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On computation of a common mean

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Abstract

Combining several independent measurements of the same physical quantity is one of the most important tasks in metrology. Small samples, biased input estimates, not always adequate reported uncertainties, and unknown error distribution make a rigorous solution very difficult, if not impossible. For this reason, many methods to compute a common mean and its uncertainty were proposed, each with own advantages and shortcomings. Most of them are variants of the weighted average (WA) approach with different strategies to compute WA and its standard deviation. Median estimate became also increasingly popular during recent years. In this paper, these two methods in most widely used modifications are compared using simulated and real data. To overcome some problems of known approaches to compute the WA uncertainty, a new combined estimate has been proposed. It has been shown that the proposed method can help to obtain more robust and realistic estimate suitable for both consistent and discrepant measurements.

1 Introduction

Computation of a common mean (CM) of several independent measurements of a physical quantity is a common procedure in scientific analysis. Typical task include combining results obtained by different analysts or results based on different measurement methods or results of several series of measurements, etc. One of the most important applications required computation of a CM is derivation of the best estimate of physical constants. Both accurate CM value and its realistic uncertainty are equally important in such computations.

Input information consists of measured values x_i, $i = 1, \ldots, n$ with associated uncertainties s_i, usually standard deviations (STD), and correlations between x_i are not available. From statistical point of view, it is a classical case of direct measurements of unequal precision. Due to lack of needed information we have to treat them as uncorrelated. Combination procedure aimed to get an estimate $\bar{x}$ of the CM x with associated uncertainty σ, which adequately reflects the scatter and uncertainties of input measurements.

There is no unambiguous solution of this problem. It is well known the the classical weighted average (WA) is unbiased CM estimate with minimum variance, provided x_i are independent unbiased estimators, and s_i^2 are true variances. A solution of the problem is not straightforward if true variances are unknown. Numerous papers are devoted to computation of a CM and its uncertainty; see e.g. Graybill and Deal (1959); Sinha (1985); Witkovský and Wimmer (2001); Zhang (2006) and references therein. Unfortunately, results are obtained under rather strong assumptions: the x_i are unbiased estimates of $\bar{x}$, s_i are normally distributed, and number of measurements n_i formed each x_i is known. Evidently, these assumptions are hardly met in scientific data analysis. The situation becomes even more complicated because small samples are are the rule rather than the exception in such tasks, which makes it difficult to efficiently apply most of statistical methods generally used.

For these reasons many alternative approaches, not always strongly justified, are mostly used, see e.g. MacMahon et al (2004), Chen et al (2011), and Dataplot software documentation[1]. We do not aim this paper at investigation of all the existing methods. Such a task seems to be impractical because some methods cannot be used in our case because we lack needed information, some are developed for specific applications, and some approaches may be too complicated for routine use, e.g. bootstrapping (Helene, 2007) or total median (Figueiredo and Gomes, 2004; Cox and Harris, 2004).

We consider two basic methods most commonly used: WA and median. As to the former, several approaches to compute its uncertainty (STD) are proposed in literature. This paper is devoted to comparison of this methods based on simulated and real data. Besides, a new combined approach is proposed to compute the WA uncertainty. This approach was proposed for the first time in Malkin (2001b) and has shown to be useful in practical applications such as computation of Earth orientation parameter (EOP) combined solution (Malkin, 2001a), radio source position catalogues combination (Sokolova and Malkin, 2007), analysis of radio source position time series (Malkin, 2008), and modeling the galactic aberration (Malkin, 2011). Special attention is given to analysis of small statistical samples.

2 Computation of CM

2.1 Basic WA estimators

The WA estimator is most widely used in various scientific and practical applications. Let we have n values x_i with associated standard deviations s_i, $i = 1 \ldots n$. Then we can compute the following statistics (e.g. Brandt (1999); Bevington and Robinson (2003))

$$p_i = \frac{1}{s_i^2} \ , \quad p = \sum_{i=1}^{n} p_i \ , \quad \bar{x}_w = \frac{\sum_{i=1}^{n} p_i x_i}{p} \ . \tag{1}$$

In result, we have the classical WA estimate $\bar{x}_w$ with weights inversely proportional to variances of input measurements s_i^2. We also can compute the following statistics also used as a measure of goodness of fit

$$H = \sum_{i=1}^{n} p_i (x_i - \bar{x}_w)^2 = \sum_{i=1}^{n} \left[\frac{(x_i - \bar{x}_w)}{s_i} \right]^2 \ , \tag{2}$$

where H has a χ^2 distribution with $n-1$ degree of freedom (dof) if s_i^2 are theoretical variances. In practice, s_i^2 are, as a rule, sample variances, but this fact is usually ignored.

