

Obtaining a Good Estimate of a Quantity

Replicate error Reading error Calibration error But what do we do when we obtain a quantity from a calculation?

$$\rho = \frac{M_F - M_E}{V_{pyc}}$$

$$\mu = \rho \alpha \Delta t$$

$$Q = \dot{m}C_p(T_{out} - T_{in})$$

etc.

Answer:

Propagate the **error** through the calculation

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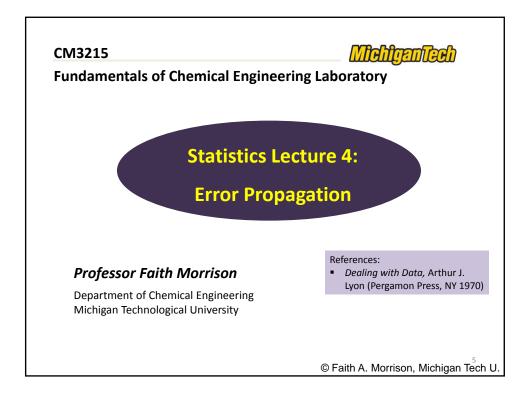
Fundamentals of Chemical Engineering Laboratory

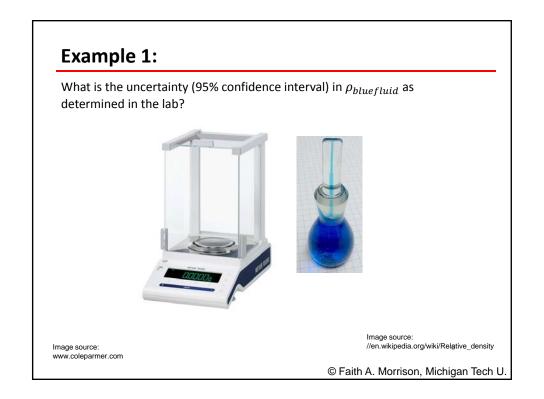
Statistics Lecture 4: Error Propagation

Professor Faith Morrison

Department of Chemical Engineering Michigan Technological University

- 1. Quick start—Replicate error
- 2. Reading Error
- 3. Calibration Error
- 4. Error Propagation
- 5. Least Squares Curve Fitting





Example 1:

What is the uncertainty (95% confidence interval) in $\rho_{bluefluid}$ as determined in the lab?



$$\rho_{bluefluid} = \frac{M_{full} - M_{empty}}{V_{pycnometer}}$$

- The value of density obtained is a function of three measurements
- Each measurement has its own uncertainty

Image source: www.coleparmer.com

Image source: //en.wikipedia.org/wiki/Relative_density

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Example 1:

 $e_{\scriptscriptstyle S} \equiv$ Standard Error

What is the uncertainty (95% confidence interval) in $\rho_{bluefluid}$ as determined in the lab?

Three error sources on each measured quantity:

$$e_{\scriptscriptstyle S} = \frac{\scriptscriptstyle S}{\sqrt{n}}$$

Standard error of replicates

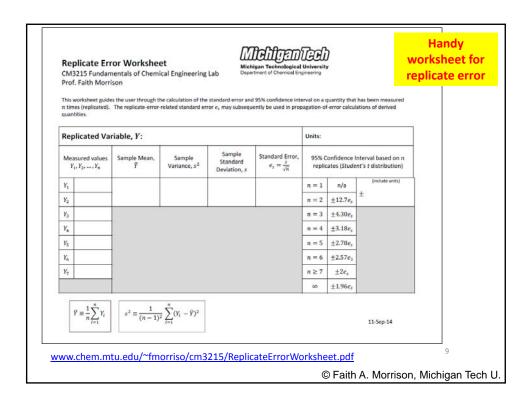
$$e_S = \frac{e_R}{\sqrt{3}}$$

Standard error due to $\ \underline{\text{Reading Error}}$

 e_S = (as determined)

Standard error due to Calibration Error

For each variable, determine the three $e_{\rm S}$, then pick the largest (or average if they are close and you want to be less conservative)



