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Basic Statistics and Uncertainty Propagation

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Overview

- **Basic Statistical Concepts**
 - Properties of the Gaussian Distribution
 - Error propagation
- **Three Example Exercises:**
 - Uranium Ratios to Determine Potential Source of a Seized Material
 - Chronometry to Estimate Age of a Seized Material
 - Estimating Amount of a Specified Component

Uncertainties

Imagine the results of an isotopic analysis measurements are:

$$^{234}\text{U} = 0.911 \pm 0.034, \ ^{235}\text{U} = 92.15 \pm 1.02, \ ^{238}\text{U} = 6.08 \pm 0.28$$

What is the true answer? What do these uncertainties tell us? What do they mean? How can we use them?

To get a better understanding of these results, lets do a thought experiment: What would happen if we repeated the measurement many times?

- The results of each measurement would not be identically the same.
- A histogram of the results would form a Gaussian distribution, centered around the true value*.
- The width of the distribution would be related to the uncertainty.

* Assumes no systematic errors.

The Gaussian Distribution

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

X = center of distribution

= average of many
measurements

σ = width of distribution

= standard deviation

after many measurements

= uncertainty determined from
counting statistics from one
measurement

For a large number of measurements, X is a good estimate of the true value.

Properties of the Gaussian Distribution

Probability within:

$$1 \sigma = \int_{-1\sigma}^{1\sigma} G(x) = 68.3\%$$

$$2 \sigma = \int_{-2\sigma}^{2\sigma} G(x) = 95.5\%$$

$$3 \sigma = \int_{-3\sigma}^{3\sigma} G(x) = 99.7\%$$

How does this relate if only **one** measurements is made?

If one measurement is made, there is a 68.3% chance that the true value is within one σ and a 95.5% chance that the true value is within two σ .

Propagation of Error

The error, σ_f , of a function, $f(x_1, x_2, \dots, x_i)$, with x_i random variables is propagated using the follow method:

$$\sigma_f^2 = \left(\frac{\partial f}{\partial x_1} \sigma_{x_1} \right)^2 + \left(\frac{\partial f}{\partial x_2} \sigma_{x_2} \right)^2 + \dots + \left(\frac{\partial f}{\partial x_i} \sigma_{x_i} \right)^2$$

For example, if $D = A - B$, then $\sigma_S = \sqrt{(\sigma_A)^2 + (\sigma_B)^2}$

if $P = A \times B$, then $\sigma_P = \sqrt{(B\sigma_A)^2 + (A\sigma_B)^2}$

A	12 ± 0.3
B	10 ± 0.4
S	2 ± 0.5
P	120 ± 5.6

$$\sigma_P = \sqrt{\left(AB \frac{\sigma_A}{A} \right)^2 + \left(AB \frac{\sigma_B}{B} \right)^2}$$

$$\sigma_P = P \sqrt{\left(\frac{\sigma_A}{A} \right)^2 + \left(\frac{\sigma_B}{B} \right)^2}$$

Examples

We will now apply these basic statistical concepts to three examples

Three Example Exercises:

- Uranium Ratios to Determine Potential Source of a Seized Material
- Chronometry to Estimate Age of a Seized Material
- Estimating Amount of a Specified Component

Uranium Ratios

- Suppose that records from Countries A, B, and C indicate the following uranium concentrations and corresponding uncertainties following their most recent processing.

Country	Isotope	Weight Percent	Standard Uncertainty
A	^{234}U	0.9449	0.0353
	^{235}U	92.8647	1.0144
	^{238}U	5.8159	0.2479
B	^{234}U	0.9678	0.0345
	^{235}U	91.4354	1.0253
	^{238}U	7.2292	0.2546
C	^{234}U	0.888	0.03
	^{235}U	74.299	0.85
	^{238}U	4.447	0.10

Uranium Ratios (cont.)

- Suppose that a particular quantity of seized material is analyzed and found to have the following uranium concentrations and corresponding uncertainties.

Isotope	Weight Percent	Standard Uncertainty
^{234}U	0.9113	0.0335
^{235}U	92.1501	1.0216
^{238}U	6.0753	0.2752

- Use this information to determine the most likely country of origin for this seized material.