[1] http://www.itl.nist.gov/div898/software/dataplot/

The H statistics is an indicator of consistency of input measurements. If the measurements are consistent, the value

$$\frac{\chi^2}{dof} = \frac{H}{n-1} \tag{3}$$

is close to unity. Otherwise one can assume that the input measurements x_i have systematic errors or s_i are underestimated.

The question is how to estimate the standard error σ of the mean? Two main approaches can be applied to compute σ. The classical WA estimate is

$$\sigma_1 = \frac{1}{\sqrt{p}} \ . \tag{4}$$

Least squares approach leads to alternative estimate of the WA uncertainty. The solution of the least square problem $x_i = \bar{x} + \varepsilon_i$ with weights p_i gives the same WA estimate $\bar{x}$, but another estimate of its uncertainty:

$$\sigma_2 = \sqrt{\frac{\sum_{i=1}^{n} p_i (x_i - \bar{x}_w)^2}{p\,(n-1)}} \ . \tag{5}$$

This estimate of the WA uncertainty is, in fact, σ_1 estimate scaled in such a way to make χ^2/dof close to unity:

$$\sigma_2 = \sigma_1 \sqrt{\frac{H}{n-1}} \ , \tag{6}$$

which is equivalent to scaling of input s_i by the factor $\sqrt{H/(n-1)}$ as recommended by Rosenfeld et al (1967) and Brandt (1999). However, such a scaling makes resulting σ estimate independent of the "scale" of input variances s_i^2, and dependent only on their ratio.

So, both approaches give the same estimate for the WA, but different estimates for the WA uncertainty. The first value σ_1 depends on s_i and does not depend on the scatter of the input values x_i. On the other hand, σ_2 depends on relative values of input variances s_i^2 and the scatter of x_i. Difference between the two σ estimates may be attributed to systematic errors in x_i or underestimated s_i.

Theoretically, choice between σ_1 and σ_2 depends on whether the scatter of x_i is a result of random error or there are systematic differences between estimates x_i. Obviously, both effects are present in most of practical applications. This is a well recognized problem in data analysis, and its rigorous solution is hardly possible due to generally biased input estimates, not always adequate reported uncertainties, and unknown error distribution.

In practice, if x_i are close each other and s_i are greater than the scatter of x_i, it seems reasonable to use σ_1. Otherwise, if s_i are much less than the scatter of the input measurements, σ_2 estimate seems to be more adequate to the data. Indeed such a way to choose the best estimate for the WA uncertainty cannot be considered satisfactory.

A possible practical, statistically based approach has been proposed by Rosenfeld et al. (1967) and Brandt (1999). According to this approach, χ^2 criteria is used to decide whether the scatter of x_i is a result of random errors. First, both uncertainty estimates σ_1 and σ_2 are computed. Then the final WA uncertainty is taken as

$$\sigma_3 = \begin{cases} \sigma_1, & \text{if } H \le \chi^2(Q, n-1) \ , \\ \sigma_2, & \text{if } H > \chi^2(Q, n-1) \ , \end{cases} \tag{7}$$

where Q is a significance level. One can see that to a first approximation $\sigma_3 = \sigma_1$ for consistent measurements and $\sigma_3 = \sigma_2$ for discrepant ones, and given Q value is used to distinguish between them. As a consequence, substantially different σ estimates can be obtained for the same input measurements (x_i, s_i) but specifying different Q.

Similar approach is discussed by Bich et al (2002). It recommends accept σ_1 as the estimate of the CM mean uncertainty if consistency check $H \le \chi^2(Q, n-1)$ passed at a significance level Q=5%; otherwise supplement studies should be performed, such check of outliers, investigation of input data, etc. Unfortunately, the latter is generally not feasible.