Handy workshee for readin error	gineering	igan Technological U	Depar	emical Engineering Lab	th Morrison	CM3215 Prof. Fait
	8271	ng-error-related	readin	gh the calculation of the standard err X and subject to reading error). The ie used in propagation of error calcula	ital readout (yielding value	or off a dig
				Reading error		
					Measured Quantity: (give symbol)	
	pplicable	Quantity or Not Ap	8 - 8	(include units)	Representative value:	
				contribution to error	issue	
			1	How much signal does it take to cause the reading to change?	Resolution	
			2	Half smallest division or decimal place	Limitation on marked scale or digital readout	
			3	(max-min)/2	Fluctuations with time of observation	Reading error, e _R :
	(units)		e _R =	Maximum of 1, 2 & 3:		
			e _s =	e _s =e _R /v3	Standard error based on reading error:	
				95% Confidence Interval on the reading: +/-1.96e,		

Michigan Technological U Department of Chemical Engli	neering			Handy worksheet fo
	ror Worksheet entals of Chemical E on			calibration er
a manufacturer or for a technical specifications constant (the viscomet uncertainty. In this cas Finally, a user may take	a particular device by son s of a device may indicate ter constant α , for examp se, the method of "least s e steps to calibrate a met	neone with authority to cert that it is accurate to a value le) may be provided by the significant digit" is appropria ter on site; this determinatio	etermined for a brand-new unit by ify the value. For example, the e ±2e _s . Alternatively, a value of a manufacturer with no specific te for evaluating the uncertainty. no ferror (likely to be greater than the particular unit in question.	
Quantity:	Symbol:	Representative value: (include units)		
		Estimate of e _g : (or Not Applicable)		
Method 1: Manufacturer maximum error allowable	2 e _s ≈			
Method 2: Least significant digit on provided value	Least significant digit varies by at least ±1			
Method 3:	2e₂ ≈			
User calibration				
User calibration	Maximum of Methods 1 - 3	e _z =	95% C.I.: quantity±2e _s	

Example 1: What is the uncertainty (95% confidence interval) in $\rho_{bluefluid}$ as determined in the lab?

First:

What are the uncertainties e_{x_i} for M_{full} , M_{empty} , and V_{pyc} ?



You try.

Image source: www.coleparmer.com

Image source: //en.wikipedia.org/wiki/Relative_density

Example 1: What is the uncertainty (95% confidence interval) in $\rho_{bluefluid}$ as determined in the lab?

First:



What are the uncertainties e_{x_i} for M_{full} , M_{empty} , and V_{pyc} ?

Standard errors:

M_{full} :	$= 30.800 \ g$
1.1	40.440

 $M_{empty}: = 13.410 g$

 $V_{pycnometer} = \overline{10.00 \, ml}$

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Example 1: What is the uncertainty (95% confidence interval) in $\rho_{bluefluid}$ as determined in the lab?

First:



What are the uncertainties e_{x_i} for M_{full} , M_{empty} , and V_{pyc} ?

Standard errors:

$$\begin{array}{ccc} M_{full} \colon &= 30.800 \; g \\ \hline M_{empty} \colon &= 13.410 \; g \\ \hline V_{pycnometer} = 10.00 \; ml \; \} \end{array}$$
 (reading)

Now, how to combine? Propagation of Errors

We seek to combine the errors associated with the various quantities in a calculation

$$\rho_{bluefluid} = \frac{M_{full} - M_{empty}}{V_{pycnometer}}$$

We use an analysis based on the calculation of <u>variance</u>. We use the Taylor series expansion of a nonlinear function.

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Error Propagation

We use an analysis based on the Taylor series expansion of a nonlinear function.

Taylor series:

(higher order terms)

$$f(x_1, x_2, x_3) = f^0 + \frac{\partial f}{\partial x_1} x_1 + \frac{\partial f}{\partial x_2} x_2 + \frac{\partial f}{\partial x_3} x_3 + h.o.t.$$

A calculation of the function $f(x_1, x_2, x_3)$ from uncertain values of x_1, x_2, x_3 is a random variable of mean \bar{f} and variance σ_f^2 :

$$\sigma_f^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 \sigma_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 \sigma_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 \sigma_{x_3}^2 + \text{Covariance terms, if } x_i \text{ are correlated}$$

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We use an analysis based on the Taylor series expansion of a nonlinear function.

