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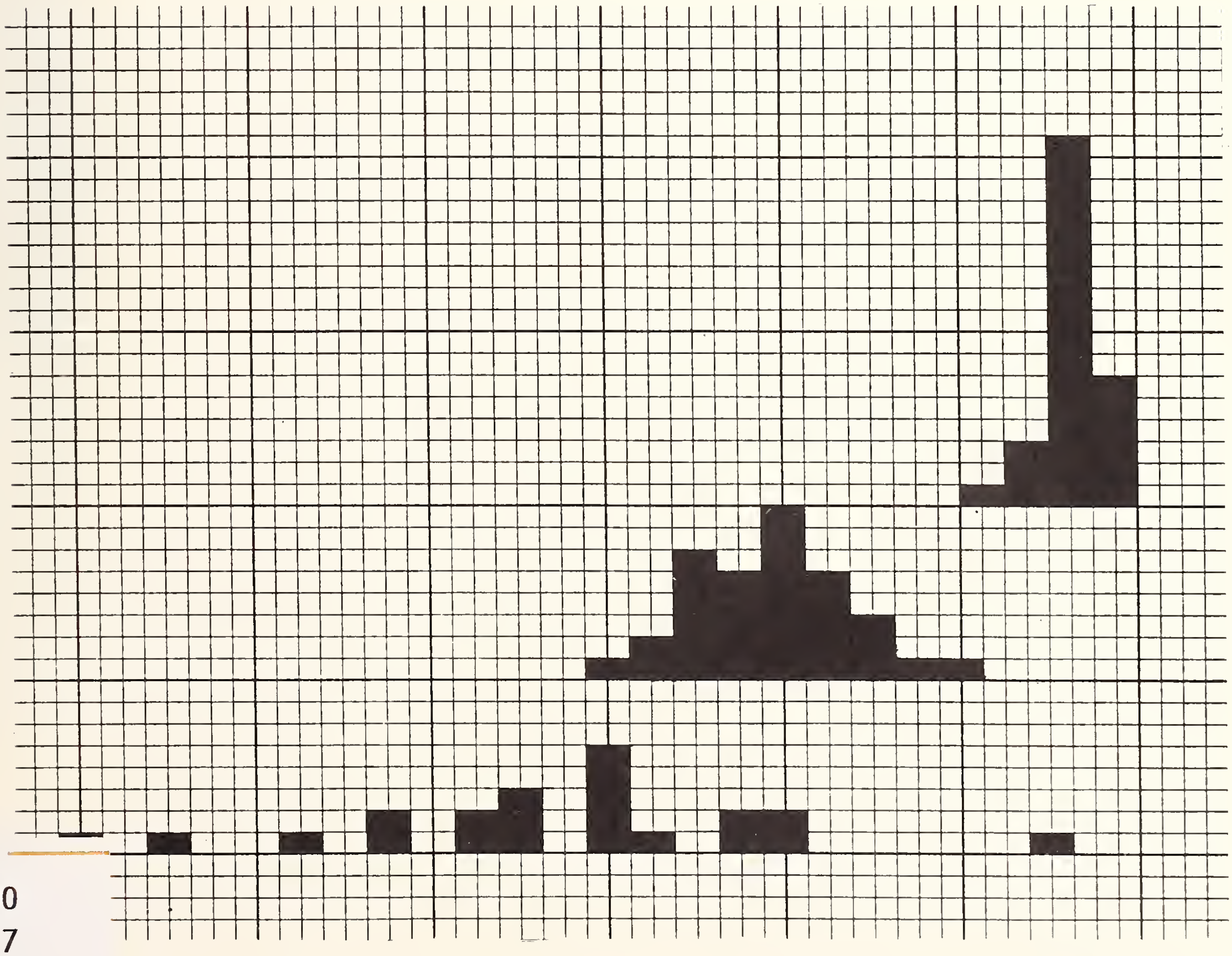
Uncertainty and Accuracy in Physical Measurements

Harry H. Ku



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UNCERTAINTY AND ACCURACY IN PHYSICAL MEASUREMENTS

Harry H. Ku*

ABSTRACT

The formulation of the "uncertainty" of a reported value always involves a certain degree of arbitrariness, depending primarily on how the value is going to be used. Currently there are at least two schools of thought on this subject: physicists interested in detecting differences among results are in favor of the recommendations of the International Bureau of Weights and Measures (BIPM/CIPM 1981), whereas those involved in calibration work and routine measurements follow the orthodox method (see e.g., NBS Special Publication 644).

