Interpretation of Lab Results

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- What am I buying?
- What does it mean?
- What do I do with it?

Reasons for Testing

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- Regulatory Compliance
- Process Verification / Change
- Stability Studies
- Problem Investigation
- Due diligence
- Other?

Interpretation

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- To even begin to interpret lab results we need some understanding of measurement uncertainty.

Measurement Uncertainty

UPPSALA UNIVERSITET

Quality of quantitative results:

"A quantitative result without any kind of uncertainty estimate is not only useless, it is dangerous because it can be misused"

Churchill Eisenhart
1952

BUT FIRST…

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This presentation is not about mathematics…

The formal approach to measurement uncertainty estimation calculates a measurement uncertainty estimate from an equation, or mathematical model. The procedures described as method validation are designed to ensure that the equation used to estimate the result, with due allowance for random errors of all kinds, is a valid expression embodying all recognized and significant effects upon the result. It follows that, with one caveat elaborated further below, the equation or "model" subjected to validation may be used directly to estimate measurement uncertainty. This is done by following established principles, based on the "law of propagation of uncertainty" which, for independent input effects is:

$$u[y(x_1,x_2,\ldots)] = \sqrt{\sum_{i=1,n} c_i^2 u(x_i)^2}$$

where *y*(*x*1,*x*2,..*xn*) is a function of several independent variables *x*1,*x*2,..., and *ci* is a sensitivity coefficient evaluated as *ci* = ∂*y*/∂*xi*, the partial differential of *y* with respect to *xi*. *u*(*xi*) and *u*(*y*) are *standard uncertainties*, that is, measurement uncertainties expressed in the form of standard deviations. Since separate *u*[*y*(*x*1,*x*2,...] is a function of several uncertainty estimates, it is referred to as a *combined standard uncertainty*.

But…

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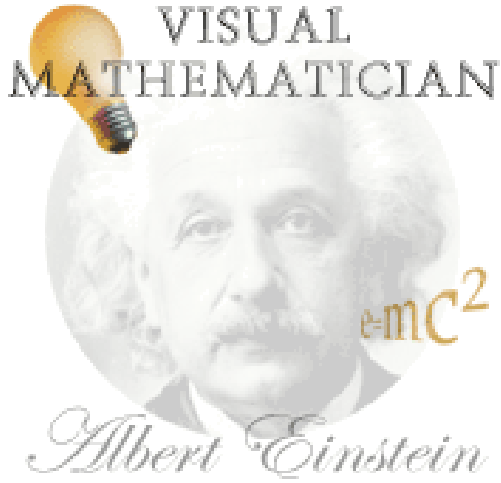
- **It helps if you know some math**
  - Means
  - Standard Deviations
  - Square root of sum of squares



This presentation

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- **Is not about "The Standard"**
  - 5.4.6.2 Testing laboratories shall have and shall apply procedures for estimating uncertainty of measurement….Reasonable estimation shall be based on knowledge of the performance of the method and on the measurement scope and shall make use of, for example, previous experience and validation data.
  - 5.4.6.3 When estimating the uncertainty of measurement, all uncertainty components which are of importance in the given situation shall be taken into account using appropriate methods of analysis.

But

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- **We should know the lab requirements**
  - Must have and apply a procedure for estimating uncertainty
  - Must report uncertainty when required
  - Must consider all sources of uncertainty
  - Must not mislead clients as to the uncertainty of a result

Definition

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- **Uncertainty is a parameter associated with a measurement that characterizes the dispersion of the values that could be reasonably attributed to the measurand**
  - VIM

What is measurement uncertainty?

- **Its not error**
  - Error is a quantity – the distance of a result from the “true” value
  - Error deals with a single measurement

Uncertainty vs. Error

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- Error tells us how much the result differs from the true value
- Uncertainty tells us the interval in which the true value is likely top fall

So…

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- Uncertainty is a quality
- A property of the analytical system (method)
- the range of values that the analyst feels could reasonably be attributed to our result

Therefore…

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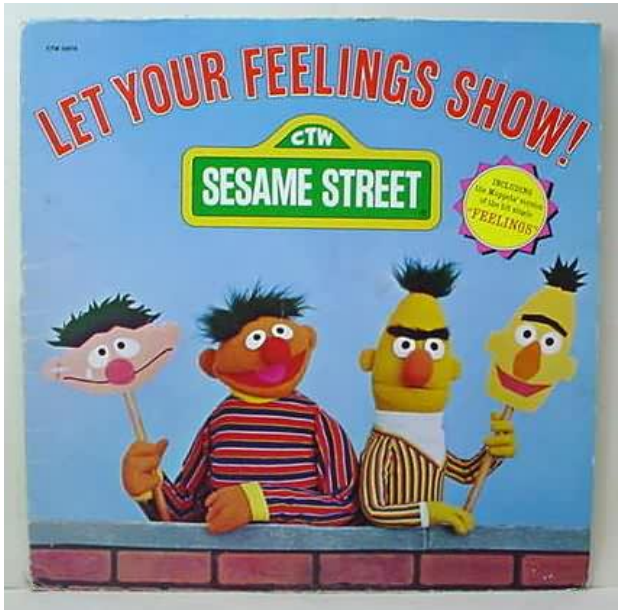
- This presentation is about feelings



Sources of Uncertainty in Analysis

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- Sample inhomogeneity
- Incomplete extraction
- Analyte decomposition, volatilty, adsorption
- Contamination
- Uncertainty of standards
- Instrument drift
- Carryover
- Imperfect selectivity (cross-talk)

Other considerations

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- **What the uncertainty does not include**
  - Field variability and transport
  - Gross in lab errors – blunders

Other considerations

- Near the detection limit the uncertainty world changes
- Uncertainty applies only to “normal” samples

Why does it Matter?

