Error Analysis in Experimentation

Experimentation involves observations, measurements, and analyses.

The quality of the final results, assessed by the reliability of data, depends on the *quality of the measurements* and the rigor with which the data are analyzed.

Central to the critical analysis of experimental data is a thorough understanding of the sources and the magnitudes of the errors associated with it.

There are always limitations in discovering the "ultimate reality" about a system that we wish to characterize.

These limitations cause discrepancies between our experimental result and the "true value" of the quantity of interest.

The fact is that the true value is defined in statistics as the mean of the sample population composed of an infinite number of measurements.

Implication: that any result obtained from a finite set of data may be in error to some extent.

The sources of error are categorized as systematic and random.

A systematic error arises from a bias that is placed on the measurement either by the instrument itself or by a consistently improper method of reading the instrument.

Random errors arise from intrinsic limitations in the sensitivity of the instrument and in the ability of the user to interpret the instrument’s output.

Many measurements of a quantity are likely to be slightly different each time the measurement is made.

These fluctuations in the reading would be caused by the inherent inability of the electronic and mechanical components of the balance to function absolutely reproducibly.

It is possible to observe a pattern in the observed random fluctuations of the measurements and they can be characterized.

There exists a distribution of such measured values and it can be expressed in a definite mathematical way (Gaussian distribution).

Accuracy and Precision

An experimental measurement has high precision if the random errors (fluctuations) are small. Many significant figures are justified.

A measurement is accurate if there are small systematic errors. If so there is no intrinsic bias to the measurement, and its value approaches the true or accepted one.

There is no relationship between accuracy and precision. An experiment can have small random errors and still give inaccurate results due to large systematic errors.

An experiment with large random errors may still be accurate in the sense that the "true" or accepted value lies within the limits of error reported.

Another type of error is sometimes referred to as a "blunder", a mistake. It is often evidenced by way the data point "sticks out".

It is considered acceptable to throw this data point out, and there are rigorous statistical tests that can be applied to justify this decision.

Systematic errors can also be *minimized* through proper instrument calibration and more careful experimental practices.

Yet another type of error, sometimes referred to as a "model error," is less obvious and potentially more serious than a blunder.

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Model errors can be difficult to detect because it is often easier to mistrust your data than to question the validity of the theory that is supposed to be demonstrated by them.

Data are the facts on which science is built, and theories that do not conform to the facts must be modified or rejected.

Estimating Properties

Mean

If a measurement of some property x of a system is repeated several times the *mean or average value of x*, on which n independent measurements have been made *is defined as*,

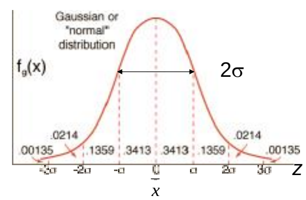
$$\bar{x} = \frac{1}{n}\sum_i x_i$$

If the *errors* associated with the measurements are completely *random in nature*, the data distribution follows a Gaussian distribution and *mean is the best* <u>*estimate*</u> *of the true value* of the property that can be obtained.

Standard Deviation, S

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/(2\sigma^2)}$$

σ = population standard deviation



The *sample variance*, S^2, which is defined as;

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

$$= \frac{n}{n-1}(\overline{x^2} - \bar{x}^2)$$

S = sample standard deviation

$S \rightarrow \sigma$ as $N \rightarrow \infty$.

S quantifies the precision/uncertainty/error (dispersion of data about the mean). For large n and data randomly distributed, ~68% of the data fall within $\pm\,\sigma$ units of the mean.

When multiple variables contribute to uncertainty, the overall variance is the sum of the variances from each variable.

Standard Error (Standard Error of the mean) S_m

If two series of measurements are made on the same system, the average value determined from the first series will in all likelihood be different from the value obtained from the second.

If a large number of these series were performed, the respective mean values would be symmetrically distributed about the "true value," and the standard deviation of the such a distribution is defined as the *standard error of the mean* would be given by,

$$S_m = \frac{S}{\sqrt{n}}$$

The precision of the mean can be raised by increasing n.