Taylor series:

(higher order

$$f(x_1, x_2, x_3) = f^0 + \frac{\partial f}{\partial x_1} x_1 + \frac{\partial f}{\partial x_2} x_2 + \frac{\partial f}{\partial x_3} x_3 + h. o. t.$$

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Note: covariance terms are not always zero o small; but they often are. For now, this is fine

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Error Propagation

(To avoid confusion with other variances, we use e_{x_i} nomenclature for errors)

$$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2$$

 $\rho_{bluefluid} = f \left(M_{full}, M_{empty}, V_{pycnometer} \right)$

 $e_{S_{M_{full}}}$ $e_{S_{M_{empty}}}$ $e_{S_{V_{pycnometer}}}$

We estimate these standard errors with our 3 worksheets

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$$e_{s_f}^2 = \left(\left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2\right)^2 + \left(\left(\frac{\partial f}{\partial x_3}\right)^2 e_{x$$

 $\rho_{bluefluid} = f \left(M_{full}, M_{empty}, V_{pycnometer} \right)$

These come from the formula for $\rho_{bluefluid}$

$$\rho_{BF} = \frac{M_F - M_E}{V_{pyc}}$$

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Error Propagation

$$e_{s_f}^2 = \left(\left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2\right)\right)$$

$$f = \rho_{BF} = \frac{M_F - M_E}{V_{pyc}}$$

$$\frac{\partial \rho_{BF}}{\partial M_F} =$$

$$\frac{\partial \rho_{BF}}{\partial M_E} =$$

$$\frac{\partial \rho_{BF}}{\partial V_{pyc}} =$$

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$$\left(\begin{array}{c}
e_{s_f}^2 \neq \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2
\end{array}\right)$$

We seek this, the standard error of the calculated property,

 $f = \rho_{bluefluid}$

$$\rho_{bluefluid} = f \left(M_{full}, M_{empty}, V_{pycnometer} \right)$$

$$\rho_{BF} = \frac{M_F - M_E}{V_{pyc}}$$

Think of the squared partial derivatives as the weighting functions for the individual squared standard errors

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CM32 Prof. F	r Propagation Worksheet 2015 Fundamentals of Chemical Engineering Lab Eaith Morrison Formula for f : (include units) (include units) Representative value of f : (include units)					Fundamentals of Chemical Engineering Lab h Morrison Formula for f : Representative value of f : (include units) (include units)					
	Measured quantities, x_i			ar	e =	Щ	, as 2	\dashv	pro	pagatio	
x_i	Symbol	Representative value		$\frac{\partial f}{\partial x_i}$	$e_{x_i} = \frac{s_i}{\sqrt{N}} \text{ or } \frac{e_{R_i}}{\sqrt{3}} \text{ or } \frac{e_{R_i}}{$	re_{s_i}	$\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$				
<i>x</i> ₁											
<i>x</i> ₂											
<i>x</i> ₃											
x4											
<i>x</i> ₅											
	$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2$	$e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 +$	$+\left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2$	$+\left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2$	$+\left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$	ŀ	$e_{s_f}^2 =$ $e_{s_f} =$	units	Standard error of calculated		



What is the uncertainty (95% confidence interval) in $\rho_{bluefluid}$ as determined in the lab?





Data:

 $M_F = 30.800 g$ $M_E = 13.410 g$

 $V_{pyc} = 10.00 \, ml$

Formula:

$$\rho_{BF} = \frac{M_F - M_E}{V_{pyc}}$$

Image source: www.coleparmer.com Image source: //en.wikipedia.org/wiki/Relative_density

