192 | -0.025259 | 0.000391 | 0.000145 |
| | 0.040673 | 0.040736 | 0.000383 | 0.000142 |
| | 0.065506 | 0.065496 | 0.000304 | 0.000135 |
| | -0.01452 | -0.014541 | 0.00021 | 0.000080 |
| BWSData_03: | -0.034783 | -0.034718 | 0.000612 | 0.000171 |
| | -0.049262 | -0.049338 | 0.000308 | 0.000110 |
| | -0.017068 | -0.017020 | 0.000308 | 0.000120 |
| | -0.032132 | -0.032109 | 0.000376 | 0.000142 |
| | -0.039959 | -0.039911 | 0.000284 | 0.000104 |
| | -0.00996 | -0.010000 | 0.000284 | 0.000129 |
| | -0.024547 | -0.024621 | 0.000404 | 0.000141 |
| | 0.039831 | 0.039883 | 0.000448 | 0.000148 |
| | 0.064648 | 0.064592 | 0.000352 | 0.000107 |
| | -0.015148 | -0.015163 | 0.000347 | 0.000118 |
| BWSData_04: | -0.033987 | -0.033880 | 0.000557 | 0.000151 |
| | -0.049309 | -0.049487 | 0.000295 | 0.000097 |
| | -0.017105 | -0.017109 | 0.000363 | 0.000129 |
| | -0.032506 | -0.032472 | 0.003 | 0.000105 |
| | -0.039734 | -0.039725 | 0.000401 | 0.000132 |
| | -0.009567 | -0.009573 | 0.000415 | 0.000136 |
| | -0.024752 | -0.024784 | 0.000262 | 0.000087 |
| | 0.039703 | 0.039722 | 0.000255 | 0.000078 |
| | 0.0645 | 0.064519 | 0.000239 | 0.000087 |
| | -0.015138 | -0.015152 | 0.000423 | 0.000110 |
| BWSData_05: | -0.033573 | -0.033409 | 0.000386 | 0.000107 |
| | -0.049118 | -0.049150 | 0.000296 | 0.000100 |
| | -0.017016 | -0.017059 | 0.000548 | 0.000149 |
| | -0.03241 | -0.032452 | 0.000364 | 0.000111 |
| | -0.040066 | -0.040067 | 0.000297 | 0.000100 |
| | -0.009969 | -0.009980 | 0.000434 | 0.000127 |
| | -0.024876 | -0.024938 | 0.000287 | 0.000104 |
| | 0.039573 | 0.039631 | 0.000311 | 0.000104 |
| | 0.064732 | 0.064737 | 0.0003 | 0.000108 |
| | -0.015002 | -0.015024 | 0.00025 | 0.000105 |
| | -0.035688 | -0.035627 | 0.00058 | 0.000174 |
| | -0.035892 | -0.035905 | 0.000333 | 0.000103 |
| | -0.051106 | -0.051118 | 0.000443 | 0.000123 |
| | -0.051004 | -0.050976 | 0.00028 | 0.000089 |

| Dataset | Mass difference [mg] | | u(mass difference) [mg] | |
|---|---|---|---|---|
| | Gauss-Jordan | Borda Weighing | Gauss-Jordan | Borda Weighing |
| BWSData_06: | -0.019324 | -0.019317 | 0.000356 | 0.000096 |
| | -0.034196 | -0.034207 | 0.000348 | 0.000103 |
| | -0.024993 | -0.025006 | 0.000253 | 0.000078 |
| | 0.040586 | 0.040609 | 0.000456 | 0.000125 |
| | 0.065387 | 0.065393 | 0.000264 | 0.000095 |
| | -0.015107 | -0.015176 | 0.000444 | 0.000134 |
| | -0.035899 | -0.035812 | 0.000619 | 0.000147 |
| | -0.050934 | -0.050974 | 0.000348 | 0.000098 |
| | -0.019182 | -0.019202 | 0.000383 | 0.000113 |
| | -0.034132 | -0.034144 | 0.00033 | 0.000102 |
| BWSData_07: | -0.039617 | -0.039603 | 0.000401 | 0.000138 |
| | -0.01023 | -0.010244 | 0.000476 | 0.000145 |
| | -0.024872 | -0.024913 | 0.00016 | 0.000080 |
| | 0.040415 | 0.040433 | 0.000316 | 0.000109 |
| | 0.065311 | 0.065333 | 0.00026 | 0.000089 |
| | -0.014927 | -0.014905 | 0.000429 | 0.000127 |

Table 15: mass differences of the weights 10g-100g

| Dataset | Mass difference [mg] | | u(mass difference) [mg] | |
|---|---|---|---|---|
| | Gauss-Jordan | Borda Weighing | Gauss-Jordan | Borda Weighing |
| | 0.72193 | 0.722203 | 0.001775 | 0.002957 |
| | 0.698775 | 0.698708 | 0.001767 | 0.002962 |
| | -0.206451 | -0.207261 | 0.001793 | 0.001575 |
| | -0.229133 | -0.228992 | 0.001882 | 0.001548 |
| Crosscheck1S3-WS1 | -0.481336 | -0.481125 | 0.001625 | 0.001041 |
| | -0.439015 | -0.438794 | 0.001561 | 0.000996 |
| | -0.46028 | -0.460012 | 0.001593 | 0.000845 |
| | -0.105501 | -0.105587 | 0.002305 | 0.000925 |
| | 0.356384 | 0.356333 | 0.002548 | 0.001790 |
| | -0.021733 | -0.021520 | 0.001678 | 0.000673 |
| | 0.72202 | 0.722367 | 0.002774 | 0.003027 |
| | 0.697758 | 0.697869 | 0.002379 | 0.003018 |
| | -0.207949 | -0.207836 | 0.003921 | 0.001758 |
| | -0.230189 | -0.229933 | 0.002958 | 0.001687 |
| Crosscheck1S3-WS2 | -0.482178 | -0.482151 | 0.001673 | 0.001002 |
| | -0.438074 | -0.437997 | 0.001905 | 0.001024 |
| | -0.46126 | -0.460349 | 0.001599 | 0.000759 |
| | -0.105894 | -0.105919 | 0.001495 | 0.000777 |
| | 0.355743 | 0.355485 | 0.002209 | 0.000846 |
| | -0.022709 | -0.022899 | 0.001839 | 0.000807 |
| | 0.7223 | 0.722993 | 0.002793 | 0.002947 |
| | 0.724041 | 0.723324 | 0.00183 | 0.002948 |
| | 0.697909 | 0.697809 | 0.002109 | 0.002962 |
| | 0.695912 | 0.695708 | 0.00391 | 0.003164 |
| Crosscheck1S3-WS3 | -0.208281 | -0.208529 | 0.002094 | 0.001643 |

| Dataset | Mass difference [mg] | | u(mass difference) [mg] | |
|---|---|---|---|---|
| | Gauss-Jordan | Borda Weighing | Gauss-Jordan | Borda Weighing |
| | -0.230435 | -0.230149 | 0.003535 | 0.001828 |
| | -0.46076 | -0.460742 | 0.001326 | 0.000825 |
| | -0.104696 | -0.104382 | 0.004869 | 0.001626 |
| | 0.355988 | 0.355894 | 0.001806 | 0.000926 |
| | -0.025466 | -0.025470 | 0.00385 | 0.001436 |
| Crosscheck1S3-WS4 (Muylwijk serie) | 0.722064 | 0.722700 | 0.00229 | 0.002978 |
| | 0.69783 | 0.697766 | 0.005664 | 0.003415 |
| | -0.206874 | -0.206890 | 0.002826 | 0.001756 |
| | -0.231532 | -0.231561 | 0.003831 | 0.001872 |
| | -0.484392 | -0.484433 | 0.002964 | 0.001400 |
| | -0.436518 | -0.436757 | 0.004784 | 0.001736 |
| | -0.104822 | -0.104752 | 0.001399 | 0.000783 |
| | 0.355349 | 0.356055 | 0.001817 | 0.000823 |
| Crosscheck1S3-WS5 | 0.723169 | 0.723611 | 0.001679 | 0.002977 |
| | 0.699214 | 0.699557 | 0.002373 | 0.003006 |
| | -0.206958 | -0.206999 | 0.002325 | 0.001626 |
| | -0.229064 | -0.229059 | 0.002257 | 0.001607 |
| | -0.4831 | -0.483605 | 0.001204 | 0.000987 |
| | -0.438431 | -0.438508 | 0.001675 | 0.001116 |
| | -0.461276 | -0.461218 | 0.001476 | 0.000919 |
| | -0.106179 | -0.106061 | 0.001528 | 0.000733 |
| | 0.355702 | 0.355272 | 0.001983 | 0.000911 |
| | -0.022448 | -0.022141 | 0.001767 | 0.000595 |
| Crosscheck1S3-WS6 | 0.7232 | 0.723517 | 0.002241 | 0.002943 |
| | 0.698929 | 0.698680 | 0.001572 | 0.002949 |
| | -0.205455 | -0.205488 | 0.001927 | 0.001566 |
| | -0.228629 | -0.228898 | 0.001462 | 0.001560 |
| | -0.48284 | -0.482763 | 0.002197 | 0.001056 |
| | -0.437989 | -0.438151 | 0.002374 | 0.001064 |
| | -0.461219 | -0.461109 | 0.001947 | 0.000793 |
| | -0.105111 | -0.104786 | 0.001509 | 0.000812 |
| | 0.356062 | 0.355854 | 0.00117 | 0.000752 |
| | -0.022341 | -0.022045 | 0.001544 | 0.000596 |

The uncertainty of $\Delta m$ determined by Borda weighing is also much smaller than the uncertainty determined by Gauss-Jordan. All the values for $\Delta m$ determined by Gauss-Jordan lie in the uncertainty of $\Delta m$ determined by Borda weighing, this also holds for all datasets.