In this note, the suggestion is made to use the word "accuracy/inaccuracy" for standards that follow BIPM's recommendation, and the word "uncertainty" for standards that follow the orthodox method. It is believed that the use of different terms for distinct purposes will resolve some of the basic difficulties facing international groups who are attempting to write their own standards.

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INTRODUCTION

"The question of what constitutes the most reliable value to be assigned as the uncertainty of any given quantity is one that has been discussed for many decades and, presumably, will continue to be discussed. It is a question that involves many considerations and by its very nature has no unique answer."

The above quotation from Raymond T. Birge in 1939 [1] can be said in 1990 just as well. In this note, we propose to look at "uncertainty" from a practical point of view, to give an interpretation of the word "uncertainty" for two main groups of users in measurement science, or metrology. In this way, we believe that intractable theoretical considerations can be avoided, and the usual emotional upheaval provoked by discussions on the subject may be minimized.

In section I we give a very brief historical background of the problems related to the use of the word "uncertainty" in metrology. In Section II we describe the objectives and needs of two groups of users, and suggest the use of the term "uncertainty" for one group, and the term "accuracy" for the other group. It is hoped that the use of those two terms may help to resolve the current debate.

I. Background

Up to about the 1980's, the "Orthodox" school of thought dominated procedures used in arriving at an uncertainty statement for reported values of repeated realizations of a particular experiment. A definitive account of this method is given in "Realistic Evaluation of the Precision and Accuracy of Instrument Calibration Systems" by Eisenhart of the National Bureau of Standards (NBS) in 1963 [2]. Recommendations for the expressions of the uncertainties of final results were published in Science in 1968 [3], and reprinted later with two additional papers in an NBS Special Publication [4]. A booklet "A Code of Practice for the Detailed Statement of Accuracy" by Campion et al. [5] of the National Physical Laboratory (NPL), reflected a similar line of reasoning.

Under this method, experimental errors are categorized into "random" and "systematic" components. The random components are those that can be treated statistically, with repeated measurements or as components of variance. Systematic components include those sources that influence in the same way all measurements which lead to the reported results. Credible (maximum) bounds to such sources of error are to be determined by the experimenters, and added linearly together as the systematic component. These two components, the random and the systematic, are propagated separately through the necessary steps, and combined at the end by linear addition if a single reported uncertainty is needed.

While the ideas underlying the traditional method are sound, they require a thorough understanding of some of the basic principles, e.g., what is a realistic "repetition" of a measurement? Are the measurements independent? Different interpretations by experimenters result, of course, in different uncertainty statements.

These difficulties have been particularly accentuated in international comparisons of standards and realization of units, where participating national laboratories report uncertainties of their measurements on different bases, with different interpretations. For those engaged in the adjustment of fundamental constants, different methods of expressing uncertainties also cause problems in weighing results reported by different experimenters. Thus in 1978 the International Bureau of Weights and Measures (BIPM) sent out a set of questionnaires on the assessment of uncertainties to more than 30 national laboratories and asked for their preference in error treatments and reasonings for their answers. The 21 replies received by BIPM were not unexpected. The only unanimous agreement was to question No. 1: "Should one recommend the use of the standard deviation to characterize the random uncertainty?" Every laboratory opted for "standard deviation of the reported value, together with its degrees of freedom."

The other questions revealed a wide divergence of opinions, especially regarding systematic errors and combination of errors to arrive at a final uncertainty statement. BIPM reported the result of its survey in 1980 [6], and convened a Working Group to study the problem. The Working Group produced a set of five rules for the report of uncertainties, which were recommended by BIPM in 1981 [7,8]. The chief sponsor of these rules was J. W. Müller, BIPM, who authored "Some second thoughts on Errors Statements" in 1979 [9]. Since that time, a working group has been drafting a "Guideline" to implement these rules, but so far nothing has been published.

The BIPM recommendations avoided the terms random and systematic uncertainties, using instead type A and type B uncertainties. Type A uncertainties are those evaluated by statistical methods, and Type B all others.