Confidence Limits

Once S_m is determined, confidence limits can be obtained. The range on both sides of the mean within which the "true value, μ" can be expected to be found for a degree of "confidence of c%"

The range ±δ is calculated from error/uncertainty δ, calculated from,

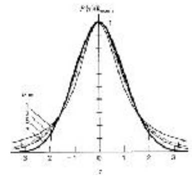
$$¢ = \pm \frac{S}{\sqrt{n}} t_{c\%}$$

t = Students t value taken from Students t table.

Student's t Distribution

In practice the replications, n ≠∞, and is finite, often n < 20. The best estimate of true value is still the average, and even though S and S_m can be calculated its usefulness is unclear because the probability distribution (Gaussian) is unknown.

The *distribution function that would apply to limited n* (therefore limited ν (=n-1) with an unknown σ is the Student's t distribution P(τ).



$$¢ = \frac{S}{\sqrt{n}} t_{c\%} = \text{c\% CL}$$

$$\Delta = t_{0.95} \frac{S}{\sqrt{n}} = \text{95\% CL}$$

Student's t distributions P(τ) for ν=1, 3, 5, ..

t depends on confidence level & n

Table 4-2 Values of Student's *t*

ν=n-1

ν Degrees of freedom	Confidence level (%) 50	90	95	98	99	99.5	99.9
1	1.000	6.314	12.706	31.821	63.657	127.32	636.619
2	0.816	2.920	4.303	6.965	9.925	14.089	31.598
3	0.765	2.353	3.182	4.541	5.841	7.453	12.924
4	0.741	2.132	2.776	3.747	4.604	5.598	8.610
5	0.727	2.015	2.571	3.365	4.032	4.773	6.869
6	0.718	1.943	2.447	3.143	3.707	4.317	5.959
7	0.711	1.895	2.365	2.998	3.500	4.029	5.408
8	0.706	1.860	2.306	2.896	3.355	3.832	5.041
9	0.703	1.833	2.262	2.821	3.250	3.690	4.781
10	0.700	1.812	2.228	2.764	3.169	3.581	4.587
15	0.691	1.753	2.131	2.602	2.947	3.252	4.073
20	0.687	1.725	2.086	2.528	2.845	3.153	3.850
25	0.684	1.708	2.060	2.485	2.787	3.078	3.725
30	0.683	1.697	2.042	2.457	2.750	3.030	3.646
40	0.681	1.684	2.021	2.423	2.704	2.971	3.551
60	0.679	1.671	2.000	2.390	2.660	2.915	3.460
120	0.677	1.658	1.980	2.358	2.617	2.860	3.373
z → ∞	0.674	1.645	1.960	2.326	2.576	2.807	3.291

t drops with increasing n

NOTE: In calculating confidence intervals, σ may be substituted for *s* in Equation 4-6 if you have a great deal of experience with a particular method and have therefore determined its "true" population standard deviation. If σ is used instead of *s*, the value of *t* to use in Equation 4-6 comes from the bottom row of Table 4-2.

Expression of numerical results:

Sample mean ± Δ (95% Confidence level, n = #)

True mean = μ.

Confidence Limits

Within what values would μ (the population mean) be, so that one can be c% confident that μ is indeed in that interval?

The confidence limits and interval are calculated using,

$$« = \bar{x} \pm ¢$$

$$\text{confidence limits} \quad \bar{x} - \frac{tS}{\sqrt{n}} \leq « \leq \bar{x} + \frac{tS}{\sqrt{n}}$$

$$\text{confidence interval} \quad \bar{x} - \frac{tS}{\sqrt{n}} \; and \; \bar{x} + \frac{tS}{\sqrt{n}}$$

Find the value of ***Student's t*** from tables relevant to (n-1) degrees of freedom at desired c% confidence.
n = # replications

Rejection of outliers: Q Test

Outliers are not always obvious. To reject a suspicious data point from set of n data points, where there is no obvious gross error, the Q test is used.