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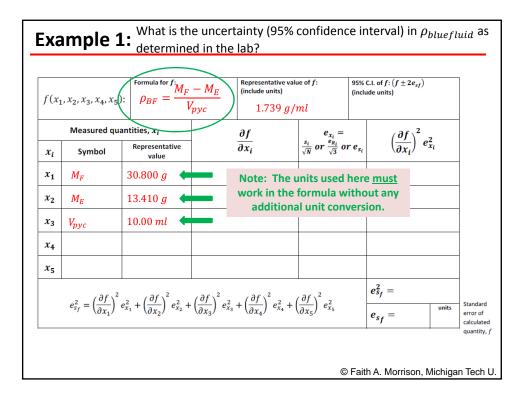
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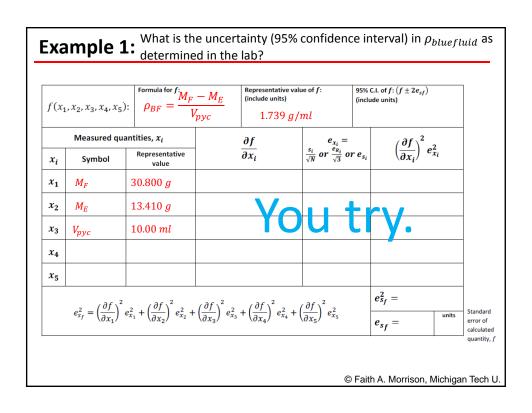
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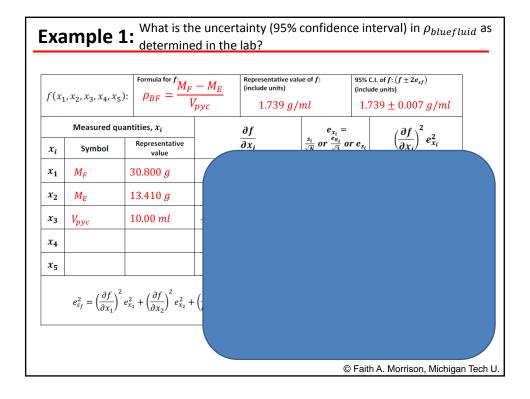
Example 1: What is the uncertainty (95% confidence interval) in $\rho_{bluefluid}$ as determined in the lab?

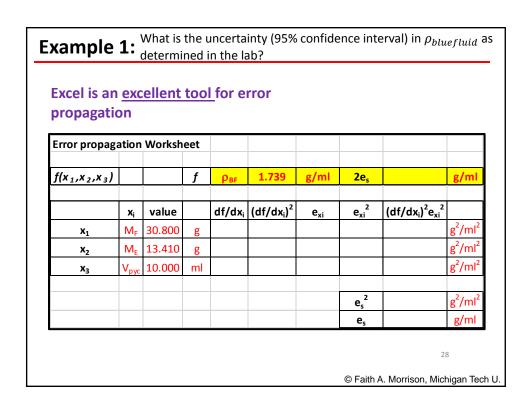
$f(x_1)$	(x_2, x_3, x_4, x_5)	Formula for $f: \rho_{BF} = \frac{M_F}{1}$	$\frac{-M_E}{V_{pyc}}$	Representative val	ue of f :		II. of f : $(f\pm 2e_{sf})$ de units)	
	Measured qua	intities, x_i		дf	$e_{x_i} =$		$(\partial f)^2$	
x_i	Symbol	Representative value		$\frac{\partial f}{\partial x_i}$	$\frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or	re_{s_i}	$\left(\frac{\partial f}{\partial x_i}\right)^2 e^{\frac{1}{2}}$	χį
<i>x</i> ₁								
<i>x</i> ₂								
<i>x</i> ₃								
x ₄								
x ₅								
·	$\partial f $	$(\partial f)^2$	$(\partial f)^2$	$(\partial f)^2$	$(\partial f)^2$		$e_{s_f}^2 =$	
	$e_{s_f}^2 = \left(\frac{s_f}{\partial x_1}\right) \ e_{s_f}^2 = \left(\frac{s_f}{\partial x_1}\right$	$e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 +$	$-\left(\frac{}{\partial x_3}\right) e_{x_3}^2$	$_3+\left(\frac{}{\partial x_4}\right) e_{x_4}^2+$	$\left(\frac{\dot{\partial x_5}}{\partial x_5}\right) e_{x_5}^2$		$e_{s_f} =$	units