2.2 Combined WA uncertainty estimator

As pointed out in the previous section, the literature recommends using either σ_1 or σ_2 depending on some criteria, which can lead to ambiguous results, keeping in mind that these two estimates may differ by several times. So, a more robust σ estimate is desirable for practical use, which would account of both the scatter of x_i and their uncertainties s_i. After investigation of behavior of all three estimates using simulated and real data, and supplement tests we decided in favor of combined estimate computed by simple formula

$$\sigma_c = \sqrt{\sigma_1^2 + \sigma_2^2} \ . \tag{8}$$

As a variant, σ_2 computed with unit weights can be used, which provides clear separation of impacts at combined estimate σ_c from the uncertainties (σ_1) and scatter (σ_2) of the input measurements. However, in this case, the result is generally more sensitive to measurements suspected to be outliers.

Unfortunately, we cannot suggest a rigorous theoretical ground of this approach, which is common for other practical recommendations too. Our considerations are as follows. Suppose we can represent each input value as $x_i = x + \varepsilon_i + \varepsilon_{0i}$, where x is the true value of the CM, ε_i is a random error distributed as $N(0, s_i^2)$ and ε_{0i} is a systematic error of the x_i measurement distributed as $N(0, \sigma_0^2)$. Here σ_0 is considered as a measure of the scatter of the set of systematic errors in input measurements. Evidently, ε_{0i} is unknown, otherwise it would be accounted for in the reported value of x_i. We can suppose that ε_{0i} biases x_i but does not bias s_i. Thus the mathematical expectation of each x_i is

$$\mathcal{E}(x_i) = x + \varepsilon_{0i} \, . \tag{9}$$

Now we can use the set of n equations (9) for $i = 1, \ldots, n$ as an equations of condition to be solved by the least squares method. As a result of this solution, we obtain an estimate of x and its uncertainty σ_0, which can be expected close to σ_2. Then we can consider $\sigma_0 \approx \sigma_2$ as an additive error in the WA uncertainty. Combining this error with σ_1 computed under the assumption of absence of systematic errors in x_i we get σ_c as defined by Eq 8.

Finally, let us notice that (8) can be rewritten as

$$\sigma_c = \sqrt{\frac{1}{p}\left(1 + \frac{H}{n-1}\right)} \ . \qquad (10)$$

So, to obtain σ_c estimate, there is no need to compute separately both σ_1 and σ_2 and then use Eq. (8).

2.3 Median

Another approach routinely used to get the estimate of a CM is computation of a median $\bar{x}_m$. The median is known as a robust statistics less influenced by outliers. However its standard definition does not provide an estimate of error of a median value (it makes it immune to unreliable uncertainties though).

A possible approach to compute a median uncertainty was proposed by Müller (1995, 2000a). Let $\bar{x}_m$ be the median of x_i, i.e. $\bar{x}_m = med\{x_i\}$. Now we can compute the median of the absolute deviations (MAD) as

$$MAD = med\{|x_i - \bar{x}_m|\} \ . \qquad (11)$$

The uncertainty of $\bar{m}$ is then taken as

$$\sigma_m = \frac{1.8582}{\sqrt{n-1}}\, MAD \ . \qquad (12)$$

One can see that this estimate of the median uncertainty depends only on the data scatter and not on input uncertainties. Later Müller (2000b) proposed a method to take account of the uncertainty in input data and thus compute weighted median and its uncertainty. However its practical realization, as pointed out by the author, is more cumbersome, and the testing results and discussion given therein do not show clear advantage of using weighted median.

3 Tests with artificial data

In this section, results of two tests with simulated data are presented. These tests were constructed to investigate in more details the behavior of the σ estimates introduced in the previous section. Indeed, many of features discussed here can be seen directly from corresponding equations, but not so demonstrative.

Table 1 shows some numerical examples of computation of WA for two measurements, and its standard deviation. To compute σ_3 we used Q=99%, which corresponds to χ^2(0.99,1)=6.635. Using Q=95%, χ^2(0.95,1)=3.841 does not change main conclusions. Note that, unlike general practice, we keep several significant digits in uncertainty just to better show the difference between various estimates.