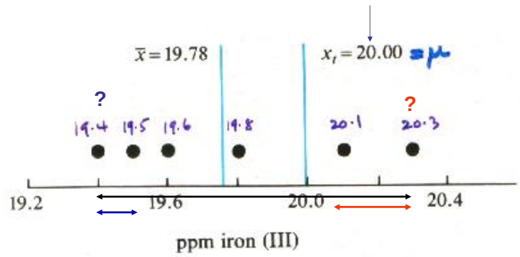
a. Arrange the data in the order of increasing value.

b. Determine the range = (x_{max} - x_{min})

c. Find the difference between the data point in question, and its nearest neighbor. gap = $|X_q - X_n|$

d. Calculate the rejection quotient Q_{calc} as; $Q_{calc} = \frac{\text{gap}}{\text{range}}$

e If $Q_{calc} < Q_{table}$ for the n, accept x_q for a given confidence level, 90% - norm. (> i.e 10% chance it is an outlier).



Outliers, if exists appear at the extremes.

Table 4-6 Values of Q for rejection of data

Q (90% confidence)[a]	Number of observations
0.76	4
0.64	5
0.56	6
0.51	7
0.47	8
0.44	9
0.41	10

a. Q = gap/range. If $Q_{calculated} > Q_{table}$, the value in question can be rejected with 90% confidence.

SOURCE: R. B. Dean and W. J. Dixon, *Anal. Chem.* **1951**, *23*, 636; see also D. R. Rorabacher, *Anal. Chem.* **1991**, *63*, 139.

Rejection of outliers: Grubbs Test

Calculate the Grubbs statistic.

$$G_{calc} = \frac{|questionable\ value - \bar{x}|}{S}$$

Compare G_{calc} vs Critical table values for G for n observations

If $G_{calc} < G_{table}$; accept the questionable value at 95% CL.

TABLE 4-5 Critical values of G for rejection of outlier

Number of observations	G (95% confidence)
4	1.463
5	1.672
6	1.822
7	1.938
8	2.032
9	2.110
10	2.176
11	2.234
12	2.285
15	2.409
20	2.557

$G_{calculated}$ = |questionable value − mean|/s. If $G_{calculated} > G_{table}$, the value in question can be rejected with 95% confidence. Values in this table are for a one-tailed test, as recommended by ASTM.

SOURCE: ASTM E 178-02 Standard Practice for Dealing with Outlying Observations, http://webstore.ansi.org; F. E. Grubbs and G. Beck, Technometrics 1972, 14, 847.

Harris, *Quantitative Chemical Analysis, 8e*

Discarding Data

Another method for deciding whether a data point can be justifiably discarded is to evaluate the mean without the 'suspect data point'.

Then determine if this point deviates from the mean by more than four times the *average deviation* of the other points.

The *average deviation* is defined as,

$$d_{av} = \frac{1}{n}\sum_{i=1}^{n}\left|x_i - \bar{x}\right|^2$$

Propagation of (Random) Errors

Once measurements (x, y, z..) are made and estimates of the uncertainties associated with each of the individual measurements have been obtained Δx, Δy, Δz .., their combined effect on the quantity of interest, F, must be assessed.

This procedure is known as the propagation of errors.

$$F = f(x, y, z,..)$$

Then, $dF = \frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial y}dy + \frac{\partial F}{\partial z}dz + ...$ for infinitesimal changes

$\Delta F = \frac{\partial F}{\partial x}\Delta x + \frac{\partial F}{\partial y}\Delta y + \frac{\partial F}{\partial z}\Delta z + ...$ for finite changes

i.e. error in F, $\Delta F = \pounds(F) = \frac{\partial F}{\partial x}\pounds(x) + \frac{\partial F}{\partial y}\pounds(y) + \frac{\partial F}{\partial z}\pounds(z) + ...$

$F = f(x, y, z, ..)$

$$£(F) = \frac{\partial F}{\partial x}£(x) + \frac{\partial F}{\partial y}£(y) + \frac{\partial F}{\partial z}£(z) + ...$$

Squaring and eliminating the high order terms leads to,

$$[£(F)]^2 = \left(\frac{\partial F}{\partial x}\right)^2 [£(x)]^2 + \left(\frac{\partial F}{\partial y}\right)^2 [£(y)]^2 + \left(\frac{\partial F}{\partial z}\right)^2 [£(z)]^2 + ...$$