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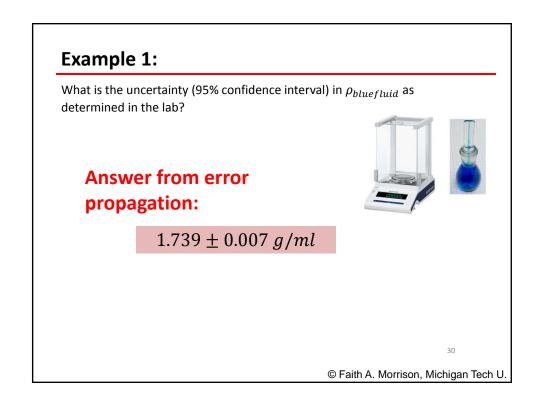








Example 1: What is the uncertainty (95% confidence interval) in $\rho_{bluefluid}$ as determined in the lab?										
Excel is an <u>excellent too</u> propagation	<u>l</u> for e	error								
Error propagation Worksheet										
				e _s ²	1.21E-05	g^2/ml^2				
				e _s	0.0035	g/ml				
			1							
					2	29				
				© Faith A	A. Morrison, Mic	chigan Tech U.				



Summary: Error Analysis with Real Numbers

 To understand the accuracy of our numbers, we need to determine a confidence interval.

 $ar{x} \pm 2e_{\scriptscriptstyle S}$ with 95.0% confidence

For replicate data with n < 7 , replace "2" with $t_{0.025,n-1}$

- The Standard error e_s for a measured quantity is the largest of:
 - e_S determined by replicates $e_S = s/\sqrt{n}$ or
 - e_s by estimate of *reading error* $e_s = e_R/\sqrt{3}$ or
 - e_s by estimate of *calibration error* $e_s = \max error/2$
- Standard error e_f for derived quantities (arrived at from equations), is obtained at through error propagation, which is a combination of variances.

3.

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Example 2: Replicates revisited

In Example 1, we calculated a value of ρ_{BF} along with its uncertainty from a single determination of density using error propagation. In lab, we have replicates of density measurements. How does the result from the single value compare to the result determined from replicates?

i	ρ_{BFi}
	g/cm
1	1.7162
2	1.7162
3	1.69942
4	1.7110
5	1.7152
6	1.70616
7	1.73097
8	1.73746
9	1.727



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Example 2: Replicates revisited

In Example 1, we calculated a value of ρ_{BF} along with its uncertainty from a single determination of density using error propagation. In lab, we have replicates of density measurements. How does the result from the single value compare to the result determined from replicates?

Re	eplicate W	orks/			
i	ρ_{BFi}		n=	9	
	g/cm		mean ρ=	1.718	g ² /ml ²
1	1.7162		s ² =	0.00015	g^2/ml^2
2	1.7162		s=	0.0121	
3	1.69942		s/sqrt(n)=	0.0040	g/cm
4	1.7110		2e _s =	0.008	g/cm
5	1.7152		te _s =	0.009	g/cm
6	1.70616				
7	1.73097				
8	1.73746				
9	1.727				





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Example 2: Replicates revisited

In Example 1, we calculated a value of ρ_{BF} along with its uncertainty from a single determination of density using error propagation. In lab, we have replicates of density measurements. How does the result from the single value compare to the result determined from replicates?

Solution:

Single measurement:

 $1.739 \pm 0.007 \ g/ml$

9 replicates:

