THE UNIVERSITY OF TEXAS AT AUSTIN — WHAT STARTS HERE CHANGES THE WORLD

CHE 379/384
From Data to Decisions:
Measurement, Uncertainty, Analysis, and Modeling

Lecture 2
Data and Measurement

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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)

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The Measurement Model

- The act of measurement requires a "paradigm"
  - A connected set of theories that relates the thing being measured to the measurement result
  - Required to design and develop a measurement system
- Some interpretation of the data is often built into the measurement model
  - We have a purpose in mind when we design a measurement, and we make assumptions about what is being measured
  - Might this purpose bias our measurement?
  - We generally don't see what we aren't looking for (http://www.simonslab.com/videos.html)

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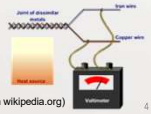
The Measurement Model

- Virtually all measurements are indirect
  - We have a set of theories that relate what is actually being measured to what we want to measure (measurement model)
- Ex: Measuring temperature with a thermometer
  - Thermal expansion of mercury (or spirits) turns length measurement into temperature measurement
  - Theory: linear model of liquid thermal expansion

- Ex: Measuring temperature with a thermocouple
  - Junction of dissimilar metals turns temperature change into voltage change (Seebeck effect)
  - Theory: polynomial model of voltage versus temperature, coupled with digital (or analog) voltage measurement



(image from wikipedia.org)

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Measurement is not a Passive Act

- Measurement can change the thing you are measuring
  - Measurement is often *not* observation without disturbance
- Example: Scanning Electron Microscope (SEM) measurement
  - Sample charging
  - Physical and chemical changes of sample due to electron bombardment (carbon deposition, etc.)
  - Effects can be current and voltage dependent

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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 (and the measurement model)

Measurement Stability

- We often make assumptions of spatial and/or temporal stability of measurements
  - Repeated measurements are taken at different times, locations, conditions, etc.
  - How constant is the sample?
  - How constant is the measurement process?
  - How constant is the measurement context?

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

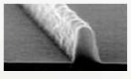
Uncertainty Components

- 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 reasonably 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)

Measurement Model Example

- How wide is this feature? 
- Most critical dimension measurement tools use a trapezoidal feature model
  - What criterion should be used to best fit a trapezoid to this complicated shape?
  - Accuracy of the width measurement is a strong function of the appropriateness of the feature model (not a good fit means not a good measurement)
- The measurement model of an SEM includes the feature model, plus a model for how electrons interact with the sample

Lecture 2: What have we learned?

- What are all the components of data?
- Explain the measurement model
- Explain the difference between precision and accuracy
- Explain the difference between repeatability and reproducibility
- Can you describe a measurement model for a measurement that we haven't discussed?