ANALYTICAL CHEMISTRY

Experimental Errors & Statistics

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Chapter Description

- Expected Outcomes
  - Differentiate the types of experimental errors in chemical analysis.
  - Understand and apply the basic concept of uncertainty in chemical analysis.
  - Understand and apply the statistical analysis into data evaluation.

Contents

- Measurement and Readings
- Errors in Chemical Analysis
- Graphs and Measurement
- Statistics to Data Evaluation
- Uncertainty in Chemical Analysis

MEASUREMENT & READINGS

Depends on what apparatus or instruments you used or read.

Example:

50 mL burette with 0.1 graduation, readings must be to the nearest 0.01 mL

Calibrated mm ruler, readings must be to the nearest 0.1 mm

Others:

Analytical balance??

Top loading balance??

pH meter??

ERRORS IN CHEMICAL ANALYSIS

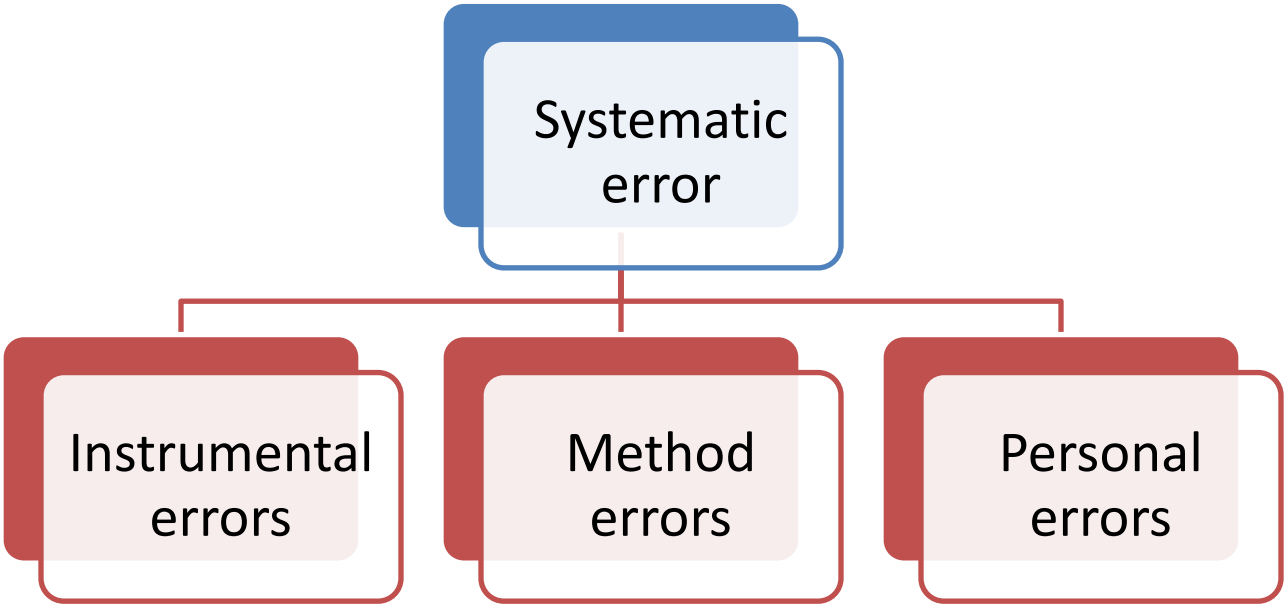
There are two types of error:

1. ***Systematic error*** - always too high or too low (improper shielding and grounding of an instrument or error in the preparation of standards).

2. ***Random error*** - unpredictably high or low (pressure changes or temperature changes).