On the base of the results using these datasets it can be said that the value of $\Delta\mu$ and $\Delta m$ determined by Borda weighing are good but that the uncertainty of $\Delta\mu$ and $\Delta m$ determined by Borda weighing are too small.

Table 16: Relative weighted residuals of 100mg-1000mg

| Equation | #02 | #03 | #04 | #05 | #06 | #07 |
|---|---|---|---|---|---|---|
| 1 | -1,11 | -1,60 | 1,91 | **2,85** | 1,49 | 1,46 |
| 2 | **2,66** | 1,03 | -1,21 | **-2,65** | -0,19 | -0,98 |
| 3 | -0,78 | 0,29 | 0,75 | 0,95 | -1,04 | 0,44 |
| 4 | -0,77 | -0,34 | -0,61 | -0,71 | 0,16 | -0,40 |
| 5 | -1,93 | -0,57 | 1,63 | 0,98 | -1,03 | 1,16 |
| 6 | 1,64 | -1,26 | -0,27 | -1,26 | 1,11 | -1,27 |
| 7 | -1,22 | 1,58 | -0,53 | 0,53 | -0,56 | -0,02 |
| 8 | 1,19 | 0,60 | -0,34 | -0,53 | 0,90 | 0,06 |
| 9 | -1,13 | -0,43 | 0,38 | 0,54 | -0,68 | -0,05 |
| 10 | -0,52 | -1,33 | 0,45 | 1,41 | -0,53 | -0,42 |

Table 17: Relative weighted residuals of 10g-100g

| Equation | #01 | #02 | #03 | #04 | #05 | #06 |
|---|---|---|---|---|---|---|
| 1 | 0,35 | 0,34 | 0,20 | 0,14 | 0,29 | 0,44 |
| 2 | -0,35 | -0,34 | 0,31 | -0,16 | -0,29 | -0,44 |
| 3 | 0,11 | -0,10 | 0,06 | 0,18 | -0,08 | 0,38 |
| 4 | -0,10 | 0,10 | -0,61 | -0,19 | 0,08 | -0,38 |
| 5 | 0,38 | 0,70 | -0,85 | 0,17 | -0,12 | 0,20 |
| 6 | -0,08 | -0,04 | 0,95 | -0,04 | 0,32 | 0,34 |
| 7 | 0,13 | 0,07 | -0,09 | -0,08 | -0,05 | -0,46 |
| 8 | -0,41 | -0,59 | 0,18 | 0,081 | -0,08 | 0,07 |
| 9 | 0,79 | 0,64 | -0,10 | | 0,10 | -0,06 |
| 10 | -0,17 | -0,56 | -0,50 | | 0,28 | 0,31 |

The fit can be remarked as a good one, because the residuals of both datasets lie between [-2.0,2.0].

# 5 Conclusions

Instead of hydrostatic weighing there is need of an alternative method to determine the volume of weights. This, because for hydrostatic weighing the weight is immersed in water and not all weights can be immersed in water. Aerostatic weighing might be such an alternative method, because it allows calibrating weights and other artefacts that cannot be immersed in water. The principle of aerostatic weighing is that the apparent mass difference between two artefacts is recorded as a function of the air density. In practice, there is another variable that may influence the measurement, namely the temperature. The temperature not only influences the air density, but also the volumes (cubic expansion) of the artefacts, so that influence needs to be taken into account.

An algorithm has been developed and implemented to process the results from aerostatic weighing. A least squares regression method has been implemented that does not rely on the assumption that one of the coordinates is without uncertainty. In order to propagate the uncertainty associated with the input variables (mass difference and air density), generalised distance regression is used, which weighs the points in the dataset on the basis of the uncertainty associated with the input quantities. The algorithm also takes care of effects of the ambient temperature on the volume of the artefacts.

The difference in true mass of T obtained by aerostatic weighing lies in the confidence interval of the difference in true mass of T obtained by hydrostatic weighing. The difference of the volume of T obtained by aerostatic weighing does not lie in the confidence interval of the difference in volume of T obtained by hydrostatic weighing, On the basis of only two datasets it can not be said that the value of the difference in true mass and the difference in volume of T calculated by aerostatic weighing is good or not. We need more datasets and calculations of the value of the difference in true mass and the difference in volume of T to do so.
After analyzing both datasets of aerostatic weighing it can be concluded that for a better regression the range covered by the air density, the range,  must be expanded.

Mass calibration is done by comparing an unknown weight with a reference mass standard by alternatively placing them on a balance, this is called Borda weighing. Usually, an assembly of weight(s) is calibrated against a (single,) already calibrated artefact. This calibration is realised by using a weighing scheme, i.e., different combinations of weights that are compared among one another. Such a weighing scheme can be designed in numerous ways. The weighing scheme used in the Netherlands for primary calibration is subjected to a rigorous mathematical optimisation.

The optimisation is carried out by first modelling the uncertainty structure of the mass differences experimentally obtained in each Borda sequence. The structure of the resulting covariance matrix is the basis for determining the mass difference in each of the Borda sequences forming the weighing scheme. Several constraints have been put in the optimisation to exclude undesired solutions, such as practically unfeasible weighing schemes. The number of Borda sequences has been limited to 14 and the number of repeated weighings in a sequence has been restricted to 30. The Gauss-Jordan elimination is used by the NMi for the determination of the mass.

The results are that the uncertainty of the deviation from the nominal mass of the weights and the difference in mass determined by Borda weighing is much smaller than the uncertainty determined by Gauss-Jordan. All the values for the deviation from the nominal mass of the weights and the difference in mass determined by Gauss-Jordan lie in the uncertainty determined by Borda weighing, this holds for all datasets. After analyzing the datasets of the weighing series it can be concluded that the value of the deviation from the nominal mass of the weights and the difference in mass obtained with the new model are good but that the uncertainty seems too small in comparison with the observed mass differences. As a result, it was impossible to perform the optimisation and to determine the optimum weighing scheme.

## References


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[4] Van der Veen A.M.H., “Regression analysis in aerostatic weighing”, Nederlands Meetinstituut, Delft, 2005

[5] Bhulai S., Breuer T., Cator E., Dekkers F., “Optimal weighing schemes”, in “Proceedings of the 52nd European Study Group with Industry”, Centrum voor Wiskunde en Informatica, Amsterdam, 2006

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## List of symbols

| | |
|---|---|
| $\mathbf{a}$ | Vector containing the regression coefficients |
| $\mathbf{f}$ | Vector of residuals |
| $\tilde{\mathbf{f}}$ | Vector of weighted residuals |
| $\varphi$ | Regression function |
| $J$ | Jacobian matrix |
| $\tilde{J}$ | Weighted Jacobian matrix |
| $L$ | Lower triangular matrix (from Cholesky factorisation) |
| $p$ | Vector containing an update to the regression coefficients |
| $Q$ | Orthogonal matrix (from $QR$–factorisation) |
| $R$ | Upper triangular matrix (from $QR$–factorisation) |
| $u$ | Standard uncertainty |
| $U$ | Expanded uncertainty |
| $V$ | Covariance matrix |
| $\mathbf{x}$ | Vector of independent variables |
| $\hat{\mathbf{x}}$ | Vector of predicted independent variables |
| $\mathbf{y}$ | Vector of dependent variables |
| $\hat{\mathbf{y}}$ | Vector of predicted dependent variables |

## List of matrices

*Matrix* — a matrix is a rectangular table of numbers. Matrices are used to describe lineair equations, keep track of the coefficients of lineair transformations and to record data that depend on two parameters. Matrices can be added, multiplied and decomposed in various ways

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

*Block matrix* — a matrix partitioned in sub-matrices called blocks

*Diagonal matrix* — a square matrix with all entries off the main diagonal equal to zero

*Block diagonal matrix* — a block matrix with entries only on the diagonal

*Identity matrix* — a diagonal matrix, with all entries on the main equal to 1, and the rest 0

$$I = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} = diag(1)$$

*Orthogonal matrix* — a matrix whose inverse is equal to its transpose, $A^{-1} = A^T$

*Square matrix* — a matrix that have the same number of rows and columns

*Covariance matrix* — Covariance is a parameter that indicates the extent to which two random variables co-vary, it measures the tendency. The covariance between two components $X_i$ and $Y_i$ is denoted by $\mathrm{cov}(X_i, X_j)$ or $\sum i, j$ and is defined by the expectation $\mathrm{cov}(X_i, X_j) = E[(X_i - \mu_i)(X_j - \mu_j)]$, where $\mu_i$ and $\mu_j$ are the means of $X_i$ and $Y_i$. Covariance are symmetric, so $\sum i, j = \sum j, i$. The covariance of any component $X_i$ with itself is that component's variance $\mathrm{cov}(X_i, X_j) = E[(X_i - \mu_i)^2] = \mathrm{var}(X_i)$. A covariance matrix given that summarizes all the covariance's of a vector $\boldsymbol{X}$:

$$\sum = \begin{bmatrix} \sum 1,1 & \sum 1,2 & \cdots & \sum 1,n \\ \sum 2,1 & \sum 2,2 & & \vdots \\ \vdots & & \ddots & \\ \sum n,1 & & \cdots & \sum n,n \end{bmatrix}$$

