Biological Chemistry Laboratory
Biology 3515/Chemistry 3515
Spring 2023

Lecture 6:
Dealing with Uncertainty

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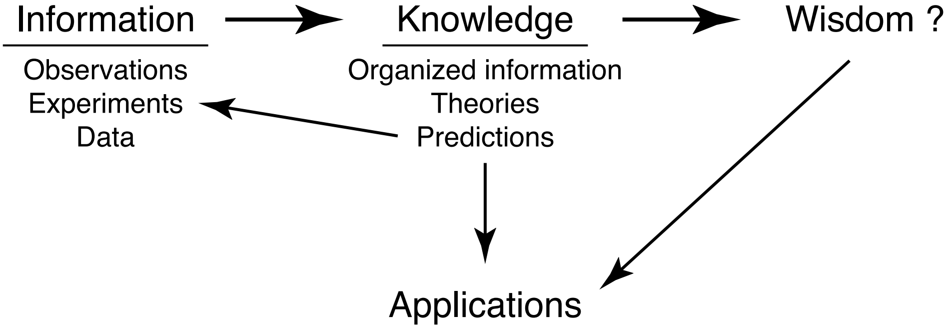
Computer Labs

- Computer Labs next week and the following week.
  - Start at 1:00 PM
  - Room 150 S. Biology Building
- Next week: Graphing and curve fitting with SciDAVis.
- Following week: Molecular modeling with PyMOL.
- We will use the computers in the lab, not personal laptops.
- But, you should still install SciDAVis and PyMOL on your own computer. Use the versions available on Canvas.

How do we know? What do we do with it?



- All of this is sometimes messy!

Dealing With Uncertainties

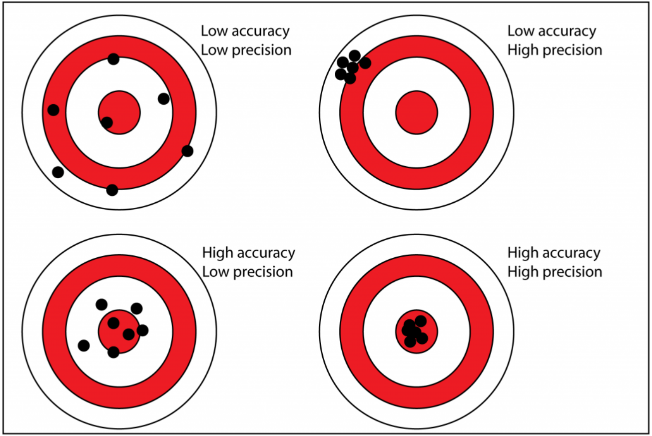
Pipette calibration data:

- Mass of water (mg) delivered from a pipette set to 20 μL:

  20.1
  18.5
  18.2
  22.4
  22.9

- mean (average) = 20.4 mg
- What is the significance of the mean?
- How do we quantify accuracy or precision?

Precision and Accuracy as Target Practice



http://www.antarcticglaciers.org/glacial-geology/dating-glacial-sediments-2/precision-and-accuracy-glacial-geology/

Precision and Accuracy in Measurement

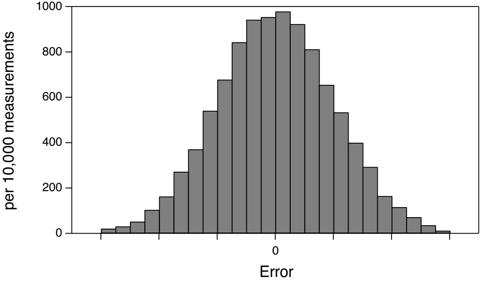
- **Precision**
  - Reproducibility of individual measurements.
  - Determined by making multiple measurements and comparing them.

- **Accuracy**
  - Consistency with an accepted value.
  - Requires comparison with an accepted standard.
  - Without high precision, we can't have high accuracy!

Dealing With Uncertainties: The Working Model

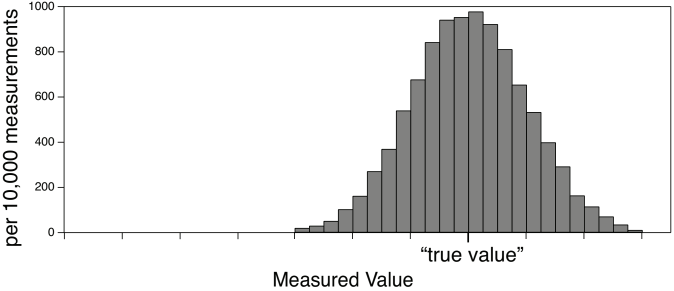
Assumptions:

- The measured values are determined by a “true” value plus random error (positive or negative).
- The random errors are distributed according to a Gaussian function, *i.e.,* a “bell curve”.



- Why is it bell shaped?

Estimating the "True" Value



- The best* estimate of the "true" value is the mean, $\bar{x}$.

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

N= number of measurements, x_i is the i^{th} measurement

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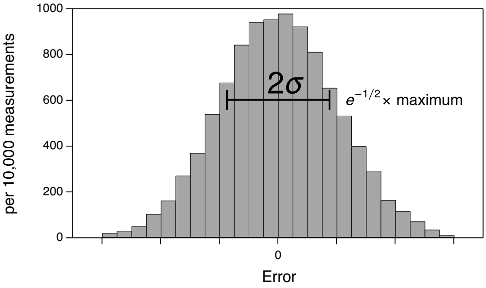
* "Best" means most likely to give the correct value.

