

COMPARISON AMONG METHODS EMPLOYED IN THE CALIBRATION OF HIGH ACCURACY MASS STANDARDS AND UNCERTAINTY VALIDATION BY NUMERICAL SIMULATION

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Abstract – The present work exposes the comparison among numerical methods used in the calibration of a set of high accuracy weights by subdivision method. This paper covers the comparison of the mean values, the uncertainties and correlations obtained with the Orthogonal, the Gauss Markov, the Ordinary Least Squares and the Weighted Least Squares (Lagrange Multiplier) methods. These methods are the most commonly used in the realization of the mass scale in the National Metrology Institutes (NMI). Also, the uncertainty evaluated by these methods was compared against the evaluation by a numerical simulation method (Monte Carlo's method).

Keywords subdivision, mass calibration, numerical multivariate simulation, Monte Carlo.

1. INTRODUCTION

In mass metrology, the use of the subdivision method is a need for the realization of the mass scale because the traceability of the mass values towards the definition of the kilogram is through 1 kg Pt-Ir prototypes, e.g., k21. Therefore, the realization of the mass scale requires the calibration of different nominal weight values, from 1 mg to 5 t, using mass standards of the same nominal value (direct comparison) or using one reference weight to calibrate a set of weights where the sum of their nominal values are the same as the reference (subdivision). The equation system is solved to find the mass values of the weights which satisfy the comparison series according to specific adjustment criteria due to the fact that the equation system is overdetermined.

The solution for this kind of systems requires a major number of measurements and the use of advanced mathematical analysis than in the calibration by direct comparison (one test weight against one reference weight), however, due to the need to realize the mass scale starting from 1 kg and the possibility to obtain reliable results by including a check standard, this method is recommended in the calibration of weights class E₁ according to OIML R-111 [1].

2. ADJUSTMENT METHODS FOR THE SUBDIVISION OF THE KILOGRAM

2.1. Least Squares

The theory used in the subdivision of the kilogram is the least squares approach. The measurement model is:

$$X\beta = Y - e \quad (1)$$

2.1. Ordinary Least Squares (OLS)

In the OLS, the function that will be minimized is [13]:

$$S^2 = (y - \hat{y})^T (y - \hat{y}) \quad (2)$$

Equation (2) represents the squared errors S^2 where \hat{y} is the estimated of vector Y . The estimated $\hat{\beta}$ is obtained by:

$$\hat{\beta}_{OLS} = (X^T X)^{-1} X^T Y \quad (3)$$

Where the elements of $\hat{\beta}_{OLS}$ are the mass values informed as corrections. The variance-covariance matrix (further called only covariance matrix) is calculated by the following expression:

$$\text{cov}(\hat{\beta}_{OLS}) = (X^T X)^{-1} \sigma^2 \quad (4)$$

The elements of the diagonal of matrix (4) are the variances of the weights, the rest of the elements are the covariance among weights. The variance due to adjustment of OLS, σ^2 , is obtained by:

$$\sigma^2 = \frac{e^T e}{m - n} \quad (5)$$

2.3 Weighted Least Squares (WLS)

The WLS are solved similar to the OLS, however the function that will be minimized is χ^2 :

$$\chi^2 = (y - \hat{y})^T W^{-2} (y - \hat{y}) \quad (6)$$

Formula (6) will have a chi-squared distribution with n degrees of freedom where vector Y has a normal distribution with variance W^{-2} . When this condition is satisfied, the system solution will be:

$$\hat{\beta}_{WLS} = (X''^T X'')^{-1} X''^T Y'' \quad (7)$$

With X'' and Y'' weighted as follows [3]:

$$X'' = W^{\frac{1}{2}} X \quad (8)$$

$$Y'' = W^{\frac{1}{2}} Y \quad (9)$$

And the covariance matrix is:

$$\text{cov}(\hat{\beta}_{WLS}) = (X''^T X'')^{-1} X''^T W^{-1} (X''^T X'')^{-1} X''^T \quad (10)$$

2.4 Weighted Least Squares by Lagrange Multiplier (WLS-LM)

This solution method is one of the most commonly used in the NMI. The solution vector (estimated mass values) will be obtained by minimizing function (6) satisfying the following condition:

$$f(\beta, y) = 0 \quad (11)$$

Matrix $(X^T X)^{-1}$ is singular; therefore it is necessary to add a restraint, in this case, the Lagrange multiplier, to remove the singularity, so the function that will be minimized is:

$$\chi^2 = (y - \hat{y})^T W^{-2} (y - \hat{y}) + 2\lambda^T f(\beta, y) \quad (12)$$

The vector with the estimated mass values of the weights is obtained with (7) and covariance matrix with (10).