*Transpose of a matrix* — The transpose of a matrix is formed by turning rows into columns and columns into rows.

$$A^T = \begin{bmatrix} a & c \\ b & d \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}$$

*Inverse of a matrix* The inverse of a square matrix $A$, is a matrix $A^{-1}$ such that $AA^{-1} = I$

$$A^{-1} = \frac{1}{ad - bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = -\frac{1}{2}\begin{bmatrix} 4 & -2 \\ -3 & 1 \end{bmatrix} = \begin{bmatrix} 2 & -1 \\ -1.5 & -0.5 \end{bmatrix}$$

*Vector* a vector is a row or column of numbers

$$V = \begin{bmatrix} 1 & 2 & 3 & 4 \end{bmatrix} \qquad W = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

## Appendix A: CIPM-81/91equation

The CIPM-81/91 equation reads as follows:

$$\rho = \frac{pM_a}{RTZ}\left[1 - x_{moi}\left(1 - \frac{M_w}{M_a}\right)\right] \qquad \text{A-1}$$

where $\rho$ denotes the air density, $M_a$ the molar mass of air, $M_w$ the molar mass of water, $Z$ the compressibility, $R$ the ideal gas constant, and $p$ the pressure. The symbols in equation (C-1) can be expressed as follows

$$x_{moi} = h \cdot f \frac{p^{sat}}{p} \qquad \text{A-2}$$

where $h$ is the relative humidity, $f$ is an enrichment factor, $p^{sat}$ is the vapour pressure of water at saturation and $p$ is the pressure. The enrichment factor $f$ can be expressed as

$$f = 1.00062 + 3.14 \cdot 10^{-8} p + 5.6 \cdot 10^{-7} t^2 \qquad \text{A-3}$$

where $t$ is the temperature in degrees Celsius. The saturation pressure of water has been expressed as follows

$$p^{sat} = \exp\left[AT^2 + BT + C + \frac{D}{T}\right] \qquad \text{A-4}$$

The coefficients of this equation (A, B, C, and D) are given in table 1 and $T$ is the absolute temperature in Kelvin. If instead of the humidity, the dewpoint temperature is measured, equation A-2, A-3 and A-4 must be replaced by

$$x_{moi} = f_{dp} \frac{p_{dp}}{p} \qquad \text{A-5}$$

$$f_{dp} = 1.00062 + 3.14 \cdot 10^{-8} p + 5.6 \cdot 10^{-7} {t_{dp}}^2 \qquad \text{A-6}$$

$$p_{dp} = \exp\left[A{T_{dp}}^2 + BT_{dp} + C + \frac{D}{T_{dp}}\right] \qquad \text{A-7}$$

with $T_{dp}$ and $t_{dp}$ the dewpoint temperature in Kelvin and Celsius respectively.

The molar mass of air ($M_a$) can be expressed as

$$M_a = \left[28{,}9635 + 12{,}011\left(x_{CO_2} - 0{,}0004\right)\right] \cdot 10^{-3} \qquad \text{A-8}$$

where $M_a$ is the mole fraction of dry air in g/mol. $x_{CO2}$ is the mole fraction $CO_2$ in the air. The equation for the compressibility of air reads as

$$Z = 1 - \frac{p}{T}\left[a_0 + a_1 t + a_2 t^2 + x_{moi}\left(b_0 + b_1 t\right) + x_{moi}^2\left(c_0 + c_1 t\right)\right] + \frac{p^2}{T^2}\left(d + e x_{moi}^2\right) \qquad \text{A-9}$$

Equation (A-1) is the best fit of several measurements and thus causes an uncertainty in the air density due to the equation itself. According to [1] this (average) relative standard uncertainty is $1 \cdot 10^{-4}$. This extra uncertainty is not taken into account for normal mass calibrations on the principle that if everybody neglects it, there is no effect on the comparison between masses. However, when the air density is used in aerostatic weighing to calculate the volume of weights, this uncertainty component can not be ignored any longer [4].

Table 18: Values of the coefficients used in equations

| Coefficient | Unit | Value |
|---|---|---|
| R | $J\ mol^{-1}\ K^{-1}$ | 8.314510 |
| A | $K^{-2}$ | $1.2378847 \cdot 10^{-5}$ |
| B | $K^{-1}$ | $-1.9121316 \cdot 10^{-2}$ |
| C | | 33.93711047 |
| D | K | $-6.3431645 \cdot 10^{3}$ |
| $a_0$ | $K\ Pa^{-1}$ | $1.58123 \cdot 10^{-6}$ |
| $a_1$ | $Pa^{-1}$ | $-2.9331 \cdot 10^{-8}$ |
| $a_2$ | $K^{-1}\ Pa^{-1}$ | $1.1043 \cdot 10^{-10}$ |
| $b_0$ | $K\ Pa^{-1}$ | $5.707 \cdot 10^{-6}$ |
| $b_1$ | $Pa^{-1}$ | $-2.051 \cdot 10^{-8}$ |
| $c_0$ | $K\ Pa^{-1}$ | $1.9898 \cdot 10^{-4}$ |
| $c_1$ | $Pa^{-1}$ | $-2.376 \cdot 10^{-6}$ |
| d | $K^2\ Pa^{-2}$ | $1.83 \cdot 10^{-11}$ |
| e | $K^2\ Pa^{-2}$ | $-0.765 \cdot 10^{-8}$ |
| $M_w$ | $g\ mol^{-1}$ | 18.0152 |

## Appendix B: Mass difference

The last input variable for the regression is the mass difference between mass standard and test weight determined by Borda-weighing. For ordinary mass calibrations the mass differences need to be corrected for air buoyancy. For aerostatic weighing the uncorrected mass difference $\Delta m_j$ is required

$$\Delta m = m_R - m_T$$

where $m_R$ is the balance reading when the mass standard is weighed and $m_T$ the balance reading when the test weight is on the scale. The mass standard and test weight placed alternately on the balance scale (using the so-called RTR method) and the whole weighing process, including reading the balance and environmental conditions, is automatized.
Because the display value of a balance always shows a small drift, a single balance reading for mass standard and test weight would not be representative. Therefore 11 weighings of the mass standard and 10 for the test weight are performed per cyclus (also called a group). After each cyclus of 21 weighings the process is repeated. The mass differences between individual weighings of a cyclus are determined by

$$\Delta m_j = m_{T_j} - \frac{m_{R_i} + m_{R_{i+1}}}{2} \quad \text{for odd values of } i$$

$$\Delta m_j = \frac{m_{T_j} + m_{T_{j+1}}}{2} - m_{R_{j+1}} \quad \text{for even values of } i$$

From the the 21 weighings per cyclus, 19 mass differences can be determined and this results in an average mass difference $\Delta\overline{m}$ for the cyclus

$$\Delta\overline{m} = \frac{\sum_{i=1}^{n} \Delta m_j}{n}$$

In this case $n$ = 19. Mass measurements are independent from the other input variables, so no correlations have to be taken into account. Though mass measurement cycli are independent of each other, there is a correlation between the individual mass differences within a group. With a correction factor for this correlation can be calculated. This correction factor approaches unity when the number of measurements increases. So because each cyclus contains 19 correlated measurements, this correction factor is generally negligible.
To incorporate an extra 'safety margin' also the 'normal' standard deviation $s$ calculated by

$$s = \sqrt{\frac{\sum_{i=1}^{n} \left(\Delta m_j - \Delta\overline{m}\right)^2}{n-1}}$$

is used in stead of $\sigma$, the standard deviation to the mean, which is given by

$$\sigma = \frac{s}{\sqrt{n}}$$

In principle the same approach will be used for aerostatic weighing, because apart from the volumes, also the true mass will be determined and it is best to use the same approach for the uncertainty analysis for all mass calibrations, regardless the method. Because of this 'safety margin' and the relative large number of measurements per cyclus, the correction factor due to correlations will be assumed negligible for now [4].

# Appendix C: Hydrostatic weighing

By determination of the conventional mass of an object in air and then in double distillated water, the air buoyancy and thus the volume and density of an object can be determined with the founded difference in mass. A different type of balance is used for the weighings. This balance is adjusted to accomplish hydrostatic weighings and is placed above a glass with double distillated water (see Fig. 32).

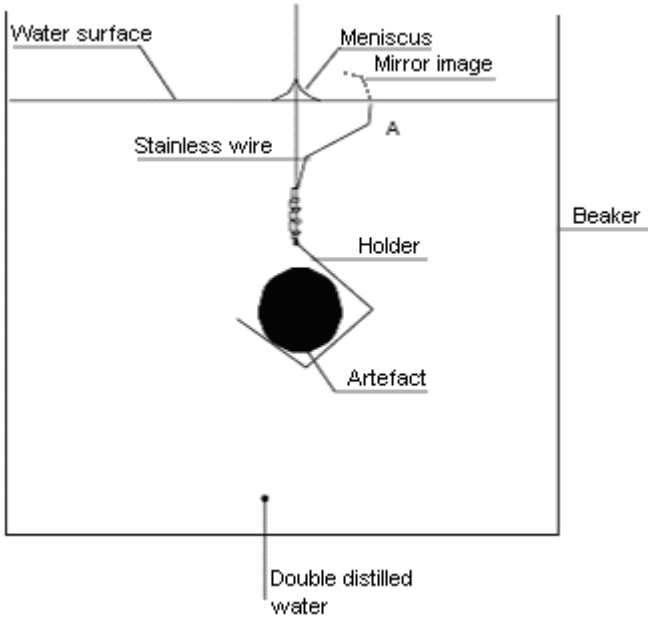



Figure 312: Hydrostatic weighing

To determine the volume of weights we mostly make use of once-only hydrostatic weighing. The disadvantage of hydrostatic weighing is that measurements cannot be repeated without losing the 'history' of the weights. Since by immersing in water the 'grow ' at the outer layer will be washed away and the regularly grow pattern will be disturbed.