Uranium Ratios (cont.)

- Our strategy will be to compare the ratios

$$\frac{{}^{234}\text{U}}{{}^{235}\text{U}} \quad \text{and} \quad \frac{{}^{234}\text{U}}{{}^{238}\text{U}}$$

for the seized material versus this same ratios for Countries A, B, and C, with an accounting for uncertainty included in the comparison.

- We will then determine whether a specific country of origin can be established with a high level of confidence.

Uranium Ratios (cont.)

- These ratios have the functional form

$$R = \frac{X}{Y}$$

- Using the propagation of error formulas, we first need the sensitivity coefficients (taking partial derivatives).

$$\frac{\partial R}{\partial X} = \frac{1}{Y} \quad \text{and} \quad \frac{\partial R}{\partial Y} = \frac{-X}{Y^2}$$

- The general error propagation approximation applied to this function (the ratio), can be expressed and simplified to the following approximation for the variance of R (assuming X and Y are independent).

$$\hat{\sigma}_R^2 \approx \left(\frac{1}{Y}\right)^2 \hat{\sigma}_X^2 + \left(\frac{-X}{Y^2}\right)^2 \hat{\sigma}_Y^2 = \left(\frac{X}{Y}\right)^2 \left[\frac{\hat{\sigma}_X^2}{X^2} + \frac{\hat{\sigma}_Y^2}{Y^2} \right]$$

Uranium Ratios (cont.)

- Using the nominal uranium concentrations and corresponding uncertainties listed in the previous tables, the error propagation approximation yields the following values:

Country	Ratio Estimate	Standard Uncertainty
A	0.01018	0.00040
	0.1625	0.0092
B	0.01058	0.00040
	0.1339	0.0067
C	0.01195	0.00043
	0.1997	0.0081
Seized Material	0.00989	0.00038
	0.1500	0.0088

Uranium Ratios (cont.)

- Note that the resulting standard uncertainties are found by taking a square root of the corresponding variance estimates.
- Applying a multiplier of 2, which represents an approximate 95% confidence level, to the resulting standard uncertainties yields “expanded uncertainties”.
- These expanded uncertainties are depicted in the following figure.
- Based on this figure, it is not likely that the seized material came from Country C.
- We cannot rule out Countries A and B as the potential country of origin for this seized material.

Uranium Ratios (cont.)

Chronometry for Age Estimation

- The following formula describes the functional relationship between the proportion of a radioactive isotope at time t (P^t) versus the amount at some starting time (P^0).

$$P^t = P^0 e^{-\lambda_P t}$$

where $\lambda_P = \frac{\ln 2}{t_{1/2}}$ and $t_{1/2}$ is the half life of the isotope of interest.

- Solving the above equation for t yields

$$t = \frac{t_{1/2} \ln\left(\frac{P^0}{P^t}\right)}{\ln 2}$$

Chronometry for Age Estimation (cont.)

- In the equation for t , assume that P^0 , P^t , and $t_{1/2}$ are considered random variables.
- Therefore, error propagation methods will be used to approximate the uncertainty associated with our estimate of t .
- We will need the following partial derivative formulas:

$$\frac{\partial t}{\partial P^0} = \frac{t_{1/2}}{P^0 \ln 2} , \quad \frac{\partial t}{\partial P^t} = \frac{-t_{1/2}}{P^t \ln 2} , \quad \text{and} \quad \frac{\partial t}{\partial t_{1/2}} = \frac{1}{\ln 2} \ln \left(\frac{P^0}{P^t} \right)$$

Chronometry for Age Estimation (cont.)

- Error propagation methodology yields the following formula for approximating the variance associated with our estimate of t (assuming P^0 , P^t , and $t_{1/2}$ are independent).

$$\hat{\sigma}_t^2 \approx \left(\frac{t_{1/2} \ln \left(\frac{P^0}{P^t} \right)}{\ln 2} \right)^2 \left[\frac{\hat{\sigma}_{t_{0.5}}^2}{t_{1/2}^2} + \frac{\hat{\sigma}_{P^0}^2}{(P^0)^2 \left[\ln \left(\frac{P^0}{P^t} \right) \right]^2} + \frac{\hat{\sigma}_{P^t}^2}{(P^t)^2 \left[\ln \left(\frac{P^0}{P^t} \right) \right]^2} \right]$$

Chronometry for Age Estimation (cont.)