2.5 Orthogonal method.

This method uses equations (3) and (4) from the solution by OLS, with a design matrix X particularly chosen to obtain non correlated values in the covariance matrix. In order to get the orthogonal design matrix X , some weighing comparisons (line vectors of X and their corresponding elements in vector Y) are repeated or removed.

2.6 Gauss Markov method (GM).

The main difference between GM and the others methods explained before is that in this method Y is assumed as a function of multiple random variables, whereas in the others Y is only a function of the variability of the indications of the balance [7]. The function that will be minimized is the same as in WLS (6), however the weighting matrix is different. The solution in GM [6] proposes a covariance matrix related to Y which includes all the uncertainty sources of the measurement model giving a complete covariance matrix [7] unlike the other methods. The covariance matrix will be:

$$W = J_u \phi J_u^T \quad (13)$$

With:

$$J_u = [J_{\Delta L} \quad J_{\rho_a} \quad J_V \quad J_{adj}] \quad (14)$$

J_u is the Jacobian of Y which, in turn, is a matrix composed by the vectors of the input quantities of the mass measurement model:

$$Y = [\Delta L \quad \rho_a \quad V \quad \varepsilon_{adj}] \quad (15)$$

ϕ will be the matrix made up of variance-covariance matrices:

$$\phi = \begin{pmatrix} \phi_{\Delta L} & \phi_{\Delta L, \rho_a} & \phi_{\Delta L, V} & \phi_{\Delta L, adj} \\ \phi_{\Delta L, \rho_a} & \phi_{\rho_a} & \phi_{\rho_a, V} & \phi_{\rho_a, adj} \\ \phi_{\Delta L, V} & \phi_{\rho_a, V} & \phi_V & \phi_{V, adj} \\ \phi_{\Delta L, adj} & \phi_{\rho_a, adj} & \phi_{V, adj} & \phi_{adj} \end{pmatrix} \quad (16)$$

Equation (13) is the matrix form of the GUM for a multivariable model. The estimated mass values are obtained with the following equation [7]:

$$\hat{\beta}_{GM} = (X^T W^{-1} X)^{-1} X^T W^{-1} Y \quad (17)$$

With the covariance matrix:

$$\text{cov}(\hat{\beta}_{GM}) = (X^T W^{-1} X)^{-1} \quad (18)$$

The methods mentioned in this paper are widely discussed in [11].

2.7 Numerical Simulation by Monte Carlo's method.

The numerical simulation by Monte Carlo's method (NSMC) combines probability distributions of the input quantities included in the measurement model giving values for the output quantity [12]. However, just like in the application of the GUM, NSMC explained in supplement 1 of GUM [12] does not consider the case for a multivariable output. In order to obtain the uncertainty of the estimated output quantities (mass values of the weights), a generalized procedure of NSMC for the multivariable case is made:

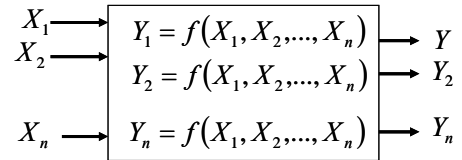


Fig 1. Measurement model with multiple input quantities and multiple output quantities.

The probability distributions of the input quantities are combined according to the corresponding measurement model, resulting in probability distributions for the output quantities. In this case, the input quantities are the mass differences, the air densities during the weighing process,

the volume of the weights, the value of the reference weight. The output quantities are the mass values of the weights under calibration.