Due to the disadvantages of hydrostatic weighing, aerostatic weighing is developed. This measurement is repeatable; the accuracy is comparable and is possibly even bigger than hydrostatic weighing.

# Appendix D: Matrix factorisations

## Cholesky decomposition

If a square matrix $A$ happens to be symmetric and positive definite, associated linear equations are often solved using Cholesky decomposition [3]. Symmetric means that $a_{ij} = a_{ji}$ for $i, j = 1,...,n$, while positive definite means that $v^T A v > 0$ for all vectors $v$.

Cholesky decomposition constructs a lower triangular matrix $L$ whose transpose $L^T$ can itself serve as the upper triangular part.

$$LL^T = A$$

This factorization is sometimes referred to as "taking the square root" of the matrix $A$. The components of $L^T$ are of course related to that of $L$ by

$$L_{ij}^T = L_{ji}$$

If we write out the equation $LL^T = A$, we obtain the following formula for the entries of $L$:

$$L_{ii} = \sqrt{\left( a_{ii} - \sum_{k=1}^{i-1} L_{ik}^2 \right)}$$

and

$$L_{ji} = \frac{1}{L_{ii}} \left( a_{ij} - \sum_{k=1}^{i-1} L_{ik} L_{jk} \right) \quad j = i+1, i+2, ...., n$$

## QR factorisation

Assume having the following overdetermined system $X\mathbf{a} = \mathbf{y}$.

The QR-factorisation of matrix $X$ is given by

$$X = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$$

where $X$ is an $n \times n$ orthogonal matrix and $R$ is an $m \times m$ upper triangular matrix. Using the fact that $\left\| Q^T \mathbf{x} \right\| = \left\| \mathbf{x} \right\|$, one gets

$$\left\| \mathbf{y} - X\mathbf{a} \right\| = \left\| Q^T \mathbf{y} - Q^T X\mathbf{a} \right\| = \left\| \begin{bmatrix} \mathbf{q_1} \\ \mathbf{q_2} \end{bmatrix} - \begin{bmatrix} R \\ 0 \end{bmatrix} \mathbf{a} \right\|$$

where $\mathbf{q_1}$ are the first $n$ and $\mathbf{q}_2$ are the second $m - n$ elements of $Q^T \mathbf{y}$. The minimisation problem is solved if **a** solves the upper triangular system

$$R\mathbf{a} = \mathbf{q_1}$$

The covariance matrix associated with **a** is given by

$$V_a = \sigma^2 \left( UU^T \right)$$

where $U$ solves the upper triangular system

$$RU = I$$

where $I$ is the identity matrix.

### Singular Value Decomposition

Assume having the following overdetermined system $X\mathbf{a} = \mathbf{y}$.

The SVD of matrix $X$ is given by

$$\begin{pmatrix} \\ X \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \mathbf{U} \\ \\ \end{pmatrix} \begin{pmatrix} W_1 & & \\ & \ddots & \\ & & W_m \end{pmatrix} \begin{pmatrix} \\ \mathbf{V^T} \\ \\ \end{pmatrix}$$

where **U** is an $n \times m$ column orthogonal matrix, the matrix **W** is an $m \times m$ diagonal matrix containing the singular values, and **V** is an $m \times m$ orthogonal matrix.

Given

$$X = \mathbf{U}\mathbf{W}\mathbf{V}^{\mathbf{T}}$$

the inverse of $X$ can be expressed as

$$X^{-1} = \mathbf{V}\left[\mathrm{diag}\left(1/W_j\right)\right]\mathbf{U}^{\mathbf{T}}$$

and hence, given the system

$$\begin{pmatrix} \\ X \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{a} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ y \\ \\ \end{pmatrix}$$

the solution **a** can be expressed as follows

$$\begin{pmatrix} \\ \mathbf{a} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \mathbf{V} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{diag}\left(1/w_j\right) \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{U^T} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{y} \\ \\ \end{pmatrix}$$

The covariance matrix $\mathbf{V_a}$ associated with the solution parameters **a** is given by $V_a = \sigma^2\left(X^T X\right)^{-1}$.

## Appendix E: Gauss-Jordan Elimination

Solving linear equations numerically is done by manipulating the given matrix using the elementary row operations to put the matrix into row echelon form [7]. To be in row echelon form, a matrix must conform to the following criteria:

- If a row does not consist entirely of zeros, then the first non zero number in the row is a 1.(the leading 1)
- If there are any rows entirely made up of zeros, then they are grouped at the bottom of the matrix.
- In any two successive rows that do not consist entirely of zeros, the leading 1 in the lower row occurs farther to the right that the leading 1 in the higher row.

From this form, the solution is easily(relatively) derived. The variation made in the Gauss-Jordan method is called back substitution. Back substitution consists of taking a row echelon matrix and operating on it in reverse order. Normally the matrix is simplified from top to bottom to achieve row echelon form. When Gauss-Jordan has finished, all that remains in the matrix is a main diagonal of ones and the augmentation, this matrix is now in reduced row echelon form. For a matrix to be in reduced row echelon form, it must be in row echelon form and submit to one added criteria:

- Each column that contains a leading 1 has zeros everywhere else.

Since the matrix is representing the coefficients of the given variables in the system, the augmentation now represents the values of each of those variables. The solution to the system can now be found by inspection and no additional work is required. Consider the following example:

Start with placing $\begin{cases} x+y+2z=8 \\ -x-2y+3z=1 \\ 3x-7y+4z=10 \end{cases}$ into an augmented matrix $\left[\begin{array}{ccc|c} 1 & 1 & 2 & 8 \\ -1 & -2 & 3 & 1 \\ 3 & -7 & 4 & 10 \end{array}\right]$

$\left[\begin{array}{ccc|c} 1 & 1 & 2 & 8 \\ -1 & -2 & 3 & 1 \\ 3 & -7 & 4 & 10 \end{array}\right]$ $R2-(-1)R1 \rightarrow R2$, $R3-(3)R1 \rightarrow R3$ $\left[\begin{array}{ccc|c} 1 & 1 & 2 & 8 \\ 0 & -1 & 5 & 9 \\ 0 & -10 & -2 & -14 \end{array}\right]$

$\left[\begin{array}{ccc|c} 1 & 1 & 2 & 8 \\ 0 & -1 & 5 & 9 \\ 0 & -10 & -2 & -14 \end{array}\right]$ $(-1)R2 \rightarrow R2$, $R3-(-10)R2 \rightarrow R3$ $\left[\begin{array}{ccc|c} 1 & 1 & 2 & 8 \\ 0 & 1 & -5 & -9 \\ 0 & 0 & -52 & -104 \end{array}\right]$

$\left[\begin{array}{ccc|c} 1 & 1 & 2 & 8 \\ 0 & 1 & -5 & -9 \\ 0 & 0 & -52 & -104 \end{array}\right]$ $\left(-\frac{1}{52}\right)R3 \rightarrow R3$, *In row echelon form* $\rightarrow$ $\left[\begin{array}{ccc|c} 1 & 1 & 2 & 8 \\ 0 & 1 & -5 & -9 \\ 0 & 0 & 1 & 2 \end{array}\right]$

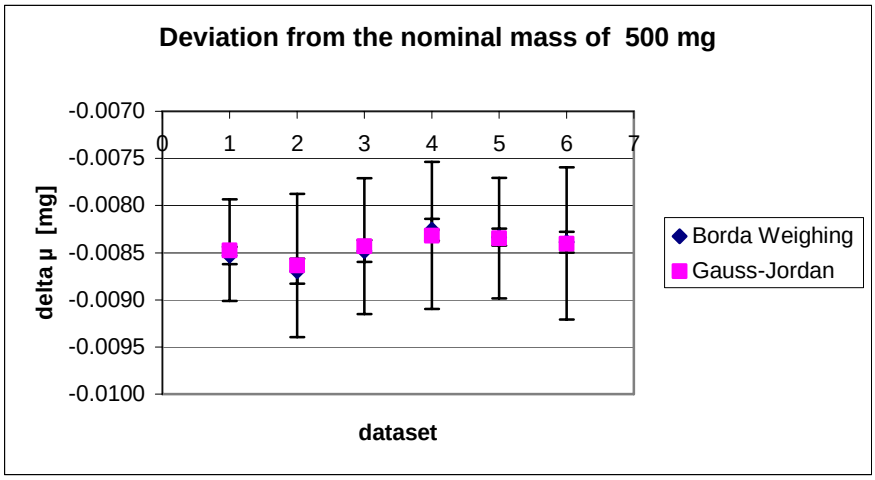
$\left[\begin{array}{ccc|c} 1 & 1 & 2 & 8 \\ 0 & 1 & -5 & -9 \\ 0 & 0 & 1 & 2 \end{array}\right]$ $R2-(-5)R3 \rightarrow R2$, $R1-(2)R3 \rightarrow R1$ $\left[\begin{array}{ccc|c} 1 & 1 & 0 & 4 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 2 \end{array}\right]$