Classical example 1 shows that σ_2 cannot provide reasonable estimate for σ whatever how large input uncertainty are given. Examples 2–7 and 8–15 show how σ estimates change with grown s_i for the same x_i. Examples 16–23 show how σ estimates change with grown x_2

for the same x_1 and s_i. One can see that no one of σ_1, σ_2, σ_3 provides a satisfactory estimate of σ for all the examples.

Several observations from Table 1 are as follows. The σ_1 estimate sometimes it is clearly underestimated (examples 8–12). Examples 2–7 and 8–15 illustrate that σ_2 (2) cannot provide satisfactory estimate, especially in the cases 7, 14, 15, where it seems to be underestimated. Estimate σ_3 gives more realistic result, but not in all the cases, e.g. 2–3 and 8–11. Moreover, σ_3 value depends not only on data sample $\{x_i,\, s_i\}$ but also on subjective choice of Q. Besides, as can be seen from this test and Eq. 7 that σ_3 may show significant jumps caused by small changes in input data or confidence level. For these reasons, it was decided not to use σ_3 in further work.

In contrast to σ_1, σ_2, and σ_3, one can see that σ_c approach can provide stable and realistic estimate of the standard deviation of the WA.

In the second test, we use the same set of five measurements with different errors (see Fig. 1). In the upper row the data have minimal uncertainties; in the middle row, all the uncertainties are increased by factor of 3; and in the bottom row, all the uncertainties are increased again by factor of 3.

From this Figure, one can see that σ_1 became greater as s_i grow, as expected. However it looks underestimated in case a. The σ_2 estimate remains the same for all three examples because it does not depend on absolute values of s_i, but only on the dispersion ratio, which is the same in all the cases. One would expect however that σ should be greater in two last examples as compared to the previous ones. Median estimate is close to σ_2 as expected because both of them depend on the x_i scatter only, and hence σ_m shows the same problems as σ_2.

The σ_c estimate appears to be optimal because it shows a steady increase from case a to case c accounting both for input s_i value and x_i scatter. In case a with small s_i values σ_c is determined mainly by the data scatter, and is close to σ_2. In case b with equal contribution of input data uncertainties and scatter ($\sigma_1 = \sigma_2$), σ_c is just greater by factor of $\sqrt{2}$. In case c, σ_c is defined mainly by s_i, which are much greater than the data scatter, and it is close to σ_1. We can say that the σ_c estimate "automatically" takes account of both input measurements scatter and uncertainties without any need in supplement assumptions or parameters like significance level.

4 Application to real data

In this section, the tests with real data are presented. In the first test, the height differences are analyzed between marks 107 and 109 of the local geodetic network of the Svetloe Radio Astronomical Observatory of the Institute of Applied Astronomy, St. Petersburg, Russia (Kazarinov and Malkin, 1997; Finkelstein et al, 2006). This analysis includes four levelling surveys performed in 1998–2003. Distance between the marks is about 135 m. Results of computations are shown in Fig 2. In this case, the scatter of the measurements is rather large as compared to measurement uncertainties. For this reason, σ_1 seems to be underestimated. Combined estimate σ_3 is close to σ_2, but may be preferable because accounts also for input uncertainties. Median uncertainty is close to σ_2. In this example, it is difficult to decide which of the two latter estimates should be preferred. Both of them looks equally realistic.

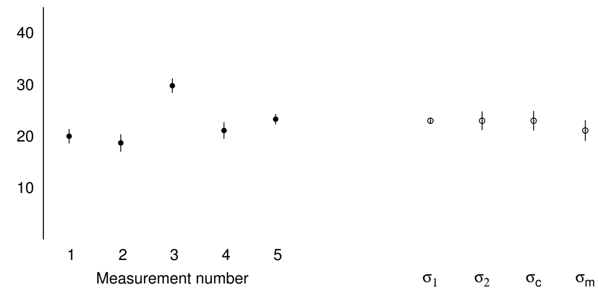
Table 1: Examples of computation of WA of two measurements x_1, x_2 with associated uncertainties s_1, s_2. Results of computations are mean $\bar{x}$ and four estimates of its uncertainty σ_1, σ_2, σ_3, and σ_c computed by (4), (5), (7), and (8) respectively. H is computed by (2) and used to compute σ_3