3. NUMERICAL EXAMPLE: MEASUREMENT DATA SET UP AND MATRIX EQUATIONS.

In this example, real calibration data were used obtained from three weighing cycles ABBA for each y_i (for each weighing comparison according to the corresponding design matrix) [2]. For all methods the mathematical model is:

$$y = \Delta m - \rho_a (V_r - V_q) - \varepsilon_{adj} \quad (19)$$

The matrices vary depending on the method and restrictions. In the Orthogonal method, the matrix equation is shown in (20). The matrix equation for both GM and OLS methods is given in equation (21) and for WLS – LM method is presented in formula (22). Table 1 shows the main data of the weights used in the calibration. Data of mass differences, air density and their uncertainties for the matrix equations in (21) and (22) are shown in table 2. In the Orthogonal method, some comparisons were eliminated and others were repeated. The mass differences, air densities and their corresponding uncertainties for matrix equation (20) are shown in table 3.

In order to compare the performance of the different adjustment methods, the uncertainty was evaluated with the same contributions (mass value of the reference weight, air density, volume of the weights, mass differences and adjustment error) following the recommended solving procedure for each method. Except for the GM method, the covariance matrix is not complete in Orthogonal, OLS and WLS-LM methods because it only covers type A uncertainty due to adjustment error. Type B uncertainties in these methods are combined with a proportionality factor according to [3].

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ -1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 0 & 1 \\ 0 & -1 & 1 & -1 & 1 \\ 0 & -1 & 1 & -1 & 1 \\ 0 & -1 & 1 & 1 & -1 \\ 0 & -1 & 1 & 1 & -1 \\ 0 & -1 & 0 & 1 & 1 \\ 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 & 1 \\ 0 & 0 & -1 & 1 & 1 \end{pmatrix} * \begin{pmatrix} 500g \\ 200g \\ 200g^* \\ 100g \\ 100g^* \end{pmatrix} = \begin{pmatrix} y_1 + m_r \\ y_2 + m_r \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \\ y_{11} \\ y_{12} \end{pmatrix} \quad (20)$$

$$\begin{pmatrix} -1 & 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 0 & 1 \\ 0 & -1 & 1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 1 & 0 & 1 \\ 0 & 0 & -1 & 1 & -1 & 1 \\ 0 & 0 & -1 & 1 & 1 & -1 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} * \begin{pmatrix} 1000g \\ 500g \\ 200g \\ 200g^* \\ 100g \\ 100g^* \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \\ m_r \end{pmatrix} \quad (21)$$

$$\begin{pmatrix} -1 & 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 0 & 1 \\ 0 & -1 & 1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 1 & 0 & 1 \\ 0 & 0 & -1 & 1 & -1 & 1 \\ 0 & 0 & -1 & 1 & 1 & -1 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} * \begin{pmatrix} 1000g \\ 500g \\ 200g \\ 200g^* \\ 100g \\ 100g^* \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \end{pmatrix} \quad (22)$$

Table 1. Data of the weights involved in the calibration process

Value g	Correction mg	$u(k=1)$ mg	volume cm^3	$u(k=1)$ cm^3
1 000	0,005	0,015	124,894	0,025
500	---	---	62,421	0,025
200	---	---	24,983	0,025
200 *	---	---	24,983	0,025
100	---	---	12,480	0,001 25
100 *	---	---	12,406	0,025

Table 2. Measurement data used in GM, OLS and WLS-LM methods

y_i	Δm mg	$u(\Delta m)$ ($k=1$) mg	ρ_a mg cm^{-3}	$u(\rho_a)$ ($k=1$) mg cm^{-3}
1	-0,141 7	0,020 41	0,961 74	0,000 10
2	-0,176 7	0,020 41	0,961 48	0,000 10
3	0,016 7	0,012 91	0,961 57	0,000 10
4	0,043 3	0,014 72	0,961 13	0,000 10
5	-0,083 3	0,011 90	0,960 73	0,000 10
6	0,038 3	0,010 80	0,960 71	0,000 10
7	0,000 0	0,002 89	0,960 32	0,000 10
8	-0,111 7	0,019 15	0,960 12	0,000 10
9	-0,096 7	0,017 80	0,960 20	0,000 10
10	0,000 0	0,002 89	0,959 94	0,000 10

Table 3. Measurement data used in GM, OLS and WLS-LM methods

The results of each method were compared with the results obtained by numerical simulation. The mathematical model used in the simulation is the same as its corresponding matrix solution method. All the simulations were performed with one hundred random data coming from each probability distribution of the input quantities (they were considered normal distributions).

