Significant figures

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The appropriate number of significant figures is important in order to have a meaningful level of resolving power when reporting analytical concentrations. Various methods or criteria can be used when estimating how many significant figures are needed. In most cases three significant figures (two true plus one uncertain) are sufficient.

Measured and/or specified uncertainty can used to estimate the number of true figures of results [1].

For quality assurance applications it is suggested to use at least one more/extra significant figure [2].

If the data handling includes manual data entry or visual inspection of results, a high number of significant figures should be avoided.

Background

The way we present numerical data in everyday life, in speech or written documents, is intuitively adjusted to convey only the necessary information about the quantities in question and to imply the inherent precision.

For example, when you are asked at the bus station, *"How long do we have to wait (until the bus is due to arrive)?"* you usually tend to give the estimated time in full minutes, even in full five minutes if the expected waiting time is long enough. In most cases this level of uncertainty is considered acceptable and also reflects the average person's time-keeping accuracy. Any requests of a more accurate estimate would be considered unreasonable.

On the other hand, if the expected waiting time is expressed including also the seconds, most people would see it as an exaggeration, even if the given waiting time is correct. The above-mentioned applies also to a more formal handling of numerical data, presentations, inserts, manuals, etc.

The information we want to transfer and how it is used influences the way we are supposed to present the numbers and how many significant figures we need to have.

Any figure of a number is significant if it is essential to fulfill the information transfer, and the true value of it is traceable to some phenomena that (sometimes) allow it to be reproduced when needed.

A simple and useful definition of significant figures is [3, 4]:

- The number of significant figures in a measured quantity is the number of digits that are known accurately, plus one that is uncertain.
- Zeroes that appear to the left of the first non-zero digit are placeholders and are not considered significant.
- Zeros located to the right of the first digit may be considered significant.

In some cases the originator of the information can provide an excess of true figures and the number is rounded off to contain only the necessary significant figures. The last significant figure is inherently uncertain because of the rounding off. The rounding-off uncertainty is usually half of the last figure's decimal-place value if no other uncertainty is expressed.

The indication of the rounding off is crucial when presenting numerical data as the dropped figures are replaced with (insignificant) placeholder zeros, if needed. If there is no indication of the uncertainty, the reader has (no other possibility than) to expect the number to contain only significant figures, the last of which is uncertain. All other interpretations can be misleading or wrong, even if based on common practices.

As a rule of thumb results of measurements and calculations have a limited number of significant figures. The results of calculations have no more significant figures than the least accurate number used in the calculations.

It should be noted that the only time that significant digits must be considered is when dealing with measured quantities. Exact or defined numbers should be considered to have an infinite number of significant digits. These are numbers that would not affect the accuracy of a calculation.

As seen above a number presented in a written document should be expressed together with the associated uncertainty if it is important to avoid any misunderstanding. And if you use a number presented in a written document, you should know the uncertainty of the number or how many significant figures it has.

How the number of significant figures reflects the uncertainty

The examples in Table I show the reported value with some of the possible interpretations of the uncertainty. Note that the values are expressed without any indication of the uncertainty or information on the number of significant figures.

The number of significant figures of a measured result can be based either on the absolute or relative accuracy of the measurement.

Significant figures on result with absolute accuracy

If the uncertainty of a result is based on the absolute accuracy of the method, the number of significant figures can be estimated using the following simple three-step procedure:

1. Round the uncertainty to two significant figures.
2. Round the result to the last figure affected by the first figure (decimal place) of the uncertainty.
3. Report the rounded result and uncertainty.

An example where the rounded value is for reporting purposes only:

The measured concentration of a D-dimer sample is 285.41 ng/mL. The (calculated, estimated, manufacturer's claim, etc.) uncertainty is 33.4875 ng/mL (11.7 %).

Start with rounding the uncertainty to two significant figures, i.e. 33 mg. Then, round the result to the one less number of decimal places as the uncertainty statement, i.e. 290 ng/mL. Report the result as 290 ng/mL ± 33 ng/mL.

Situation	Value reported	Possible interpretation of uncertainty	Significant digits in value
The waiting time when asked at the bus station	4 min	± 30 sec	1
	10 min	± 5 min	1
		± 30 sec	2
Patient's CKMB concentration	200 ng/mL	± 50 ng/mL	1
		± 5 ng/mL	2
		± 0.5 ng/mL	3
Number of people attending a meeting	100 persons	± 50 persons	1
		± 5 persons	2
		± 0 persons	3
Patient's troponin I concentration	0.071 ng/mL	± 0.0005 ng/mL	2
	4.03 ng/mL	± 0.005 ng/mL	3

TABLE I: Reported values and interpretation of uncertainty

Relative standard deviation	Standard deviation	Significant figures of result
1 % > RSD ≥ 0.1 %	0.001	4
10 % > RSD ≥ 1 %	0.01	3
20 % > RSD ≥ 10 %	0.1	2
RSD ≥ 20 %	0.2	1

TABLE II: Significant figures based on relative standard deviation

285.41 ng/mL ± 33.4875 ng/mL -> 290 ng/mL ± 33 ng/mL

Significant figures on result with relative accuracy

If the uncertainty of the result is based on the relative accuracy (Relative Standard Deviation, RSD) of the measuring method, the suitable number of significant figures can estimated using the following rule of thumb.