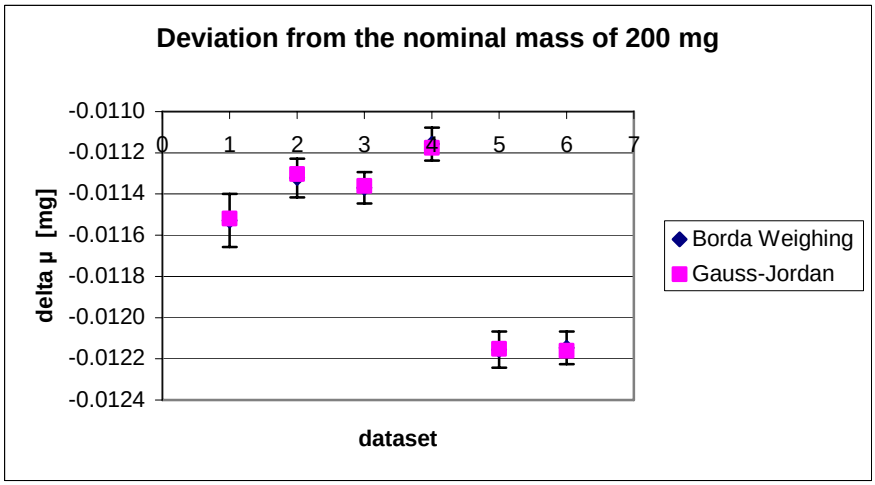
$$\left[\begin{array}{ccc|c} 1 & 1 & 0 & 4 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 2 \end{array}\right] \qquad \begin{array}{l} R1 - R2 \rightarrow R1 \\ In\ reduced\ row\ echelon\ \ form \rightarrow \end{array} \left[\begin{array}{ccc|c} 1 & 0 & 0 & 3 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 2 \end{array}\right]$$

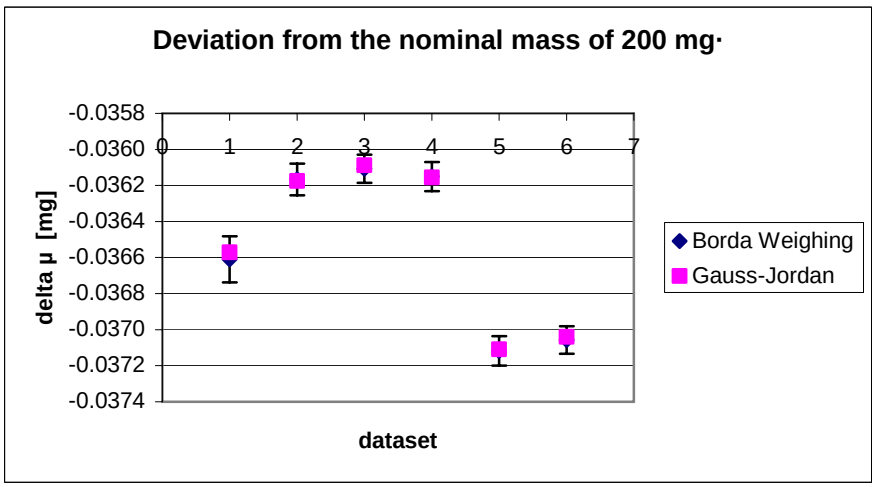
The solution to this linear system is x = 3, y = 1, and z = 2.
There are some problems that could arise while searching for these solutions. If the lines are parallel then they will not intersect and thus provide no solution. In three dimensions the problem of skewing is possible. Lines are skewed if they lie in parallel planes yet have different slopes. If this problem occurs, it will made evident in the matrix by a row (or more than one) of zeros being present when the matrix is in row echelon form. Another problem that may arise is a division by zero. If a zero is placed in the main diagonal of the row being operated on, when you divide that row by the diagonal number the division by zero error will occur. To trap this error, simply check the diagonal number being worked with. If it is zero, exchange that row with the row below it. Exchanging rows is a legal elementary row operation.

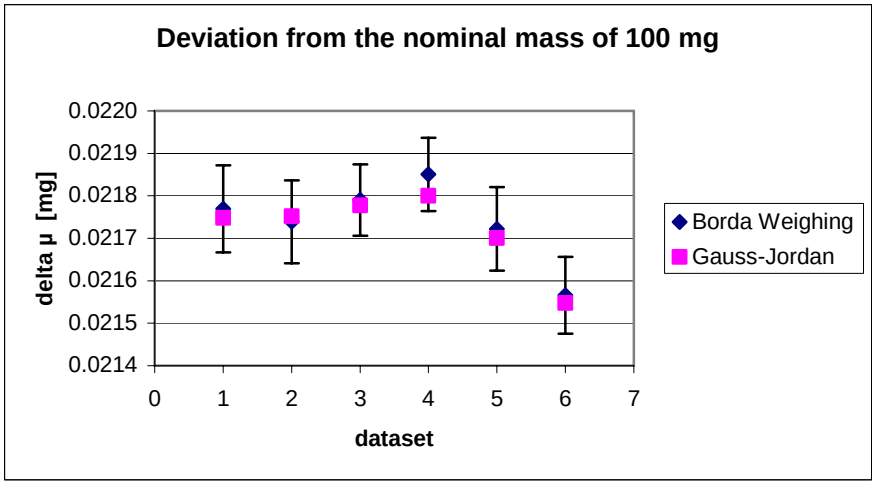
If a matrix is ill-conditioned, bad round off errors may occur. Since a large number of multiplications and divisions are performed, if the numbers are not of relative size then round off error will be apparent. If the matrix is small then the error won't have time to propagate; but if the matrix is large, the round off error could deem the output solution unreliable.

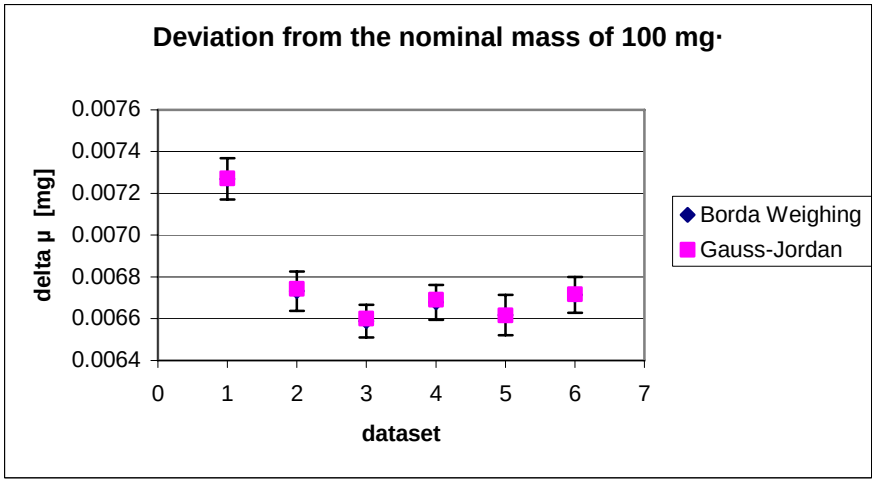
# Appendix F: Results datasets weighing series