4. NUMERICAL EXAMPLE: RESULTS

4.1 Estimated mass values and uncertainties

The results obtained with the matrix solution and with the numerical simulation for each method are presented in tables 4 to 7. Figures 2 to 6 show the results for each calibration weight. Each colour represents the solution method, where the first result corresponds to the numerical simulation and the second is the matrix solution by the generalization of the GUM.

4.2 Correlations of the calibration weights.

Except for the GM method, the methods studied in this work do not have a complete covariance matrix because only type A uncertainty due to error adjustment is considered. However, in the estimated mass values by NSMC it is possible to obtain the linear correlation coefficients from the one hundred data outputs. Tables 8 to 11 show the estimated correlation coefficients from the NSMC of each method. Table 12 provides the correlation coefficients obtained by the covariance matrix (18) of GM.

Pesa	Simulación		Matricial	
	$\hat{\beta}$ (mg)	u (k=1) (mg)	$\hat{\beta}$ (mg)	u (k=1) (mg)
500 g	-0,118	0,029	-0,118	0,014
200 g	0,009	0,025	0,009	0,008
200 g *	-0,012	0,025	-0,012	0,008
100 g	-0,039	0,006	-0,039	0,007
100 g	-0,159	0,007	-0,159	0,007

Table 4. Results of the Orthogonal Method.

Pesa	Simulación		Matricial	
	$\hat{\beta}$ (mg)	u (k=1) (mg)	$\hat{\beta}$ (mg)	u (k=1) (mg)
500 g	-0,117	0,029	-0,117	0,031
200 g	0,000	0,025	0,000	0,016
200 g *	-0,004	0,025	-0,004	0,016
100 g	-0,060	0,006	-0,060	0,020
100 g *	-0,138	0,007	-0,138	0,020

Table 5. Results of the WLS-LM Method.

Pesa	Simulación	Matricial
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	$\hat{\beta}$ (mg)	u (k=1) (mg)	$\hat{\beta}$ (mg)	u (k=1) (mg)
500 g	-0,118	0,029	-0,118	0,032
200 g	0,007	0,025	0,007	0,018
200 g *	-0,010	0,025	-0,010	0,018
100 g	-0,052	0,007	-0,052	0,017
100 g *	-0,146	0,007	-0,146	0,017

Table 6. Results of the GM Method.

Pesa	Simulación		Matricial	
	$\hat{\beta}$ (mg)	u (k=1) (mg)	$\hat{\beta}$ (mg)	u (k=1) (mg)
500 g	-0,118	0,029	-0,118	0,023
200 g	0,007	0,025	0,007	0,013
200 g *	-0,010	0,025	-0,010	0,013
100 g	-0,048	0,007	-0,048	0,013
100 g *	-0,150	0,007	-0,150	0,013

Table 7. Results of the OLS Method.

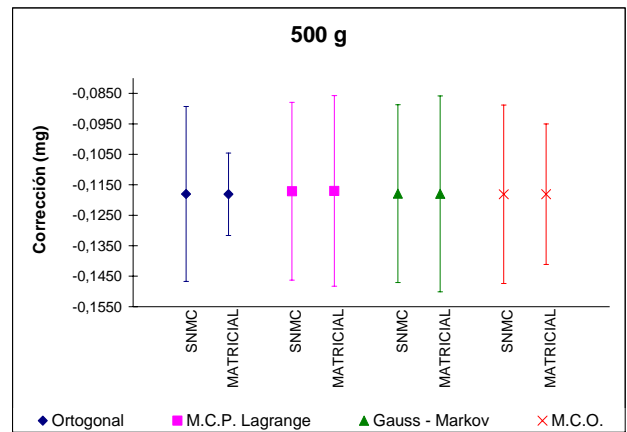


Figure 2. Comparison among values for 500 g weight. Uncertainty bars are with k=1.

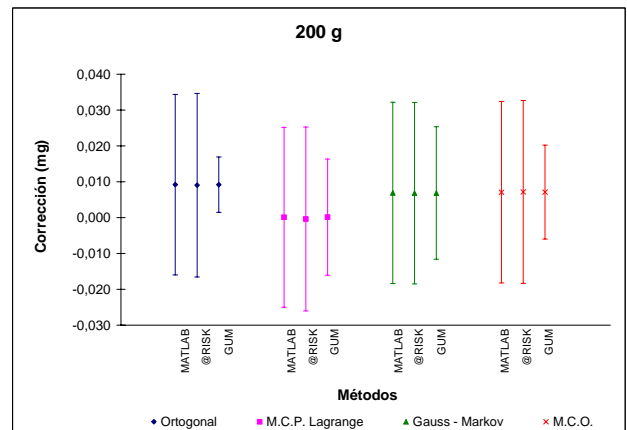


Figure 3. Comparison among values for 200 g weight. Uncertainty bars are with k=1.