Assuming uncertainty $£(F) = S(F)$; $[£(F)]^2 = S^2(F)$

analogously, $S^2(F) = \left(\frac{\partial F}{\partial x}\right)^2 S^2(x) + \left(\frac{\partial F}{\partial y}\right)^2 S^2(y) + \left(\frac{\partial F}{\partial z}\right)^2 S^2(z) + ...$

and $\Delta^2(F) = \left(\frac{\partial F}{\partial x}\right)^2 \Delta^2(x) + \left(\frac{\partial F}{\partial y}\right)^2 \Delta^2(y) + \left(\frac{\partial F}{\partial z}\right)^2 \Delta^2(z) + ...$

Only variances are additive, not standard deviations!

$$£(F) = \frac{\partial F}{\partial x}£(x) + \frac{\partial F}{\partial y}£(y) + \frac{\partial F}{\partial z}£(z) + ...$$

and $\Delta^2(F) = \left(\frac{\partial F}{\partial x}\right)^2 \Delta^2(x) + \left(\frac{\partial F}{\partial y}\right)^2 \Delta^2(y) + \left(\frac{\partial F}{\partial z}\right)^2 \Delta^2(z) + ...$

and $\Delta^2(F) = (Dx)^2 (\Delta x)^2 + (Dy)^2 (S\Delta y)^2 + (Dz)^2 (S\Delta z)^2 + ...$

$S^2(F) = (Dx)^2 (Sx)^2 + (Dy)^2 (Sy)^2 + (Dz)^2 (Sz)^2 + ...$

$S^2(F) = (Dx)^2 (Sx)^2 + (Dy)^2 (Sy)^2 + (Dz)^2 (Sz)^2 + ...$

Some general examples:

1. For $F = ax \pm by \pm cz$,

$$\Delta^2(F) = a^2\Delta^2(x) + b^2\Delta^2(y) + c^2\Delta^2(z)$$

2. For $F = axyz$ (or axy/z or ax/yz or a/xyz),

$$\frac{\Delta^2(F)}{F^2} = \frac{\Delta^2(x)}{x^2} + \frac{\Delta^2(y)}{y^2} + \frac{\Delta^2(z)}{z^2}$$

3. For $F = ax^n$,

$$\frac{\Delta^2(F)}{F^2} = n^2\frac{\Delta^2(x)}{x^2} \rightarrow \frac{\Delta(F)}{F} = n\frac{\Delta(x)}{x}$$

4. For $F = ae^x$,

$$\Delta^2(F) = a^2e^{2x}\Delta^2(x) \rightarrow \frac{\Delta(F)}{F} = \Delta(x)$$

5. For $F = a \ln x$,

$$\Delta^2(F) = \frac{a^2}{x^2}\Delta^2(x) \rightarrow \Delta(F) = a\frac{\Delta(x)}{x}$$

$$F = C\frac{x^2}{y} \qquad \Delta^2(F) = \left(\frac{2Cx}{y}\right)^2\Delta^2(x) + \left(\frac{Cx^2}{y^2}\right)^2\Delta^2(y)$$

$$F = C\frac{x^2}{y}$$

If the general approach using the following expression;

$$\Delta^2(F) = \left(\frac{\partial F}{\partial x}\right)^2 \Delta^2(x) + \left(\frac{\partial F}{\partial y}\right)^2 \Delta^2(y)$$

We get, $\Delta^2(F) = \left(\frac{2Cx}{y}\right)^2\Delta^2(x) + \left(\frac{Cx^2}{y^2}\right)^2\Delta^2(y)$

The expression for F is can be such that the functional form requires care to justify a breakdown of the procedure into steps.