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Comparison to a regulatory limit

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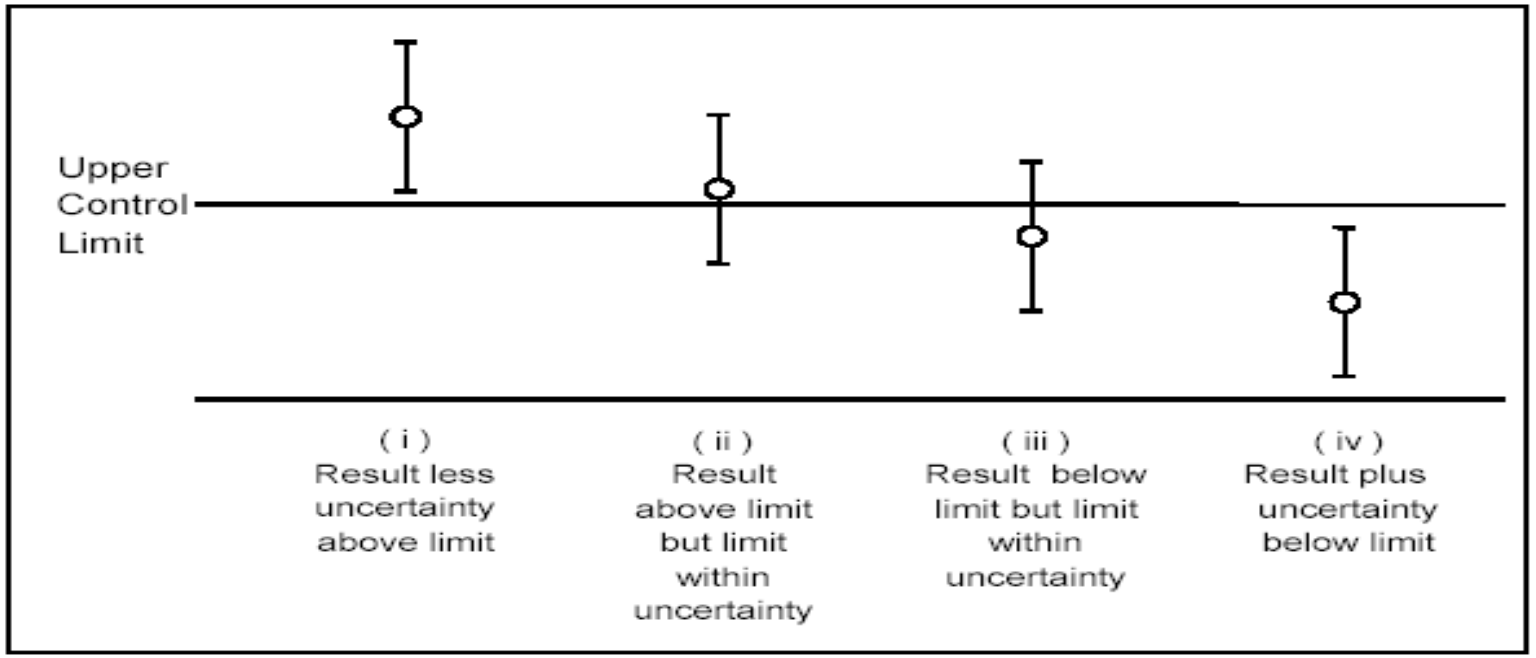

Comparison of Results

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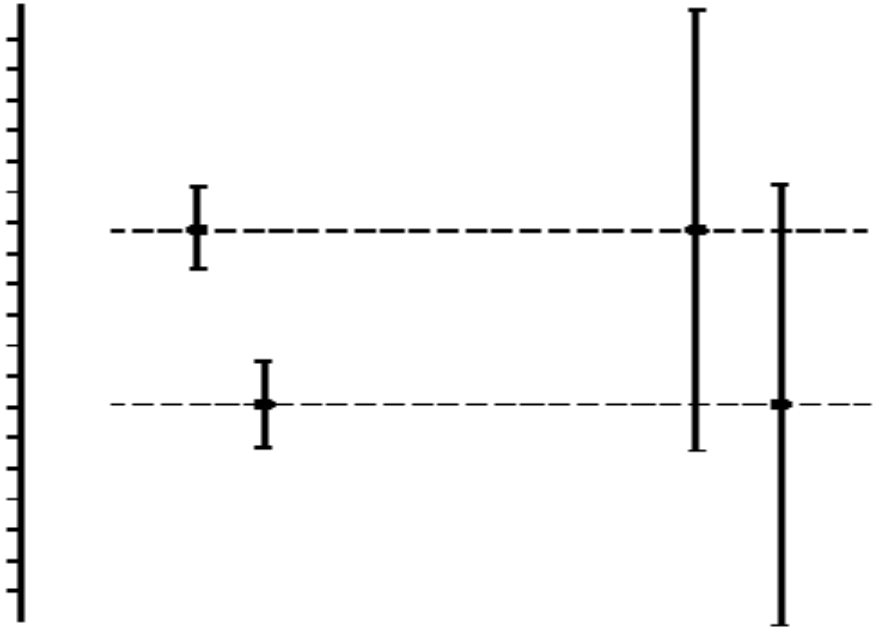

Considerations

- **Risk of a false non-compliant finding (alpha error)**
- **Risk of a false compliant finding (beta error)**
- **How was the limit/specification set?**
  - With uncertainty in mind?
- **Performance properties of the analytical method**

Lesson Learned

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- You are not buying a number but rather, a range that the number may be in
- The range gives you a probability of compliance/non-compliance
- Confer with the lab ahead of time to use a method that gives the (un)certainty required for a good decision
- You (or the regulator) decides based on the probability of error. The Decision Limit.

Questions?

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