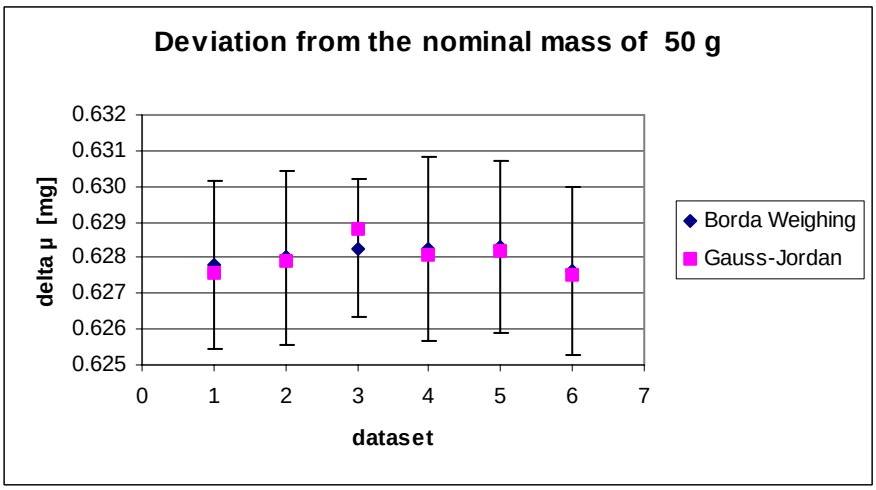


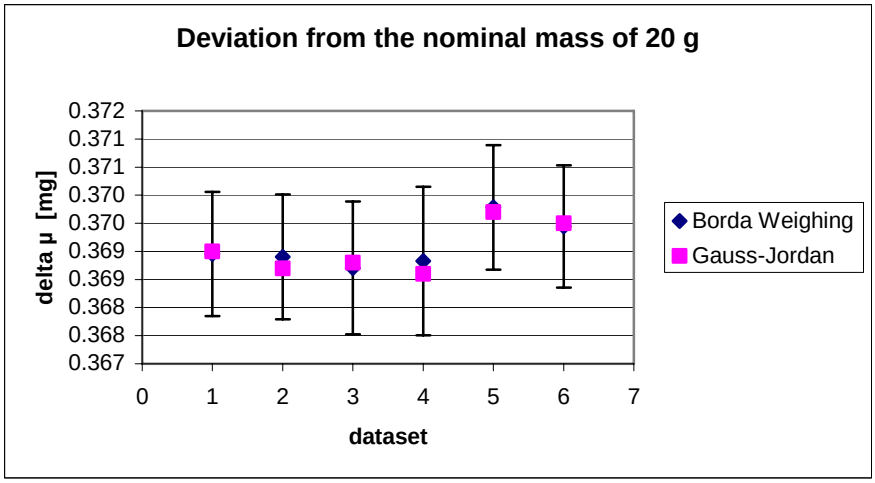



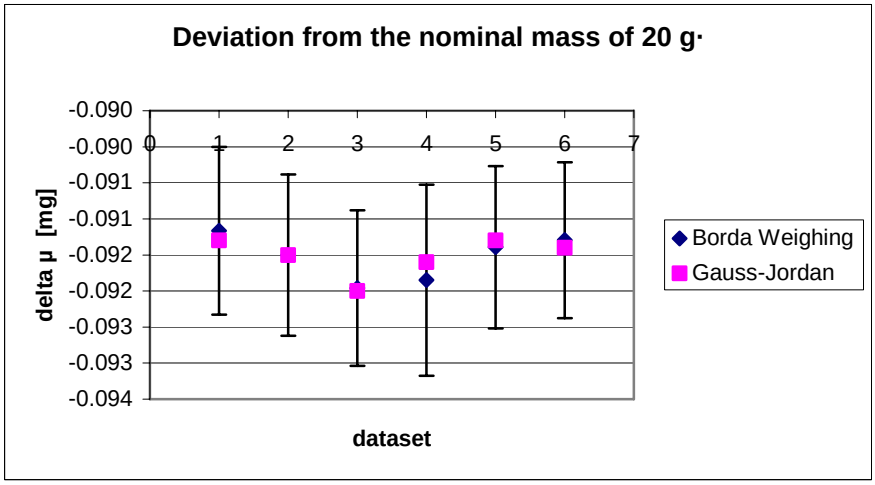



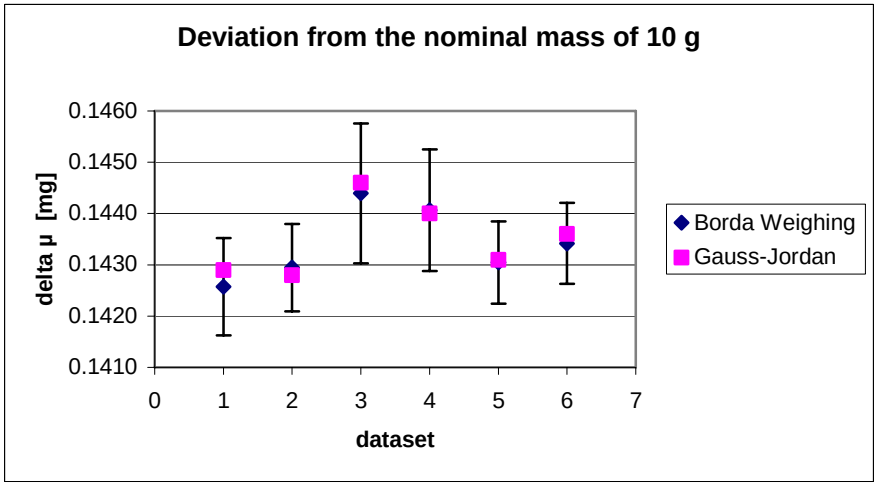

Deviation from the nominal mass of 100 mg
delta µ [mg]
0.0220
0.0219
0.0218
0.0217
0.0216
0.0215
0.0214
0 1 2 3 4 5 6 7
dataset
Borda Weighing
Gauss-Jordan

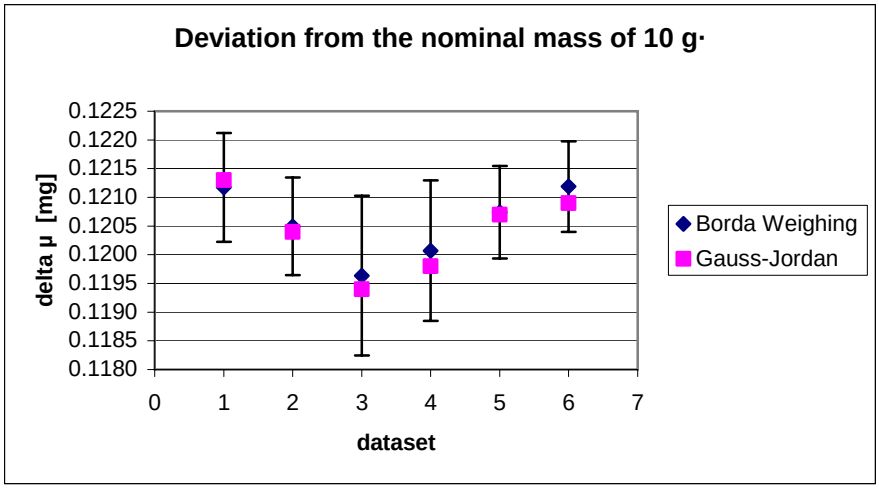

Deviation from the nominal mass of 100 mg·
delta µ [mg]
0.0076
0.0074
0.0072
0.0070
0.0068
0.0066
0.0064
0 1 2 3 4 5 6 7
dataset
Borda Weighing
Gauss-Jordan

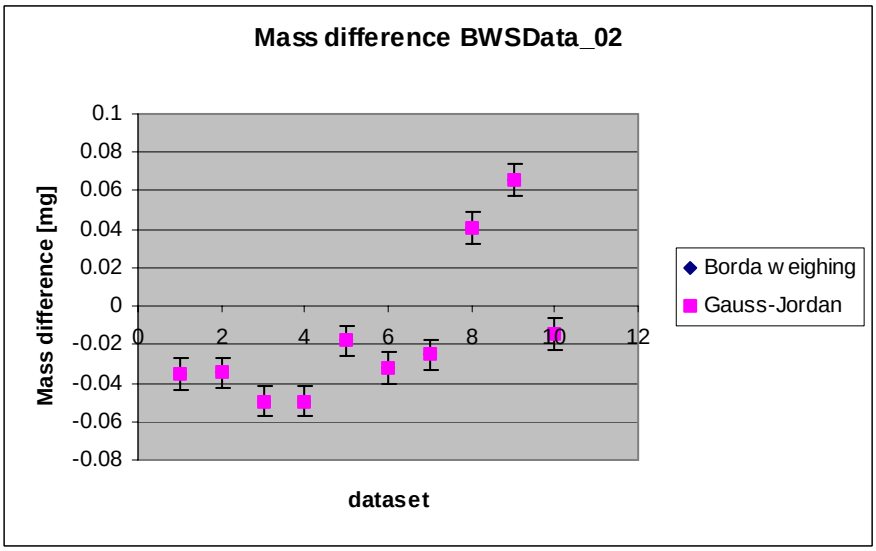

Deviation from the nominal mass of 50 g
delta µ [mg]
0.632
0.631
0.630
0.629
0.628
0.627
0.626
0.625
0 1 2 3 4 5 6 7
dataset
Borda Weighing
Gauss-Jordan

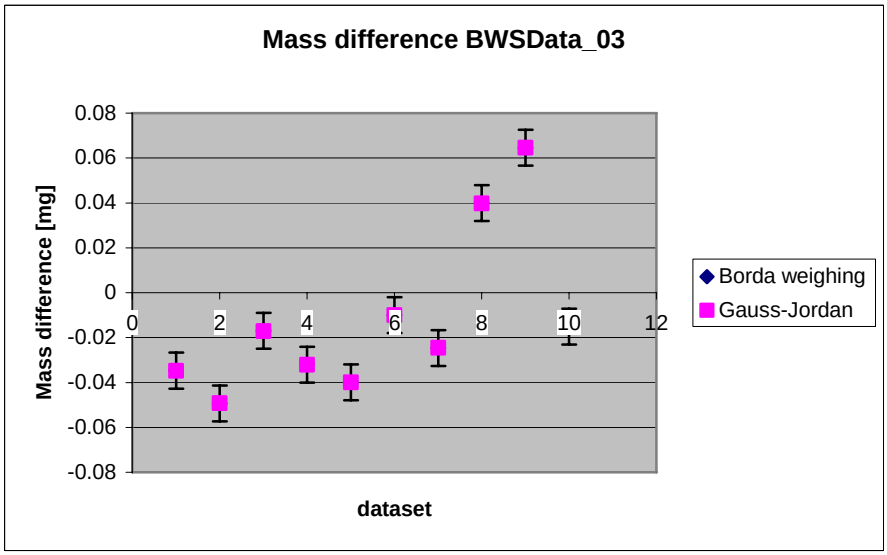

Deviation from the nominal mass of 20 g
delta µ [mg]
0.372
0.371
0.371
0.370
0.370
0.369
0.369
0.368
0.368
0.367
0 1 2 3 4 5 6 7
dataset
Borda Weighing
Gauss-Jordan