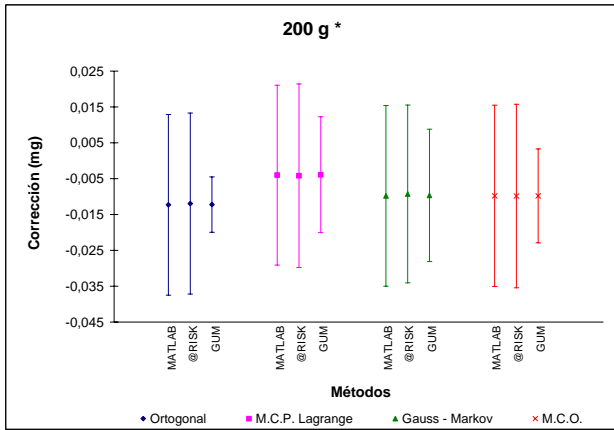


Figure 4. Comparison among values for 200 g* weight. Uncertainty bars are with k=1.

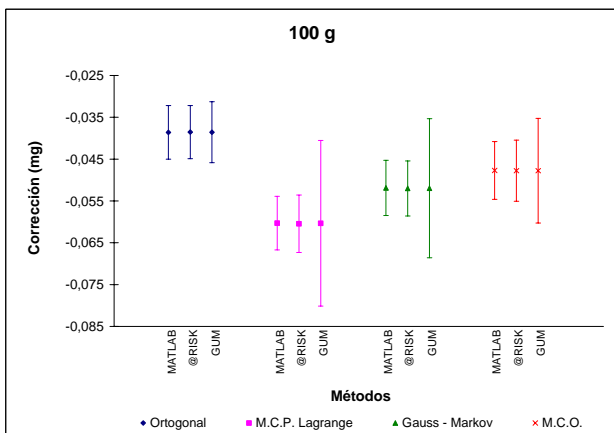


Figure 5. Comparison among values for 100 g weight. Uncertainty bars are with k=1.

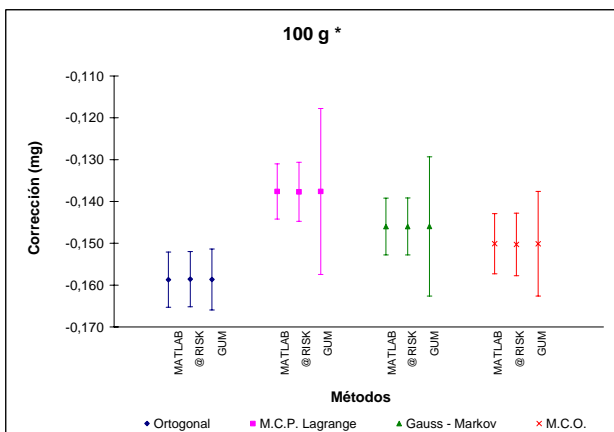


Figure 6. Comparison among values for 100 g* weight. Uncertainty bars are with k=1.

	500 g	200 g	200 g *	100 g	100 g *
500 g	1,00	0,11	0,12	0,22	0,20
200 g		1,00	0,06	0,07	0,05
200 g *			1,00	0,07	0,07

100 g				1,00	0,43
100 g *					1,00

Table 8. Correlation coefficients among weights for NSMC with the Orthogonal method.

	1 000 g	500 g	200 g	200 g *	100 g	100 g *
1 000 g	1,00	0,26	0,12	0,12	0,23	0,22
500 g		1,00	0,12	0,13	0,24	0,23
200 g			1,00	0,08	0,05	0,05
200 g *				1,00	0,05	0,05
100 g					1,00	0,86
100 g *						1,00

Table 9. Correlation coefficients among weights for NSMC with the WLS-LM method.