A "standard-deviation" like quantity is to be estimated by the experimenters for type B uncertainties and all uncertainties are to be combined by root-sum-of-squares. At the very end, the combined uncertainty <u>may</u> be multiplied by a factor k, where k might typically be 2 or 3. A comparison of the Orthodox and BIPM recommendation is shown on the next page. These two boxes are reproduced from a paper by Colclough of NPL in 1987 [10]. Colclough's paper made detailed studies and criticisms of both methods, and is recommended reading for serious students of uncertainty assessment.

Thus it appears that the orthodox method could be somewhat on the conservative side (leading to a potential overestimate of uncertainties) in requiring linear addition of all major systematic uncertainties. On the other hand, the root-sum-of-squares treatment of all uncertainties in the BIPM recommendation is too liberal (leading to a potential underestimate of uncertainties), and the estimation of a standard-deviation-like quantity for a systematic error leads to new problems. I believe, however, each method has its own field of application, depending on the <u>use</u> at which the uncertainty statement is aimed.

In international comparisons of standards, the aim is to put all national laboratories on the same basis, and thus one is looking for differences among laboratories. Large uncertainties reported by laboratories would only camouflage such differences, i.e., lead to the conclusion that these results are comparable, whereas, in fact, they may show discrepancies the analysis of which would be desirable.

Furthermore, systematic or type B errors usually dominate in upper echelon laboratories. Linear addition of these errors would result in a large uncertainty that defeats the purpose of international comparison. Hence, BIPM's rules, even taken as a committee decision, do serve the

Box 1. The BIPM's Recommendation for the Combination of Experimental Uncertainties

1. The uncertainty in the result of a measurement generally consists of several components which may be grouped into two categories according to the way in which their numerical value is estimated:

A - those which are evaluated by statistical methods,
B - those which are evaluated by other means.

There is not always a simple correspondence between the classification into categories A or B and the previously used classification into "random" and "systematic" uncertainties. The term "systematic uncertainty" can be misleading and should be avoided.

Any detailed report of the uncertainty should consist of a complete list of the components, specifying for each the method used to obtain its numerical value.

2. The components in category A are characterized by the estimated variances s_i^2, (or the estimated "standard deviations" s_i) and the number of degrees of freedom, ν_i. Where appropriate, the covariances should be given.

3. The components in category B should be characterized by quantities u_j^2, which may be considered as approximations to the corresponding variances, the existence of which is assumed. The quantities u_j^2 may be treated like variances and the quantities u_j like standard deviations. Where appropriate, the covariances should be treated in a similar way.

4. The combined uncertainty should be characterized by the numerical value obtained by applying the usual method for the combination of variances. The combined uncertainty and its components should be expressed in the form of "standard deviations."

5. If, for particular applications, it is necessary to multiply the combined uncertainty by a factor to obtain an overall uncertainty, the multiplying factor used must always be stated.

From ref. [10]

Box 2. Representative Orthodox Recommendations for the Combination of Experimental Uncertainties

The uncertainty on a measurement should be put into one of two categories depending on how the uncertainty is derived: a random uncertainty is derived by a statistical analysis of repeated measurement while a systematic uncertainty is estimated by nonstatistical methods.*

When combining the uncertainties on individual measurements in a complex experiment involving measurements on several physical quantities the two categories of uncertainties should be kept separate throughout.

In such an experiment the total random uncertainty should be obtained from the combination of the variances of the means of the individual measurement together with those associated with any constants, calibration factors, etc.

The component systematic uncertainties should be estimated in the form of maximum values or overall limits to the uncertainties.

In reporting measurements of the highest accuracy, a full statement of the result of an experiment should be in three parts, the mean corrected value, the random uncertainty, and the systematic uncertainty. The components that have contributed to the final uncertainty should be listed in sufficient detail to make it clear whether they would remain constant if the experiment were repeated. The estimate of the total systematic uncertainty should be stated. Each component of the systematic uncertainty should be listed, expressed as the estimated maximum value of that uncertainty. The method used to combine these component (systematic) uncertainties should be made clear.

The combination of random and systematic uncertainties to give an "overall uncertainty" is deprecated, but if in a particular case this is thought to be appropriate then it should be given in addition to the two uncertainties, together with the method of combination.

From ref. [10]

* I would prefer to rephrase the last part to: "... while a systematic uncertainty is estimated as a credible bound to an error that is likely to affect all the measurement in the same manner".

purpose. In fact, for those engaged in the adjustment of fundamental constants, the "k" factor is taken to be unity to sharpen the tools for the detection of discrepancies.