- Suppose a particular quantity of seized material contains some proportion of ^{241}Am as well as ^{241}Pu , as described in the table below. Assume a half-life of 14 years for ^{241}Pu .

Random Variable	Nominal Value	Standard Uncertainty
$t_{1/2}$	14	0.001
$^{241}\text{Pu}: P^0$	1	0.005
$^{241}\text{Pu}: P^t$	0.9317	0.004

- Use this information to estimate the age of the seized material (time since last processing/separation).
- Calculate an approximation for the standard uncertainty associated with your estimate of the material's age.

Chronometry for Age Estimation (cont.)

- The assumed inputs yield the following estimates:
- $t = 1.43$ years (the estimated age of the material, the time since the material was last processed).
- The standard uncertainty associated with our estimate of t is $\sigma_t = 0.13$ years. This is the square root of the variance estimate.
- Therefore, there is a
 - 69% confidence that the true age is 1.43 ± 0.13 years
 - 95% confidence that the true age is 1.43 ± 0.26 years
 - 99.7% confidence that the true age is 1.43 ± 0.39 years

Estimating the Amount of a Specified Component

- Suppose that the measured total mass of a particular seized material is M .
- A sample of the material is taken to be analyzed. The measured mass of the sample is m .
- The analyzed amount of the component of interest in the sample is x .
- Estimate the amount X of the specified component in the entire quantity of the seized material, and the associated standard uncertainty.

Estimating the Amount of a Specified Component (cont.)

- Assuming the proportion of the specified component is the same for both the entire quantity of seized material and the analyzed sample,

$$\frac{X}{M} = \frac{x}{m}$$

- Solving this equation for X yields:

$$X = M \frac{x}{m}$$

Estimating the Amount of a Specified Component (cont.)

- Assume that M , x , and m are random variables with nominal values and associated uncertainties given in the table below.

Random Variable	Nominal Value	Relative Standard Uncertainty	Standard Uncertainty
M	2450 g	1%	24.50 g
x	4 g	3%	0.12 g
m	210 g	1%	2.10 g

- We will need the following partial derivatives:

$$\frac{\partial X}{\partial M} = \frac{x}{m}, \quad \frac{\partial X}{\partial x} = \frac{M}{m}, \quad \text{and} \quad \frac{\partial X}{\partial m} = \frac{-Mx}{m^2}$$

Estimating the Amount of a Specified Component (cont.)

- Error propagation methodology yields the following formula for approximating the variance associated with our estimate of X (assuming M , x , and m are independent).

$$\hat{\sigma}_X^2 \approx \left(\frac{Mx}{m} \right)^2 \left[\frac{\hat{\sigma}_M^2}{M^2} + \frac{\hat{\sigma}_x^2}{x^2} + \frac{\hat{\sigma}_m^2}{m^2} \right]$$

Estimating the Amount of a Specified Component (cont.)

- The assumed inputs yield the following estimates:
- $X = 46.7$ g.
- The standard uncertainty associated with our estimate of X is $\sigma_X = 1.6$ g. This is the square root of the variance estimate.
- Therefore, there is a
 - 69% confidence that the true mass is 46.7 ± 1.6 grams
 - 95% confidence that the true mass is 46.7 ± 3.2 grams
 - 99.7% confidence that the true mass is 46.7 ± 4.8 grams

Summary

Understanding the uncertainties is critical to draw conclusions about a measurement.

When performing calculations of measured quantities, one must correctly propagate the errors to get the uncertainty of the calculated quantity.

A 1σ uncertainty will result in a confidence level of 68.3%

A 2σ uncertainty will result in a confidence level of 95.5%

A 3σ uncertainty will result in a confidence level of >99%