F = f (A, B) where A = f(x_1, x_1, ..) and B = f(y_1, y_1, ..) with A and B independent.

$$\Delta^2(F) = \left(\frac{\partial F}{\partial A}\right)^2\Delta^2(A) + \left(\frac{\partial F}{\partial B}\right)^2\Delta^2(B) \cdot$$

$$\Delta^2(A) = \left(\frac{\partial A}{\partial x_1}\right)^2\Delta^2(x_1) + \left(\frac{\partial A}{\partial x_2}\right)^2\Delta^2(x_2)$$

$$\Delta^2(B) = \left(\frac{\partial B}{\partial y_1}\right)^2\Delta^2(y_1) + \left(\frac{\partial B}{\partial y_2}\right)^2\Delta^2(y_2)$$

If the terms A, B, etc.. are not independent the error calculated in this manner will be incorrect.

e.g. F = a($e^{\lambda x}$ -1) + b(y-cx) = A + B

$$\Delta^2(F) = \Delta^2(A) + \Delta^2(B)$$

~~$\Delta^2(A) = (ake^{kx})^2\Delta^2(x)$~~ $\qquad \Delta^2(B) = b^2\Delta^2(y) + b^2c^2\Delta^2(x)$

If the general approach using the following expression;

$$\Delta^2(F) = \left(\frac{\partial F}{\partial x}\right)^2 \Delta^2(x) + \left(\frac{\partial F}{\partial y}\right)^2 \Delta^2(y)$$

Would result in, $\Delta^2(F) = (ake^{kx} - bc)^2\Delta^2(x) + b^2\Delta^2(y)$

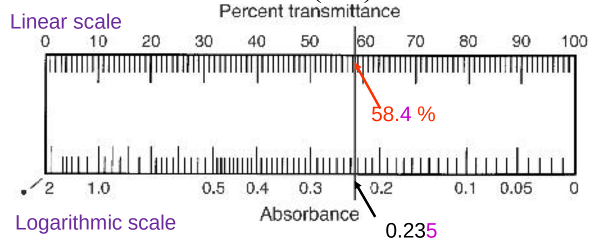
Single measurements:

measurement: *number* *unit*

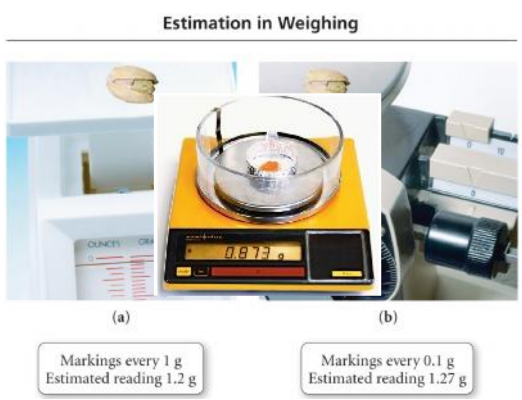
The accuracy of the *measurement* is limited by the capability of the measuring instrument.

The last digit of the *number* of a measurement is a *considered judgment, estimate*. (a source of uncertainty).

$$A = \log\left(\frac{100}{\%T}\right)$$



58.4 means actual value is between 58.0 and 59.0.
0.235 means actual value is between 0.230 and 0.240.



Better instruments will allow more precise measurements - better estimates - uncertainty can be minimized but never eliminated.

Significant figures:

measurement - 104.036 m

↑

uncertain, but *must be included* in the number

The uncertain position in the number limits the number of digits in a measurement, hence the need for the definition of significant figures.

Significant figures:

measurement - 104.036 m

↑

Expressed in scientific notation:

$$104.036 = 1.04036 \times 10^2 \quad (6)$$

$$= 0.104036 \times 10^3$$

$$= 0.0104036 \times 10^4$$

↑ ↑

pre-exponent exponent

significant figures = non-place-holding digits in a reported measurement = # of digits in the pre-exponent.

ZEROs of a number are significant in a number if (i) in the middle of a number (ii) at the end on the rhs of decimal point.

1) All non-zero digits are significant
   1.5 has 2 sig. figs.
2) Interior zeros are significant
   1.05 has 3 sig. figs.
3) Leading zeros are **NOT** significant
   0.001050 has 4 sig. figs.
   1.050×10^{-3} has 4 sig. figs.
4) Trailing zeros may or may not be significant
   i. Trailing zeros after a decimal point are significant
      1.050 has 4 sig. figs.
   ii. Zeros at the end of a number without a written decimal point are *ambiguous* and should be avoided by using scientific notation
      if 150 has 2 sig. figs. then 1.5×10^2
      but if 150 has 3 sig. figs. then 1.50×10^2

ALL DIGITS OF A MEASUREMENT INCLUDING THE UNCERTAIN ONE are called SIGNIFICANT FIGURES.