No.	x_1	x_2	s_1, s_2	$\bar{x}$	H	σ_1	σ_2	σ_3	σ_c
1	1.0	1.0	0.5	1.0	0.00	0.354	0.000	0.354	0.354
2	1.0	2.0	0.1	1.5	50.00	0.071	0.500	0.500	0.505
3			0.2		12.50	0.141	0.500	0.500	0.520
4			0.3		5.56	0.212	0.500	0.212	0.543
5			0.5		2.00	0.354	0.500	0.354	0.612
6			1.0		0.50	0.707	0.500	0.707	0.866
7			2.0		0.12	1.414	0.500	1.414	1.500
8	10.0	20.0	0.1	15.0	5000.00	0.071	5.000	5.000	5.000
9			0.5		200.00	0.354	5.000	5.000	5.012
10			1.0		50.00	0.707	5.000	5.000	5.050
11			2.0		12.50	1.414	5.000	5.000	5.196
12			3.0		5.56	2.121	5.000	2.121	5.431
13			5.0		2.00	3.536	5.000	3.536	6.124
14			10.0		0.50	7.071	5.000	7.071	8.660
15			20.0		0.12	14.142	5.000	14.142	15.000
16	10.0	10.0	1.0	10.0	0.00	0.707	0.000	0.707	0.707
17	10.0	11.0		10.5	0.50	0.707	0.500	0.707	0.866
18	10.0	12.0		11.0	2.00	0.707	1.000	0.707	1.225
19	10.0	13.0		11.5	4.50	0.707	1.500	0.707	1.658
20	10.0	14.0		12.0	8.00	0.707	2.000	2.000	2.121
21	10.0	15.0		12.5	12.50	0.707	2.500	2.500	2.598
22	10.0	16.0		13.0	18.00	0.707	3.000	3.000	3.082
23	10.0	17.0		13.5	24.50	0.707	3.500	3.500	3.571

a

$x_1 = 20.0 \pm 1.4$
$x_2 = 18.7 \pm 1.7$
$x_3 = 29.8 \pm 1.4$
$x_4 = 21.1 \pm 1.6$
$x_5 = 23.3 \pm 1.0$

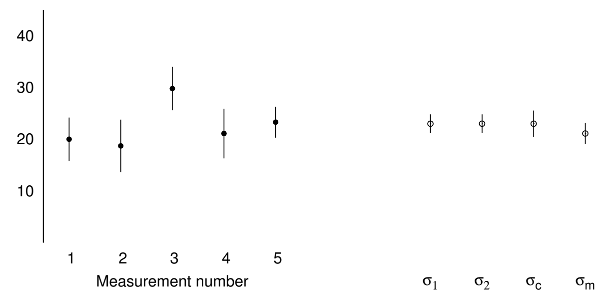
$\bar{x}_{w1} = 23.00 \pm 0.60$
$\bar{x}_{w2} = 23.00 \pm 1.81$
$\bar{x}_{wc} = 23.00 \pm 1.91$
$\bar{x}_m = 21.10 \pm 2.04$



b

$x_1 = 20.0 \pm 4.2$
$x_2 = 18.7 \pm 5.1$
$x_3 = 29.8 \pm 4.2$
$x_4 = 21.1 \pm 4.8$
$x_5 = 23.3 \pm 3.0$

$\bar{x}_{w1} = 23.00 \pm 1.81$
$\bar{x}_{w2} = 23.00 \pm 1.81$
$\bar{x}_{wc} = 23.00 \pm 2.56$
$\bar{x}_m = 21.10 \pm 2.04$



c

$x_1 = 20.0 \pm 12.6$
$x_2 = 18.7 \pm 15.3$
$x_3 = 29.8 \pm 12.6$
$x_4 = 21.1 \pm 14.4$
$x_5 = 23.3 \pm 9.0$

$\bar{x}_{w1} = 13.00 \pm 5.42$
$\bar{x}_{w2} = 13.00 \pm 1.81$
$\bar{x}_{wc} = 13.00 \pm 5.71$
$\bar{x}_m = 11.10 \pm 2.04$