In many cases the observed relative measurement error is in the order of 1-10 % of the measured value. This uncertainty level suggests using no more than three figures when reporting the results.

Calculations

If the result is intended to be used as an intermediate part of calculations, one or more figures can be added to assure more accurate calculation results [1].

The data used in the quality assessment calculations can be considered to be an intermediate part of the calculations and thus the rounding off is not applied or is different (one more significant figure) until all the calculations (coefficient of variation, mean, etc.) have been completed. If an insufficient number of significant figures are used (in the evaluation of methods), significant errors in estimating the statistical parameters can result [2].

Data entry into calculators or computers should include all of the available digits from the instrument generating the data. Some instrument outputs contain an excessive number of figures. In these cases data entry should be at least five figures (if available) to prevent error due to successive rounding.

Once the appropriate number of significant figures has been established, the excessive figures can be cut off.

Rounding-off rules

There is no law against reporting (too) many figures if they are considered to be accurate, but an excessive number of significant figures can lead to unnecessary confusion.

The rounding off is an integral part of the numerical data presentation. The general rules applied, for example by spreadsheet calculators, are usually satisfactory to drop off the excess decimals. There are, however, some special cases where it is preferable to apply more sophisticated methods.

Once the number of wanted significant figures in the result is established, rounding off the excessive figures follows the standard rules.

Basic rounding-off rules are based on the value of the first dropped figure:

- Less than 5, round down
(2.6342 to two decimal places => 2.63)
- Higher than 5, round up
(2.6351 to two decimal places => 2.64)
- Exactly 5 (only zeros follow), round up
(2.6350 to two decimal places => 2.64)

Please note that the National Institute of Standards and Technology (NIST) and NCCLS suggest rounding off to the closest even figure in case the first dropped figure is exactly 5. This secures more balanced statistics if there is a lot of data that has 5 as the last non-zero figure.

The uncertainty caused by the rounding to three figures is in the order of ± 0.5 % or less, which in the majority of cases is considered to be acceptable for all analytes and concentration ranges.

Extra significant figures of a reported result can lead to unnecessary confusion when evaluating the result against acceptance criteria (limits) expressed as concentration units.

Let us assume that the measured value is expected to be less or the same (≤) as the limit concentration.

The reported value is 2003 ng/mL and the acceptance criterion is ≤ 2000 ng/mL. Let us further assume that the measurement uncertainty is specified to be < 5 % suggesting a rounding off to be done at three significant figures (two true figures plus one uncertain). Using the simple rules above the measured concentration would be reported as 2000 ng/mL.

The rounded off concentration value can be accepted without compromising the quality criterion. The result with four reported figures would lead to false rejection unless extra steps were taken to accept the result.

Table III and Table IV present two examples of 21 measured values. The original data has five significant figures.

These data has been rounded off to respectively four, three and two significant figures, the respective coefficient of variation (CV) are calculated and the quality control test status (passed or check) is reported. All the CVs are reported with two decimal places for the sake of demonstrating differences.

Significant figures				Significant figures			
5	4	3	2	5	4	3	2
Measured concen-tration	Reported concentration			Conclusion based on reported concentration Acceptance criterion: concentration ≤ 2.50			
2.3895	2.390	2.39	2.4	Passed	Passed	Passed	Passed
2.4005	2.401	2.40	2.4	Passed	Passed	Passed	Passed
2.4116	2.412	2.41	2.4	Passed	Passed	Passed	Passed
2.4226	2.423	2.42	2.4	Passed	Passed	Passed	Passed
2.4337	2.434	2.43	2.4	Passed	Passed	Passed	Passed
2.4447	2.445	2.44	2.4	Passed	Passed	Passed	Passed
2.4558	2.456	2.46	2.5	Passed	Passed	Passed	Passed
2.4668	2.467	2.47	2.5	Passed	Passed	Passed	Passed
2.4779	2.478	2.48	2.5	Passed	Passed	Passed	Passed
2.4889	2.489	2.49	2.5	Passed	Passed	Passed	Passed
2.5000	2.500	2.50	2.5	Passed	Passed	Passed	Passed
2.5111	2.511	2.51	2.5	Check	Check	Check	Passed
2.5221	2.522	2.52	2.5	Check	Check	Check	Passed
2.5332	2.533	2.53	2.5	Check	Check	Check	Passed
2.5442	2.544	2.54	2.5	Check	Check	Check	Passed
2.5553	2.555	2.56	2.6	Check	Check	Check	Check
2.5663	2.566	2.57	2.6	Check	Check	Check	Check
2.5774	2.577	2.58	2.6	Check	Check	Check	Check
2.5884	2.588	2.59	2.6	Check	Check	Check	Check
2.5995	2.600	2.60	2.6	Check	Check	Check	Check
2.6105	2.611	2.61	2.6	Check	Check	Check	Check
CV, %				Fraction of rejected results			
2.74	2.74	2.77	3.10	10/21	10/21	10/21	6/21