On the other hand, in measurement situations where a series of results is continuously monitored for an established measurement process, such as a calibration system for a standard, it might be undesirable to suspect a large percent of the results (k = 1) and try to search for assignable causes of error. Linear addition of major systematic errors plus a suitable measure of imprecision as suggested by the orthodox school serves the purpose much better. See for example, the concept of Measurement Assurance Program [11] adopted in the calibration of basic standards at NBS, now National Institute of Standards and Technology (NIST).

Up to the present time, much effort has been spent on arriving at a unique, correct, way of expressing uncertainty of reported results, neglecting the fact that different groups of users of the term have distinct purposes in mind. Any unique way of expressing uncertainty for one group of users cannot be satisfactory to the other group, and any compromise would fail both groups. Fortunately both the BIPM and the Orthodox recommendations include a requirement for a complete list of components of errors and how the numerical values are obtained. An excellent example is given in "A Measurement of the NBS Electrical Watt in SI Units" by P. Thomas Olsen et al. [12] where nine possible sources of error are listed and discussed in detail. With a detailed description of sources of error and their numerical magnitudes, users can then decide which of these errors are of concern to them and how they should be treated.

II. Different Objectives in the Use of the Term "Uncertainty"

We have stated in section I that there are two main groups of users of the term "uncertainty" in metrology, and each group uses the term to fulfill what they believe is the objective of their experiment(s). We will try to describe the work involved in the two groups, say: Group I and Group II.

Group I

Rolf is in charge of a calibration laboratory of a large aerospace concern, and is responsible for the accuracy of all calibrations performed in his laboratory. For a particular type of calibration, he has studied the physical theory in support of the method of calibration, purchased the necessary equipment and instruments, trained operators, and established the laboratory procedure to be followed for each operation. In addition, he has established the stability of his calibration process, both in long term mean values and variability of the results, by using a "check standard[1]." Since the test items are measured in the same manner as the check standard, he feels sure that the precision (σ) obtained from the series of measurements on the check standard will apply also to the test items.

There are about 1000 test items to be calibrated a year. Rolf has no reason to believe that any particular item would behave differently from the others since they are all treated in the same way. Being realistic, though, he knows that a small percentage will not be as close to what they should be purely by chance. Being conservative, he adopts $\pm 3\sigma$ limits as the random part of the uncertainty of

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[1] See, for example, section 3 of ref. [11].

his calibration. Rolf feels comfortable that more than 99 percent of his calibrated items will have random errors less than these limits.

Rolf realizes that there are errors inherent in his standards, instruments, operators, and procedures. These errors, however, affect all of his calibration results in the same direction and with the same magnitude. Hence, these errors are systematic in nature, i.e., they remain constant for each and every test item calibrated. Since they do not behave in the same manner as the random part of measurement, these errors should be kept separate from the random part. If two test items are calibrated by the same process, the systematic errors cancel out when the values of the two items are compared.

There are never enough resources and time to determine the systematic errors. Rolf studies the literature and manufacturer's claims, and estimates bounds to these errors. He reasons that, based on his judgment and experience, he would have noticed a departure if the actual errors were larger than his estimated bounds. Fortunately in his case, most of these errors are small compared to his random uncertainty.

Combining these systematic errors in his preferred fashion, Rolf reports uncertainty of the calibration results by the "Orthodox" method, i.e., 3σ limits for the random component, and an estimated bound for the systematic errors. Thus Rolf feels that the accepted value of the measurement is included in his uncertainty limits, so the user of his calibrated item does not have to worry about being wrong using his report. Let us call Rolf's uncertainty the "uncertainty." He is aiming for the coverage of his many results.

GROUP II

Richard is an outstanding physicist in a national laboratory. His work on the frontiers of experimental physics is recognized internationally. He has just developed an improved method to measure the lattice parameter of crystals. Using this method together with two other physical properties of silicon crystals, he feels that the value of a fundamental constant can be improved by an order of magnitude.

It took several years for Richard to build his instruments, refine his technique, and coordinate work performed by his colleagues in measuring the other two properties. His final result was published in a short note in Physics Review Letters, with an uncertainty of 1 ppm. This uncertainty, representing one standard deviation of the reported value, is computed from the standard deviations of the lattice parameter and the other two properties through error propagation. Essentially Richard followed the BIPM recommendations in arriving at his uncertainty. We shall call an uncertainty derived in this manner the "accuracy," because the focus here is for the closeness of this result to the quantity of interest.