	1 000 g	500 g	200 g	200 g *	100 g	100 g *
1 000 g	1,00	0,26	0,12	0,12	0,22	0,21
500 g		1,00	0,13	0,13	0,23	0,22
200 g			1,00	0,07	0,05	0,05
200 g *				1,00	0,05	0,06
100 g					1,00	0,59
100 g *						1,00

Table 10. Correlation coefficients among weights for NSMC with the OLS method.

	1 000 g	500 g	200 g	200 g *	100 g	100 g *
1 000 g	1,00	0,26	0,11	0,12	0,23	0,22
500 g		1,00	0,12	0,13	0,24	0,23
200 g			1,00	0,06	0,05	0,05
200 g *				1,00	0,06	0,06
100 g					1,00	0,77
100 g *						1,00

Table 11. Correlation coefficients among weights for NSMC with the GM method.

	1 000 g	500 g	200 g	200 g *	100 g	100 g *
1 000 g	1,00	0,50	0,34	0,35	0,19	0,19
500 g		1,00	0,24	0,24	0,13	0,13
200 g			1,00	0,17	0,04	0,04
200 g *				1,00	0,05	0,05
100 g					1,00	0,29
100 g *						1,00

Table 12. Correlation coefficients among weights for the GM method matrix solution.

4. DISCUSSION

The difference among the estimated mass values obtained with the different matrix solution methods are within the combined uncertainty at confidence level of

approximately 95% (normalized error). The difference in the estimated mass values by solving matrix equations exists due to that in GM and WLS-LM methods the y_i data are being weighted; in the other hand, Orthogonal method uses a different design matrix. However, the estimated mass values obtained with the different methods do not differ significantly [6,9]. The estimated mass values obtained with NSMC agree with their corresponding matrix solution, however, the uncertainty evaluation is different from the matrix method (GUM generalization).

The mass values obtained from SNMC are equal to those values obtained from the matrix method; however there are significant differences between the matrix estimation of the uncertainty and SNMC estimation of uncertainty.

The uncertainty values calculated with SMNC are the same between all the tested methods.

For the 500 g weigh the estimated uncertainties for MCP-ML and GM are almost the same compared to SNMC, however there is an underestimation for the 200 g, and an overestimation for the 100 g weighs compared to its SNMC.

The MCO method underestimates the uncertainty of the 500 g and 200 g weighs. And overestimates the uncertainty compared with the SNMC

The Orthogonal method underestimates all the weigh values but the 100 g in relation to SNMC.

The correlation coefficient for the 100 g and 100 g*, obtained from the matrix GM gives 0,29 in comparison with the value obtained in SNMC 0,77, which is significantly different.

The correlation coefficients between the 100 g weighs, obtained from the SNMC for orthogonal model is 0,43. The lowest coefficients obtained were in this method.

The correlation coefficients between the 100 g weighs, obtained from the SNMC for MCP-ML model is 0,86. Thus implies a highly lineal dependence between these weighs.

5. CONCLUSIONS.

The most commonly matrix solution methods used in the NMI's in the calibration of weights by subdivision method and the comparison against their numerical simulation by Monte Carlo's method were studied in this work.

The best estimated mass values obtained both by NSMC and by matrix solution methods do not differ significantly from one to another.

The uncertainty calculated by the NSMC differs from the calculation by the matrix methods in higher or lower degree of impact, but indeed differs from the matrix calculation.

The uncertainty values obtained by NSMC for all the mathematical models (Orthogonal, OLS, WLS-LM and GM) are almost the same, meaning that probability distributions of the input quantities propagate in the same way no matter the method employed.

The SNMC gives the possibility of calculate the correlation between mass values. The traditional orthogonal method don not allows it, because the method only estimates the Type A correlation, and thus if the correlation of the design matrix is zero the resultant correlation will be zero.

In conclusion, the authors recommend calculate estimated values of vector β and their associated uncertainties using the numerical simulation by Monte Carlo's method of the GM matrix equation.

For the same nominal values of mass there are no significant differences between SMNC and GUM generalization (Matrix methods) [10], however for the subdivision are different, and it could be because the configuration of the design matrix

In conclusion, the authors recommend calculate estimated values of vector β and their associated uncertainties using the numerical simulation by Monte Carlo's method of the GM matrix equation.

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