TABLE III: Effect of significant figures on acceptance, example 1

Significant figures				Significant figures			
5	4	3	2	5	4	3	2
Measured concen-tration	Reported concentration			Conclusion based on reported concentration Acceptance criterion: concentration ≤ 23400			
22940	22940	22900	23000	Passed	Passed	Passed	Passed
22986	22990	23000	23000	Passed	Passed	Passed	Passed
23032	23030	23000	23000	Passed	Passed	Passed	Passed
23078	23080	23100	23000	Passed	Passed	Passed	Passed
23124	23120	23100	23000	Passed	Passed	Passed	Passed
23170	23170	23200	23000	Passed	Passed	Passed	Passed
23216	23220	23200	23000	Passed	Passed	Passed	Passed
23262	23260	23300	23000	Passed	Passed	Passed	Passed
23308	23310	23300	23000	Passed	Passed	Passed	Passed
23354	23350	23400	23000	Passed	Passed	Passed	Passed
23400	23400	23400	23000	Passed	Passed	Passed	Passed
23446	23450	23400	23000	Check	Check	Passed	Passed
23492	23490	23500	23000	Check	Check	Check	Passed
23538	23540	23500	24000	Check	Check	Check	Check
23584	23580	23600	24000	Check	Check	Check	Check
23630	23630	23600	24000	Check	Check	Check	Check
23676	23680	23700	24000	Check	Check	Check	Check
23722	23720	23700	24000	Check	Check	Check	Check
23768	23770	23800	24000	Check	Check	Check	Check
23814	23810	23800	24000	Check	Check	Check	Check
23860	23860	23900	24000	Check	Check	Check	Check
CV, %				Fraction of rejected results			
1.22	1.22	1.25	2.13	10/21	10/21	9/21	8/21

TABLE IV: Effect of significant figures on acceptance, example 2

In these two data sets the observed CV is relatively stable, the rounding off starts to change the statistics only at the two-significant-figures level. The fraction of rejected results is affected more, the change from 10/21 to 6/21 (example 1) or 8/21 (example 2) is significant.

It should be noted that the change had been to higher fraction of rejected results had the acceptance criterion been set differently (< 2.50 instead of ≤ 2.50 or < 23400 instead of ≤ 23400).

The calculated CV values and the fraction of rejected results in the examples suggest to choose the number of significant figures according the resolving power of the method and the quality control needs.

The data of the examples also stress the importance of using a sufficient number of significant figures when calculating the statistical parameters. The coefficient of variation is often reported with one decimal place or two significant figures, whichever is greater. Using less than three/four significant figures in the calculations can affect the results.

Method 1	Method 2
0.54233	0.64513
0.62127	0.52462
0.59184	0.54628
0.54113	0.52272
0.63299	0.62152
Average	Average
0.585912	0.572054

TABLE V: Method comparison

	Significant figures				
	All	5	4	3	2
Average method 1	0.585912	0.585910	0.5859	0.586	0.59
Average method 2	0.572054	0.572050	0.5721	0.572	0.57
Difference method 1 - method 2	0.013858	0.01386	0.0138	0.014	0.02
Mean method 1 - method 2	0.578983	0.57898	0.5790	0.579	0.58
Difference % method 1 - method 2	2.394	2.394	2.383	2.418	3.448

TABLE VI: Calculations based on method comparison

Table V and Table VI show a simple example of how the rounding off affects the calculated relative difference between the two methods' averages.

Again, the optimum number of significant figures seems to be approximately three or four figures. If the data handling includes any kind of manual data entry or visual inspection of results, it is advisable to limit the number of figures to four if there is no specific reason to keep it higher.

References

1. EURACHEM / CITAC Guide CG 4, Quantifying Uncertainty in Analytical Measurement, Second Edition, QUAM:2000.1

2. CLSI/NCCLS EP13-R. Laboratory Statistics – Standard Deviation; A Report.

3. PPI Guide to Significant Digits and Rounding Numbers.

4. NREL/TP-510-42626, Technical Report, Rounding and Significant Figures