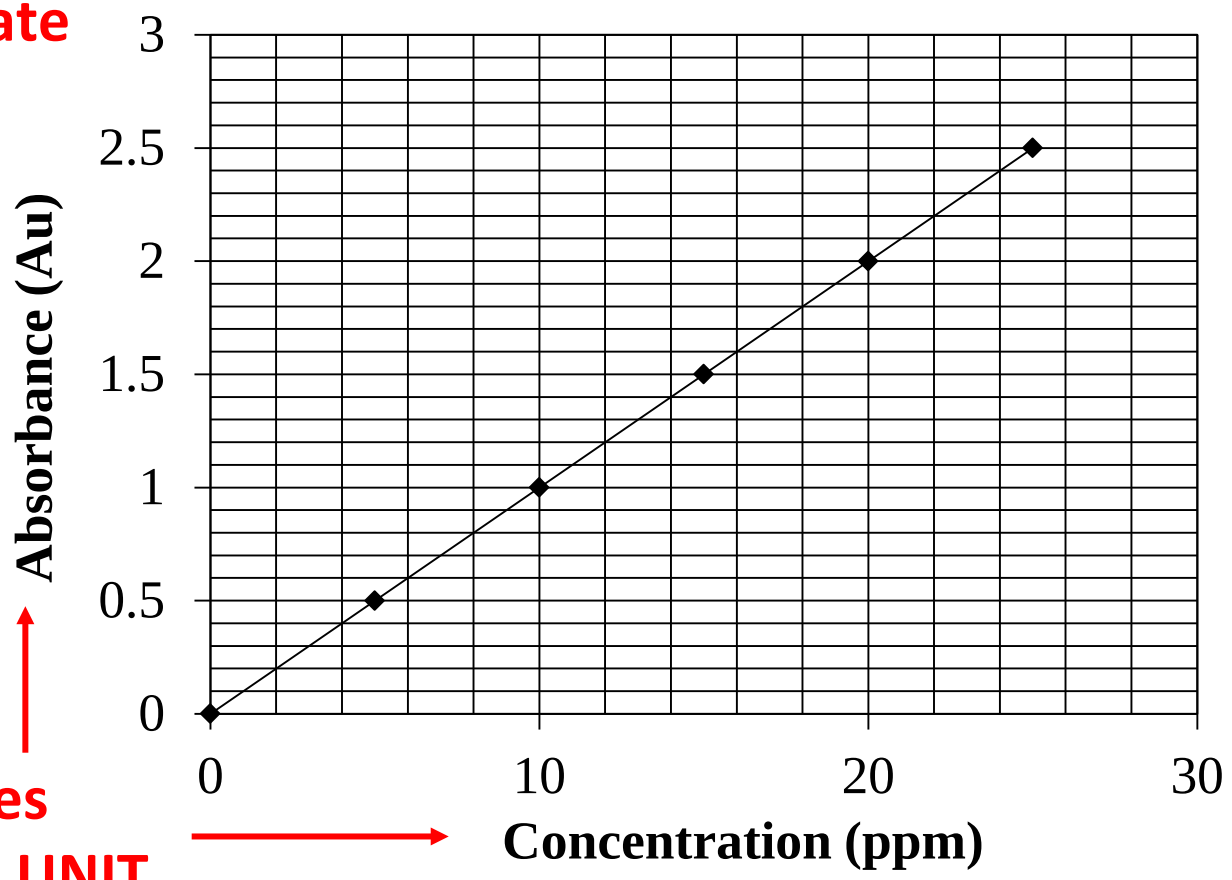
Precision = ability to control random error.
Accuracy = ability to control systematic error.

TYPES OF SYSTEMATIC ERROR



GRAPH & MEASUREMENT

1. Choose appropriate types of graph



2. Label both axes completely with UNIT

3. Plan the coordinates of graph

GRAPH & MEASUREMENT

Cartesian graph – most commonly used graph in analytical chemistry

Log-log graph – linear response runs over a very wide range of analyte concentration

Showing precise value using graph – must have tick marks on both scales

STATISTICS TO DATA EVALUATION

- Rejection of outliers
- Defining the confidence interval
- Determination of number of replicate measurements required
- Estimating the probability that an experimental mean and true value are different or that two experiments are different.
- Treating calibration data

STATISTICS TO DATA EVALUATION

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Statistics

t-test

- Compared measured result with a known value
- Compare replicate measurement
- Compare individual differences

Different from known value if $t_{calc} > t_{table}$

F-test

- To test whether Method 1 is more precise than Method 2
- To test whether Method 1 and 2 differ in their precision

Reject null hypothesis if $F_{calc} > F_{crit}$: Method 1 less precise than Method 2