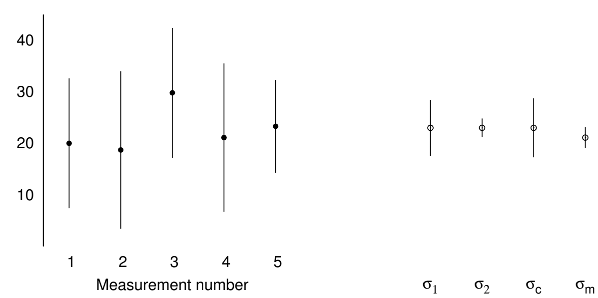


Figure 1: Testing four methods to compute CM with simulated data. The left group of points (discs) represents measurements, and the right group of points (circles) represents CM estimates. In all three examples, averaged measurements x_i are the same, but their uncertainties differ. Uncertainties in example b are three times greater than those in example a, and uncertainties in example c are three times greater than those in example b; $\bar{x}_{w1}$ is the WA computed by Eq. (1) with the uncertainty σ_1 computed by (4). $\bar{x}_{w2}$ is the same WA with the uncertainty σ_2 computed by (5), $\bar{x}_{wc}$ is the same WA with the uncertainty σ_c computed by (8), $\bar{x}_m$ is the median with the uncertainty σ_m computed by (12)

$$x_1 = 3847.5 \pm 0.4$$
$$x_2 = 3847.9 \pm 0.4$$
$$x_3 = 3846.6 \pm 0.5$$
$$x_4 = 3848.1 \pm 0.2$$

$$\bar{x}_{w1} = 3847.83 \pm 0.16$$
$$\bar{x}_{w2} = 3847.83 \pm 0.26$$
$$\bar{x}_{wc} = 3847.83 \pm 0.31$$
$$\bar{x}_m = 3847.70 \pm 0.32$$

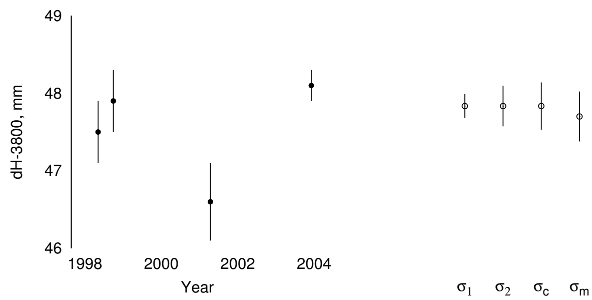


Figure 2: Testing four methods to compute a CA with real data: a case of determination of the height difference between two geodetic marks. The designations are the same as in Fig 1

$$x_1 = 15.0 \pm 0.8$$
$$x_2 = 14.4 \pm 1.2$$
$$x_3 = 11.3 \pm 1.1$$
$$x_4 = 14.8 \pm 0.8$$
$$x_4 = 14.5 \pm 1.5$$

$$\bar{x}_{w1} = 14.21 \pm 0.44$$
$$\bar{x}_{w2} = 14.21 \pm 0.65$$
$$\bar{x}_{wc} = 14.21 \pm 0.79$$
$$\bar{x}_m = 14.50 \pm 0.28$$

$$x_1 = -10.0 \pm 1.2$$
$$x_2 = -12.0 \pm 2.8$$
$$x_3 = -13.9 \pm 0.9$$
$$x_4 = -12.4 \pm 0.6$$
$$x_4 = -12.0 \pm 3.0$$

$$\bar{x}_{w1} = -12.42 \pm 0.45$$
$$\bar{x}_{w2} = -12.42 \pm 0.59$$
$$\bar{x}_{wc} = -12.42 \pm 0.74$$
$$\bar{x}_m = -12.00 \pm 0.37$$