Or

Significant figures is the *proper number of digits* in the number.

Exact numbers have an *unlimited number* of significant figures (meaning there are no uncertainties – do not worry about it's sig. figs.).

A number (e.g. integers) whose value is known with complete certainty **(exactly)** are

a. integral powers of 10

b. numbers from counting individual objects (integers)

c. numbers from definitions and defined constants
1 cm = 0.01 m; c = 299792458 m s^{-1} (vacuum)
http://physics.nist.gov/cuu/Constants/

and d. integer values (in equations)

$$\text{radius of a circle} = \frac{\text{diameter of a circle}}{2}$$

a. addition and subtraction:
i. add numbers
ii. round off at the proper decimal place

Result has decimal places same as the # with the *least* decimals

12.0
3.0045
61.830452
76.834952 (calculator)

76.834952 (roundoff); 76.8

Express all numbers with *same* exponent

1.632×10^5	$1.632\ \ \times10^5$	
4.107×10^3 →	0.04107×10^5	
0.934×10^6	$9.34\ \ \times10^5$	
	11.51307×10^5	11.51×10^5

b. multiplication and division:

Result has the same # sig. fig. as the # with the least # sig. fig.

Integers and powers of 10 has no uncertainty

$$x = \frac{41.3600\times0.02328\times\frac{122.123}{1000}}{3.4842}\times100$$

x = 3.374876 = 3.375 (note *rounding off)*

i. perform the calculation
ii. round off at the proper decimal place

Rounding Off:

Look at the left most digit to be dropped

<5, no change of retained digit
>5, increase retained digit by 1
=5, increase *retained digit* as is, if *it* is odd

$$69.5\text{in}\times\frac{1\text{yd}}{36\text{in}}\times\frac{1\text{m}}{1.0936\text{yd}}=1.765321466\text{m}=1.76\text{m}$$

c. logarithms: log 25.158 = 1.40070 (6)
↑ characteristic ↑ mantissa

mantissa has the same # sig.fig. as that of the number.
round off at the correct position.

d. antilogs:
will carry sig. figs. equal to the number of digits in the mantissa.

antilog (1.4007)=25.16 (4)
↑ round off such that it contains same # sig. fig. as mantissa

e. y=√x y has same # sig. figs. as x

Arithmetic operations:

The precision of a calculated result is determined by the number with the lowest precision.

a. addition and subtraction:

Result has decimal places same as the # with the *least* decimals.

b. multiplication and division:

Result has the same # sig. fig. as the # with the least # sig. fig.

Disregard the uncertainty of **integers and powers of 10**, because they are **exact**.

Std. deviation of computed results, propagation of errors:

a. addition & subtraction

$$y = (k_1a_1 + k_2a_2 - k_3a_3) \quad or$$
$$y = (k_1a_1 + k_2a_2 + k_3a_3) \quad or....$$

Calculate y in the usual manner.

Do not round or adjust for sig. figs. until s is calculated.

$$s = \sqrt{(k_1s_1)^2 + (k_2s_2)^2 + (k_3s_3)^2}$$

(same approach for σ, use σ in place of s)

b. multiplication & division

$$y = k\frac{a_1 \times a_2}{a_3} \quad or \quad y = k\frac{a_1}{a_2 \times a_3} \quad \text{or ...}$$

first calculate y and the relative errors,

$$\frac{s}{y} = \sqrt{(\frac{s_1}{a_1})^2 + (\frac{s_2}{a_2})^2 + (\frac{s_3}{a_3})^2}$$

Calculate y in the usual manner.

Do not round or adjust for sig. figs. until s is calculated.

$$s = \sqrt{(\frac{s_1}{a_1})^2 + (\frac{s_2}{a_2})^2 + (\frac{s_3}{a_3})^2} \times y$$

(same approach for σ), the significant figure of the final result must be consistent with uncertainty.