We note that:

1. This experiment will never be performed again using the same instrumental setup and procedures.
2. The result of this experiment will be compared with the results of all other experiments for the quantity of interest, perhaps using entirely different theories and approaches.

3. In comparing this result with other results, physicists are interested in differences only. The differences may indicate unknown systematic errors, or perhaps defects in theories. The advance of physics depends heavily on understanding and finding out why these differences exist.
4. If the orthodox uncertainty is used here, many of the differences could be camouflaged, and no additional insight gained.

Let us call Richard's uncertainty the "accuracy." He is aiming to discover differences between results.

OTHER USERS

The two main groups of users discussed above are certainly not exhaustive. Uncertainty introduced by errors in sampling, i.e., variabilities among the items measured, is usually not an essential part of a measurement system devoted to obtaining a single numerical characteristic of a single item, or of a group of highly homogeneous items. However, such problems do exist for some sectors of the scientific community, e.g., the tabulator of atomic weights table.

We look for the atomic weight of silicon in a table. The numerical value we find in the table is supposed to apply to all "pure" silicons irrespective of source. Thus the "uncertainty" attached to this value must include a component due to variabilities of isotopic composition of terrestrial silicons. Uncertainties due to measurements are only a small part of the total.

In other applications, the sources of variabilities may be so diverse and numerous as to defy an exhaustive analysis. In such cases, the only objective is to write a Standard so that all concerned parties will use the same method of calculation. An example is ANSI/ASME Performance Test Codes 19.1-1985 [13].

III. CONCLUSIONS

In the above section we have identified two main groups of users of the term "uncertainty" in the field of metrology. Group I uses the term to denote the "sameness" of their repeated measurement results, and Group II uses the term as a yard stick to measure "differences" between results. Since their objectives are basically at odds, there is no way to define uncertainty uniquely to satisfy both groups. One solution to this quandary is to define uncertainty for those who are worried about type-I error, false findings of differences between results, and accuracy for those who are worried about type-II error, or false findings of agreement between results. Using orthodox recommendations, one arrives at uncertainty. Using BIPM recommendations, one arrives at accuracy.

In Table 1 we summarize and compare the two groups and give examples to illustrate likely members of each group.

Table 1

THE TWO FACES OF UNCERTAINTY

Group I	Group II
Experimental Set-Up	
· Established measurement process	· Highly individualized experiments
· Repeated realizations	· Parameters changing from experiment to experiment
· Precision "σ" known, Components of variance allowed for	· Precision "s" computed from within experiment
· Systematic errors treated separately	· Type B errors treated in the same way as precision
Frame of Reference	
· Results produced by the particular measurement process in a laboratory	· Results of any and all experiments leading to the quantity of interests
Emphasis	
· "Sameness" of measured values	· Detection of differences in results that may contribute to theory, or to the next experiment
· Results intended for a large group of users	· Results compared to results of other individual experiments
Examples	
· Calibrations of standard items	· Fundamental constants
· Standard reference materials	· International comparisons
· Test methods	· Breakthrough experiments
· Clinical laboratories	· Counterexamples to theories
· Most macroscopic measurements	· Most atomic-scale measurements
Suggested Terms to be Used for the Expression of Dubiety	
· Uncertainties (applicable to a large number of results)	· Accuracy (to within xx of the quantity of interest)
· Orthodox recommendations: 2 or 3σ added linearly to estimated bounds of systematic errors	· BIPM recommendations: 1s added to type-B uncertainties by root-sum-of-squares

* * * * *

"Obtaining a valid measure of uncertainty is not just a matter of looking up a formula."
Mosteller and Tukey

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The formulation of the "uncertainty" of a reported value always involves a certain degree of arbitrariness, depending primarily on how the value is going to be used. Currently there are at least two schools of thought on this subject: physicists interested in detecting differences among results are in favor of the recommendations of the International Bureau of Weights and Measures (BIPM/CIPM 1981), whereas those involved in calibration work and routine measurements follow the orthodox method (see e.g., NBS Special Publication 644).

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12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)

accuracy; BIPM recommendations; inaccuracy; orthodox method; standards; uncertainty

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