Q-test

- Rejecting outliers

$$Q_{exp} = \frac{gap}{range}$$

***Reject if $Q_{exp} > Q_{table}$**

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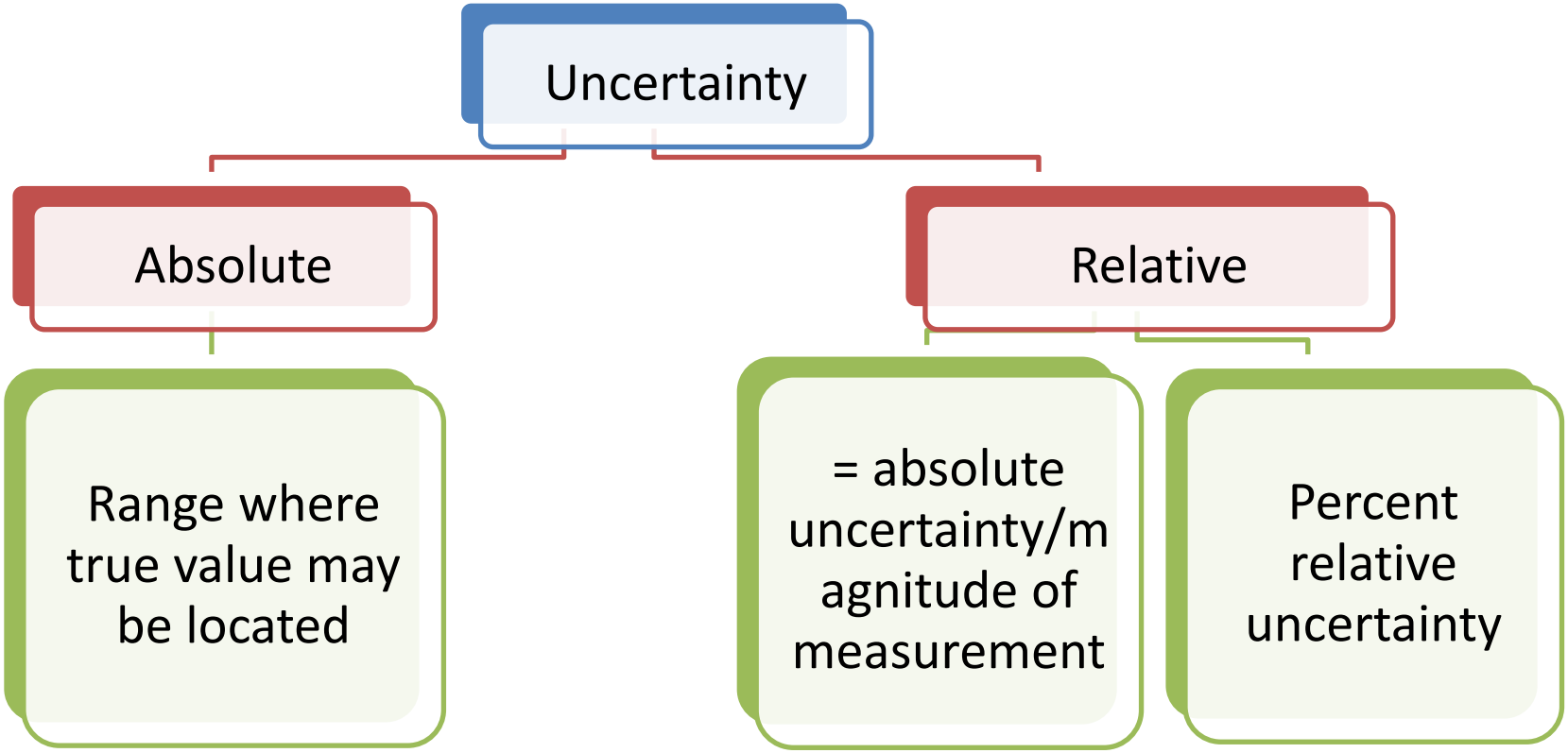
http://ocw.ump.edu.my/course/view.php?id=467

UNCERTAINTY IN CHEMICAL ANALYSIS



PROPAGATION OF UNCERTAINTY

Function	Uncertainty
$y = x_1 + x_2$	$e_y = \sqrt{e_{x_1}^2 + e_{x_2}^2}$
$y = x_1 - x_2$	$e_y = \sqrt{e_{x_1}^2 + e_{x_2}^2}$
$y = x_1 \times x_2$	$\%e_y = \sqrt{\%e_{x_1}^2 + \%e_{x_2}^2}$
$y = \frac{x_1}{x_2}$	$\%e_y = \sqrt{\%e_{x_1}^2 + \%e_{x_2}^2}$
$y = x^a$	$\%e_y = a\%e_x$
$y = \log x$	$e_y = \frac{1}{\ln 10\, x}\frac{e_x}{x}$
$y = \ln x$	$e_y = \frac{e_x}{x}$
$y = 10^x$	$\frac{e_y}{y} = (\ln 10)e_x$
$y = e^x$	$\frac{e_y}{y} = e_x$

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