Rounding Off:

Look at the left most digit to be dropped

<5, no change of retained digit
>5, increase retained digit by 1
=5, increase *retained digit* by 1, if *it* is odd

$$69.5\text{in} \times \frac{1\text{yd}}{36\text{in}} \times \frac{1\text{m}}{1.0936\text{yd}} = 1.765321466\text{m} = 1.77\text{m}$$

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antilog (1.4007)=25.16 (4)
↑ round off such that it contains same # sig. fig. as mantissa

e. y=√x y has same # sig. figs. as x

Table 2-2 Tolerances of Class A burets

Buret volume (mL)	Smallest graduation (mL)	Tolerance (mL)
5	0.01	±0.01
10	0.05 *or* 0.02	±0.02
25	0.1	±0.03
50	0.1	±0.05
100	0.2	±0.10

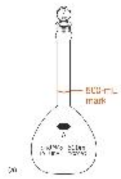

Table 2-3 Tolerances of Class A volumetric flasks

Flask capacity (mL)	Tolerance (mL)
1	±0.02
2	±0.02
5	±0.02
10	±0.02
25	±0.03
50	±0.05
100	±0.08
200	±0.10
250	±0.12
500	±0.20
1 000	±0.30
2 000	±0.50

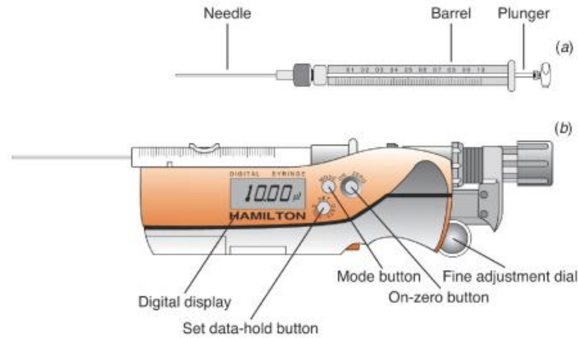

Table 2-5 Manufacturer's tolerances for micropipets

Pipet volume (μL)	At 10% of pipet volume: Accuracy (%)	At 10% of pipet volume: Precision (%)	At 100% of pipet volume: Accuracy (%)	At 100% of pipet volume: Precision (%)
Adjustable pipets				
0.2–2	±8	±4	±1.2	±0.6
1–10	±2.5	±1.2	±0.8	±0.4
2.5–25	±4.5	±1.5	±0.8	±0.2
10–100	±1.8	±0.7	±0.6	±0.15
30–300	±1.2	±0.4	±0.4	±0.15
100–1 000	±1.6	±0.5	±0.3	±0.12
Fixed pipets				
10			±0.8	±0.4
25			±0.8	±0.3
100			±0.5	±0.2
500			±0.4	±0.18
1 000			±0.3	±0.12

SOURCE: Data from Hamilton Co., Reno, NV.

Significant figures of a calculated result is determined by the ***first*** *non zero digit* of the uncertainty (σ or s) associated with it. Calculate the uncertainty first before deciding on the significant figures of the final computed value. Both the computed result and the uncertainty must be consistent in terms of the number of digits beyond the decimal point.

4 $$\frac{0.002364 \pm 0.000003}{0.02500 \pm 0.00005} = 0.0946 \pm 0.0002$$ 3

4 $$\frac{0.002664 \pm 0.000003}{0.02500 \pm 0.00005} = 0.1066 \pm 0.0002$$ 4

3 $$\frac{0.821 \pm 0.002}{0.803 \pm 0.002} = 1.022 \pm 0.004$$ 4

Estimating uncertainty of a single measurement

Sometimes the uncertainty is not expressed explicitly, for a single measurement. Then the error is considered to be at the last digit (*or* last two digits) of the significant digits of the measurement given. Uncertainty has one significant digit, usually. The number of decimals of both value and error are same.

e.g. a single measurement like 1.047m has an uncertainty of ± 0.001 m.

R = 8.3144621 ± 0.0000075 $JK^{-1}mol^{-1}$ (best available, n large)

R = 8.3145 ± 0.0001 $JK^{-1}mol^{-1}$

Unit conversion relations are not considered in significant digit assignments. http://www.onlineconversion.com/