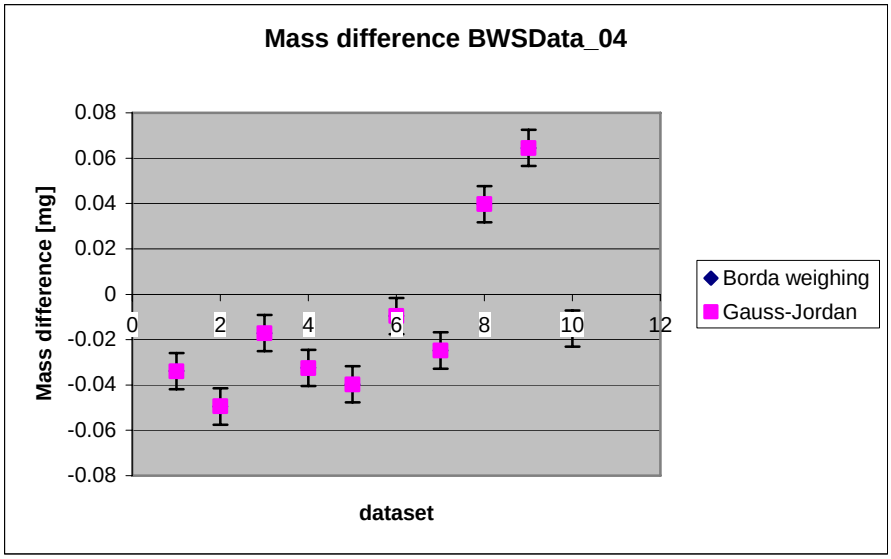

Deviation from the nominal mass of 20 g·
delta µ [mg]
-0.090
-0.090
-0.091
-0.091
-0.092
-0.092
-0.093
-0.093
-0.094
0 1 2 3 4 5 6 7
dataset
Borda Weighing
Gauss-Jordan

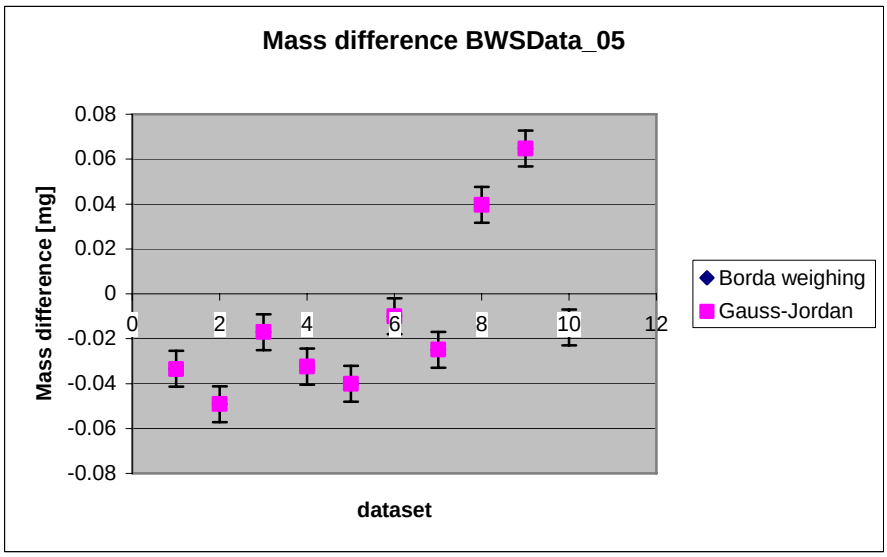

Deviation from the nominal mass of 10 g
delta µ [mg]
0.1460
0.1450
0.1440
0.1430
0.1420
0.1410
0 1 2 3 4 5 6 7
dataset
Borda Weighing
Gauss-Jordan

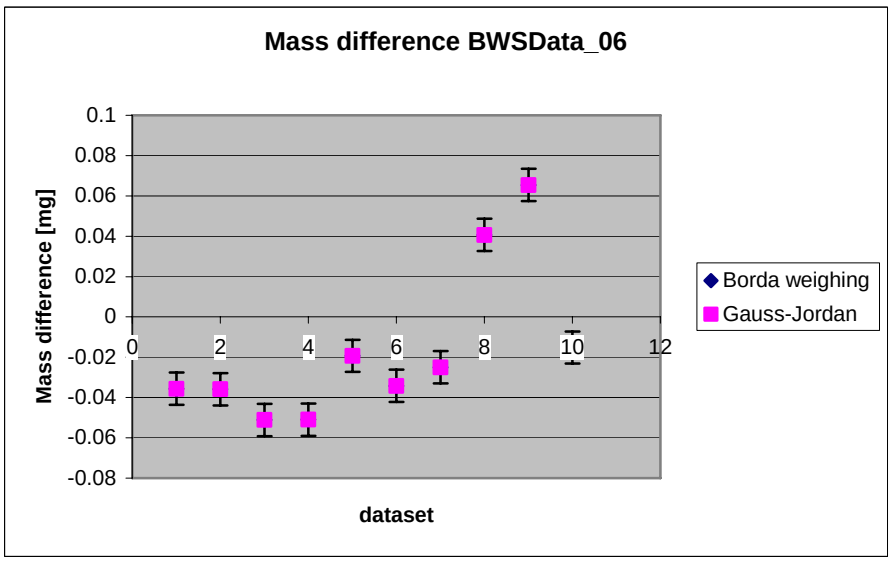

Deviation from the nominal mass of 10 g·
delta µ [mg]
0.1225
0.1220
0.1215
0.1210
0.1205
0.1200
0.1195
0.1190
0.1185
0.1180
0
1
2
3
4
5
6
7
dataset
Borda Weighing
Gauss-Jordan

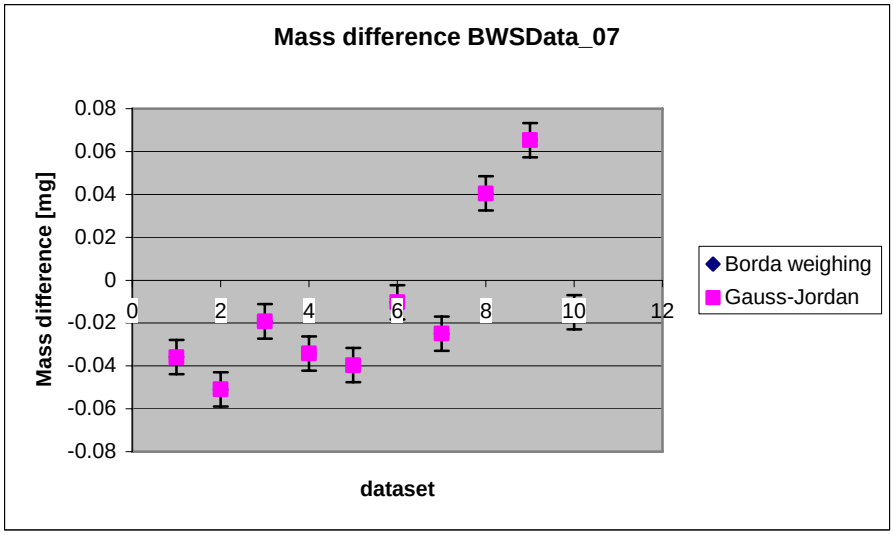

Mass difference BWSData_02
Mass difference [mg]
0.1
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
0
2
4
6
8
10
12
dataset
Borda w eighing
Gauss-Jordan

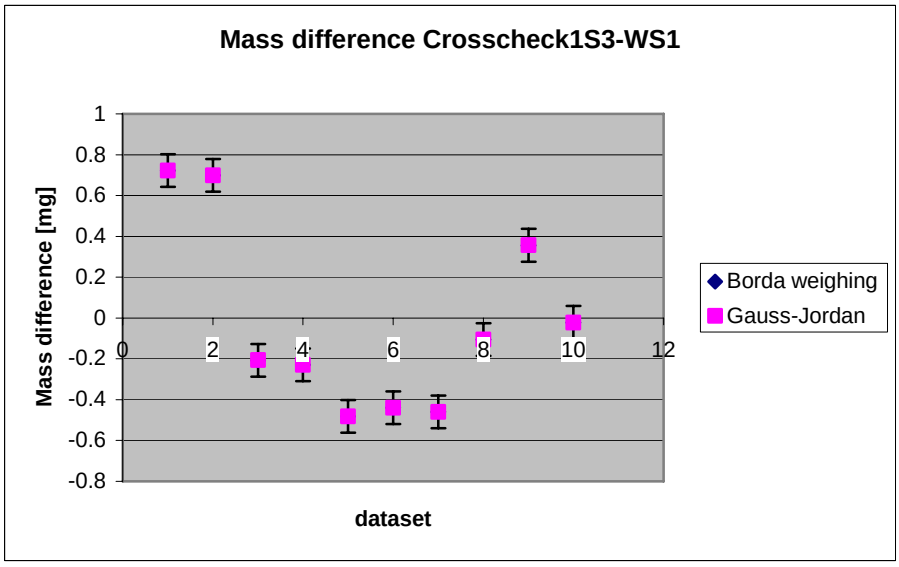

Mass difference BWSData_03
Mass difference [mg]
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan

