CHE384, From Data to Decisions: Measurement, Uncertainty, Analysis, and Modeling

Lecture 29
Measurement Uncertainty

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All Measurements are Uncertain

- Measurement error exists, but we do not know what it is
  - If we new the measurement error, we would subtract it out!
  - Unknown errors are called uncertainties
- Our goal is to estimate the uncertainty in our measurements
  - Random errors can be estimated using repeated measurements
  - Systematic errors require a sophisticated understanding of the measurement process

Why Evaluate Uncertainty?

- To allow realistic comparison of results
  - Different experiments, experimenters, over time, etc.
- To allow for more rigorous use of the data
  - Regression, model building, etc.
- Understanding the sources of uncertainty allows one to validate, and possibly improve, measurement procedures
  - How can we reduce uncertainty?
- Evaluating uncertainty means you can report uncertainty – a requirement of good science

What is Data?

Data = the results of a measurement

- Definition of the thing being measured
- Measurement value (number plus units)
- Estimate of the uncertainty of each measurement
- Experimental context (measurement method + environment)
- Context uncertainty (uncertainty of controlled and uncontrolled input parameters)
- Measurement model (theory, assumptions and definitions used in making the measurement)

The Measurement Model

- The act of measurement requires a "paradigm"
  - A connected set of theories in a framework
  - Used to design and develop the measurement system
  - Almost all measurements are indirect (theories relate what is actually measured to what we want to measure)
- Measuring temperature (an example)
  - Thermometer: assumes linear coefficient of thermal expansion to convert length to temperature
  - Thermocouple: uses Seebeck effect to convert voltage difference into temperature difference
  - Resistance thermometer: relates change in resistance to change in temperature

Measurement Terms

- Metrology: the science of measurement
- Measurand: the thing being measured
- True Value: the unknown (and unknowable) thing we wish to estimate
- Error: true value – measured value
- Measurement Uncertainty: an estimate of the dispersion of measurement values around the true value

Uncertainty Components

- Systematic errors
  - Produce a bias in the measurement result
  - We look for and try to correct for all systematic errors, but we are never totally successful
  - We try to put an upper limit on how big we expect systematic errors could be
- Random errors
  - Can be evaluated statistically, through repeated measurements

Other Measurement Terms

- Accuracy: the same as error, it can never be known, but is estimated as the maximum systematic error that might exist
- Precision: the standard deviation of repeated measurements (random error component)
- Repeatability: standard deviation of repeated measurements under conditions as nearly identical as possible
- Reproducibility: standard deviation of repeated measurements under conditions that vary in a typical way (different operators, instruments, days)

Uncertainty Types

- Type A: uncertainty estimates obtained by statistical analysis of repeated measurements
  - Standard uncertainty = standard deviation of repeated measurements
  - Fundamentally caused by fluctuations in nature (shot noise, Brownian motion, Boltzmann statistics, etc.) that propagate through the measurement model
- Type B: uncertainty estimates evaluated by other techniques (scientific judgment)
  - Prior experience or data, manufacturer's specs, calibration reports, reported uncertainty value

Sources of Type B Uncertainty

- Incomplete definition of the measurement
- Imperfect realization of the procedure
- Sample is not representative
- Environmental conditions
- Biases in reading analog scales
- Instrument resolution
- Values of constants used in calculations
- Changes in measuring instrument performance since last calibration
- Approximations/assumptions in the measurement model

Combined Uncertainty (u_c)

- Combine individual standard uncertainties (u_i) arising from Type A and/or Type B evaluation (including their covariances)

$$u_c^2 = u_1^2 + u_2^2 + 2cov(1,2)$$

- We usually use a propagation of uncertainties approach

Expanded Uncertainty

- The combined standard uncertainty (u_c) is a standard deviation
- We often express our uncertainty as a multiple of the standard deviation

$$U = ku_c$$

  - U = expanded uncertainty
  - k = coverage factor (typically 2, or up to 3)

Effective Degrees of Freedom

- When using the combined uncertainty, we usually assume that our measurement is t-distributed
- The effective number of degrees of freedom is given by the Welch-Satterthwaite approximation:

$$df_{eff} = \frac{\left(\sum u_i^2\right)^2}{\sum\left(u_i^4/df_i\right)}$$

- We often use this to calculate a coverage factor for a given probability (e.g., 95%)