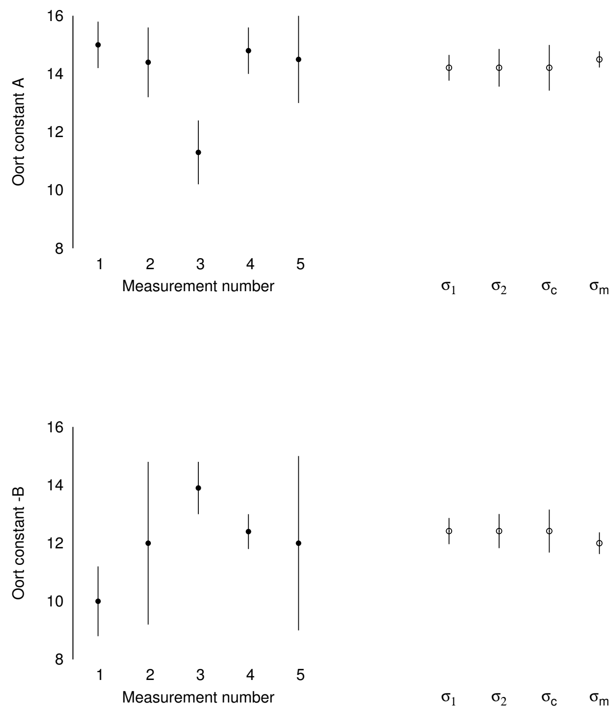


Figure 3: Testing four methods to compute a CA with real data: a case of determination of the Oort constants A (top) and B (bottom). The designations are the same as in Fig 1

In the second test, results of determination of average values of the Oort constants in Klačka (2009) are revised (see Fig 3). For comparison, the author's estimates are 14.2 ± 0.5 for A, and -12.4 ± 0.5 for B, with uncertainties computed as σ_1 and evidently rounded up. This value of the WA uncertainty is likely underestimated as compared to input data uncertainties and scatter. Median uncertainty also seems underestimated because it accounts only for relatively small scatter, and ignores relatively large measurement uncertainties. In this example, σ_c estimate again looks the most realistic and corresponding to input data.

5 Conclusion

Although computation of a CM, in particular WA, is widely used in data analysis, this problem has no definite, unambiguity solution yet. In particular, a very important problem in most of applications is to obtain a "realistic" estimate for the CM uncertainty. Both underestimation and overestimation are equally undesirable.

In this study, we mostly investigated several basic approaches to compute a WA. Currently used methods for computation of the WA uncertainty do not provide satisfactory result for many practical tasks. The classical WA uncertainty estimate σ_1 often yields underestimated value because it is rigorously justified for unbiased x_i only. Another estimate σ_2, which can be derived from a least squares solution or by appropriate scaling of the input uncertainties, does not take account of input uncertainties, but only of the variance ratio.

In this paper, we propose a new approach to compute the WA uncertainty, combined estimate σ_c given by (8) and (10), which is able to account for both uncertainties and scatter of input data. We did not propose a rigorous statistical background for this estimate. However, it can be shown that in the case when input values x_i are obtained from a normally distributed populations, and each value x_i has a normally distributed systematic error, proposed estimate σ_c can be derived from a least squares solution. It appears probable that this estimate is suitable for practical use until the deviation from normality is very large.

Several tests with simulated and real measurements have demonstrated that using σ_c is a simple and effective approach equally suitable for both discrepant and consistent measurements. It is also important that it provides realistic σ estimate even for very small samples of 2–3 measurements.

As to the median approach, it is known as a more robust CM estimate, but computation of its uncertainty is not so straightforward. A simple approach by Müller (1995, 2000a) seems to be not satisfactory in some cases, as follows from our tests. In this respect, the bootstrap method and extended bootstrap method (MacMahon et al, 2004) deserve consideration; this methods may be too complicated for routine use though.

In conclusion, one should never forget the following. Despite the method used, the CM uncertainty is only a part of real measurement accuracy, namely a Type A uncertainty according to the standard metrological terminology. By definition, Type A uncertainty is computed from data using statistical procedures, while a Type B uncertainty is obtained using supplement information and theoretical considerations (see e.g. Bucher (2004). Sometimes, the type B uncertainty is evaluated from supplement testing data processing, e.g. using subsets of the original data set. It can also be a result not of mathematical computation, but considerations based on the knowledge of the measurement procedures, observational history, and previous experience. Such procedures were used e.g. to derive the best estimates of some quantities related to Solar System dynamics (Pitjeva EV, 2009), and to compute realistic errors in radio source positions for the second realization of the International Celestial Reference Frame (Ma et al, 2009).

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