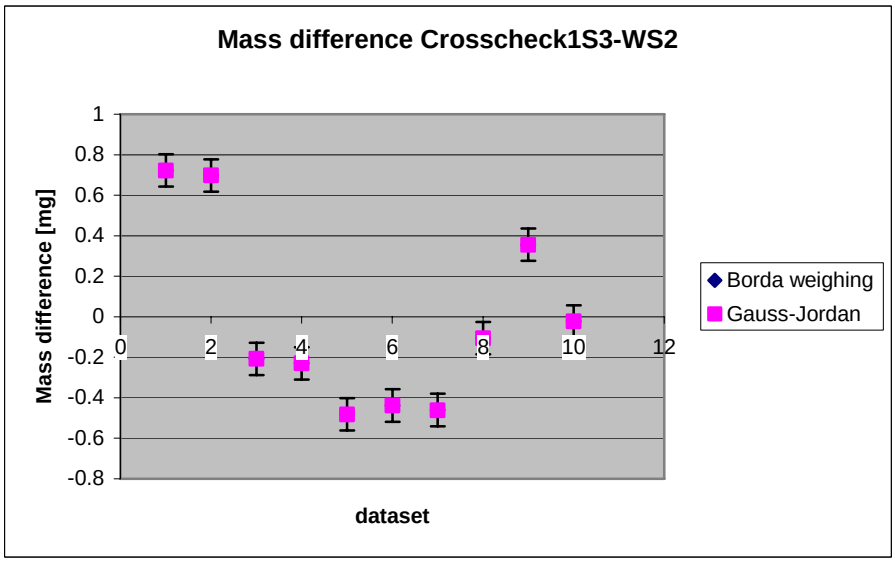

Mass difference BWSData_04
Mass difference [mg]
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan

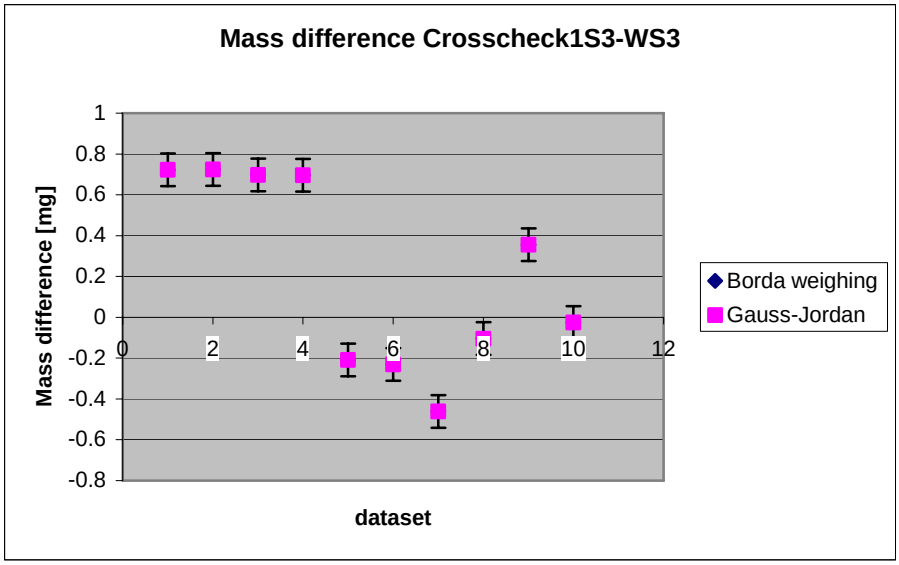

Mass difference BWSData_05
Mass difference [mg]
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan

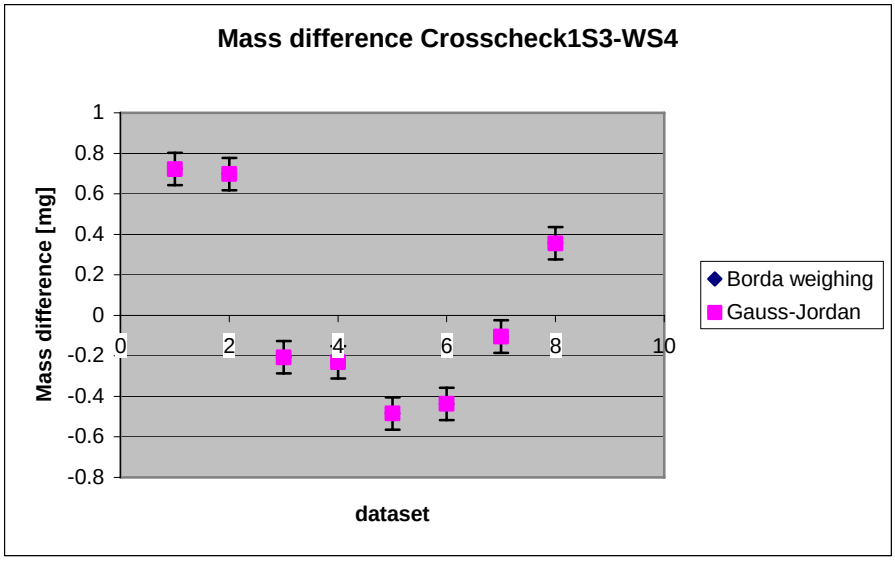

Mass difference BWSData_06
Mass difference [mg]
0.1
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan

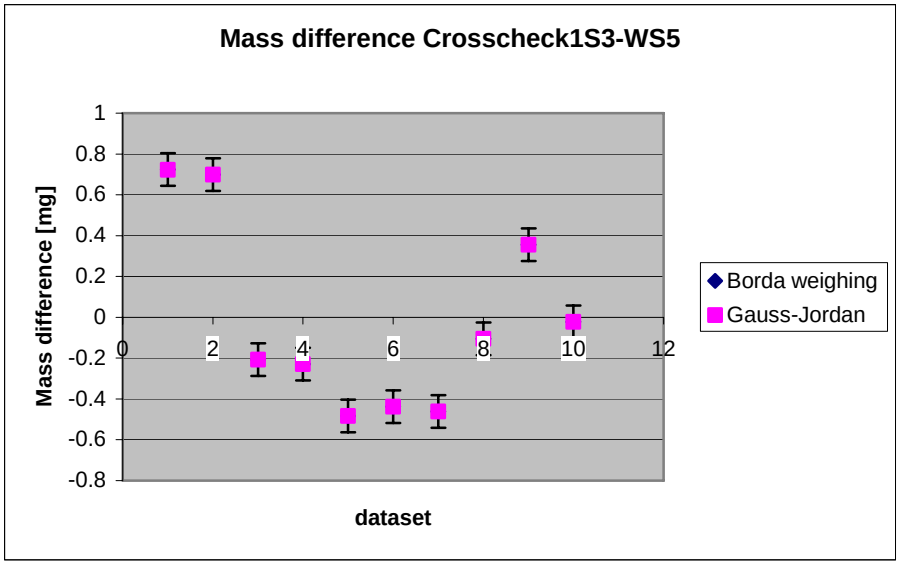

Mass difference BWSData_07
Mass difference [mg]
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
-0.08
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan

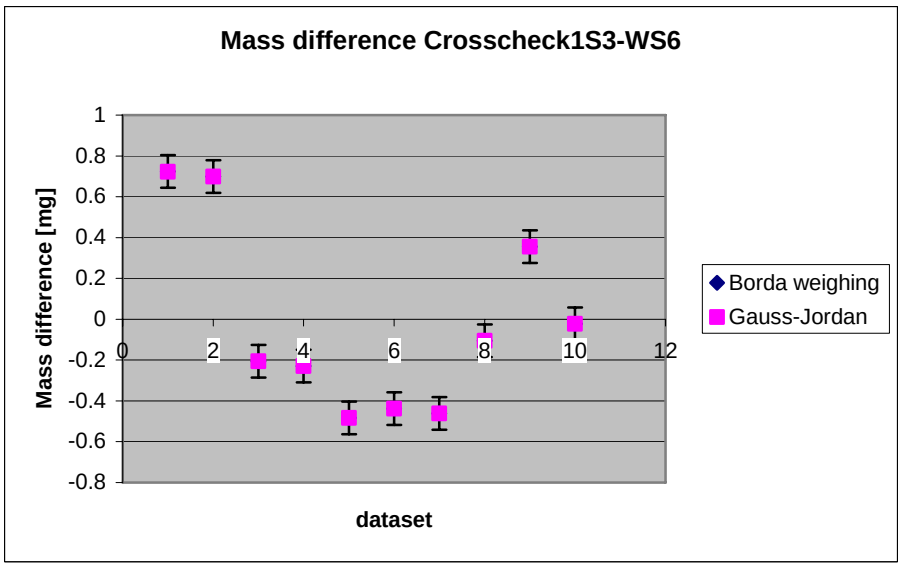

Mass difference Crosscheck1S3-WS1
Mass difference [mg]
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan


Mass difference Crosscheck1S3-WS2
Mass difference [mg]
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan


Mass difference Crosscheck1S3-WS3
Mass difference [mg]
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan


Mass difference Crosscheck1S3-WS4
Mass difference [mg]
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
2
4
6
8
10
dataset
Borda weighing
Gauss-Jordan


Mass difference Crosscheck1S3-WS5
Mass difference [mg]
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan


Mass difference Crosscheck1S3-WS6
Mass difference [mg]
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
2
4
6
8
10
12
dataset
Borda weighing
Gauss-Jordan