Estimating the Distribution Width (σ)

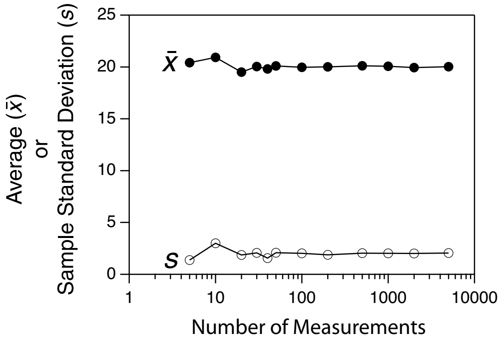


Two ways to estimate σ, the standard deviation:

- From a histogram (takes lots of measurements!)
- The sample standard deviation, s:

$$s = \sqrt{\frac{\sum (x - \bar{x})^2}{N - 1}}$$ an <u>estimate</u> of σ

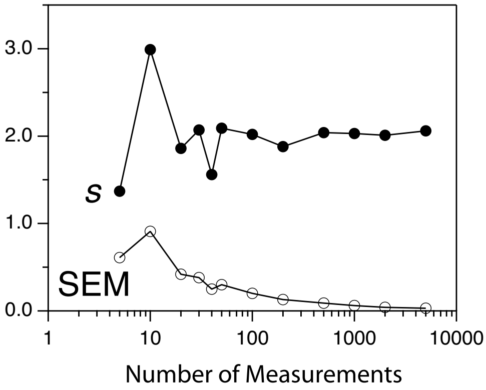
Estimates Improve With More Measurements (A Simulation)



- Estimate of true value ($\bar{x}$) approaches a limiting value (20 mg)
- Estimate of standard deviation (s) approaches a limiting value (2 mg)
- s doesn't approach zero.

Another Useful Statistic:
The Standard Error of the Mean (SEM)

$$\text{SEM} = \sqrt{\frac{\sum(x - \bar{x})^2}{(N-1)N}} = s/\sqrt{N}$$



- The standard error of the mean represents the uncertainty in the estimate of the mean, $\bar{x}$
- The uncertainty in $\bar{x}$ decreases with more measurements.
- The uncertainty in the mean can be made as small as we like, if we make enough measurements! (Assumes that errors are truly random.)
- Decreasing the uncertainty by half requires four times as many measurements.

Clicker Question #1

If I want to report on how reproducible my pipette (and technique) is, which statistic should I use?

A) The sample standard deviation

B) The standard error of the mean

Clicker Question #2

If I want to report on how reliably I have measured the average volume delivered by my pipette, which statistic should I use?

A) The sample standard deviation

B) The standard error of the mean

- Whatever you report, be clear! (and specify N)

Significant Figures

- The basic idea: The number of digits used to report a measurement should reflect the precision of the measurement.
- Reporting more digits than justified by the measurements is dishonest!
- A precise definition of ‘significant figures’ is not so simple!

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https://en.wikipedia.org/wiki/Significant_figures

Rules for Significant Figures

- All non-zero digits are significant.

number	sig. figs.
12	2
12.5	3

- Zeros between non-zero digits are significant.

number	sig. figs.
102	3
12.05	4

Rules for Significant Figures

- Trailing zeros to the right of a decimal point are significant.

number	sig. figs.
12.00	4
12.500	5

- Leading zeros to the left are *not* significant.

number	sig. figs.
012	2
0.0012	2

- What about trailing zeros without a decimal point?

number	sig. figs.
1200	2?

Rules for Significant Figures

- Avoid Ambiguity with Scientific Notation

number	sig. figs.
1200	2?
1.2×10^3	2
1.20×10^3	3
1.200×10^3	4
1200.	4

Rules for Significant Figures

- Numbers with unlimited significant figures:
  - Integers or ratios of integers (rational numbers), such as 2, $1/2$ or $2/3$.
  - Defined irrational numbers, such as $\sqrt{2}$, π or e.
  - Other numbers that are not derived from measurements, including most conversion factors.

Rules for Significant Figures

- Multiplication and division:

  The calculated result should contain the number of significant figures of the measured quantity with the smallest number of significant figures.

$$15\,\mathrm{g} \div 121.1\,\mathrm{g/mol} = 0.12\,\mathrm{mol}$$

$$\begin{aligned} 15\,\mathrm{mM} \times 25\,\mu\mathrm{L} &= 0.015\,\mathrm{moles/L} \times 2.5 \times 10^{-5}\,\mathrm{L} \\ &= 3.8 \times 10^{-7}\,\mathrm{moles} \\ &= 0.38\,\mu\mathrm{moles} \end{aligned}$$

Rules for Significant Figures

- For addition and subtraction:
  - The last decimal place of the result is determined by last decimal place of the measured quantity with the smallest number of decimal places.

    $$125\,\mathrm{g} + 0.035\,\mathrm{g} = 125\,\mathrm{g}$$

  - Adding a more precise value to a less precise one doesn't increase the precision of the sum!
  - The big message: The number of significant figures in a calculated value should not imply more precision than is present in the values going into the calculation!