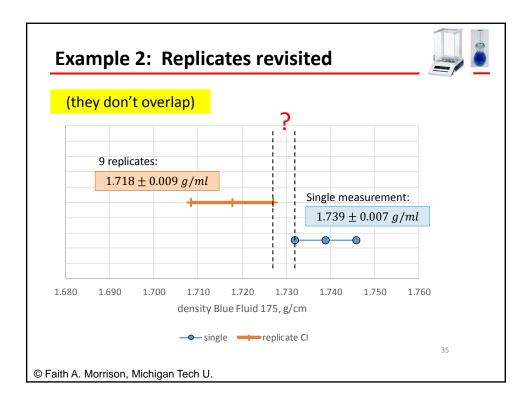
 $1.718 \pm 0.009 \ g/ml$

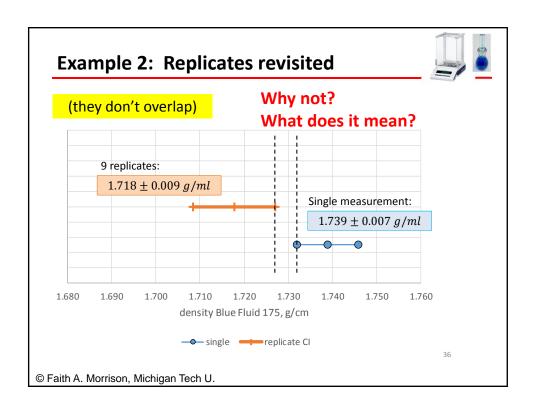


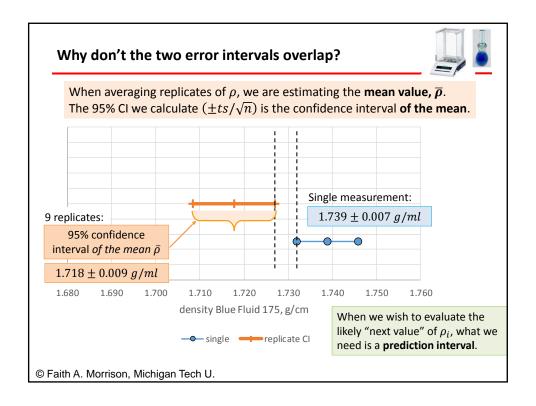


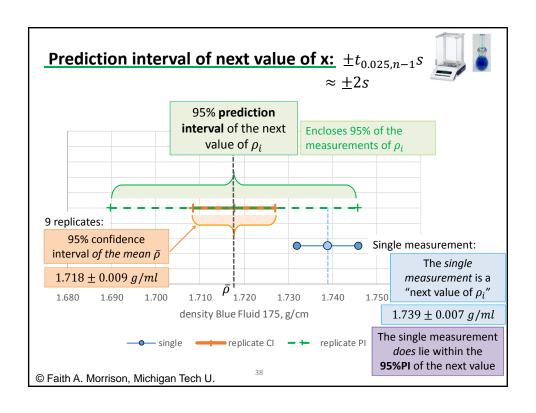
Do they agree?

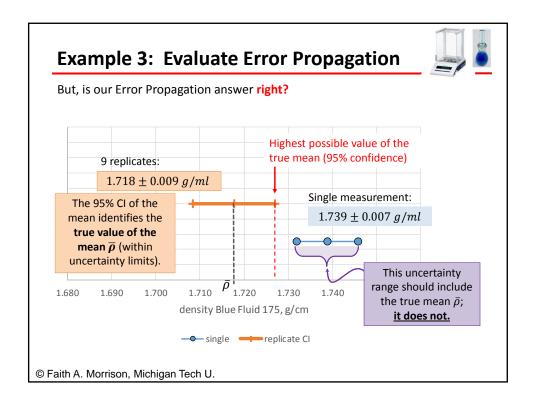
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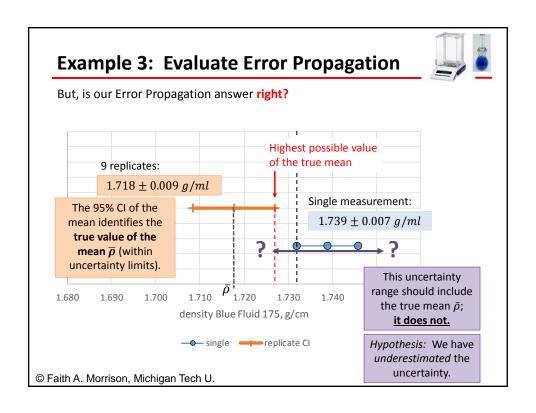


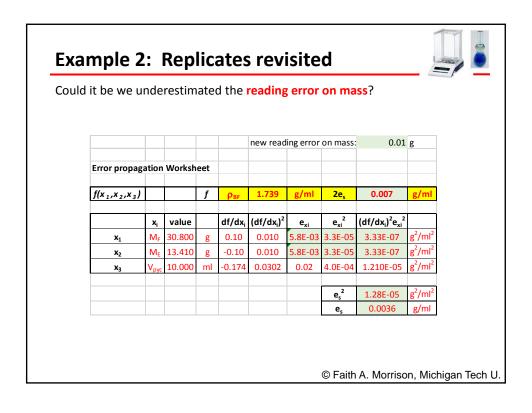


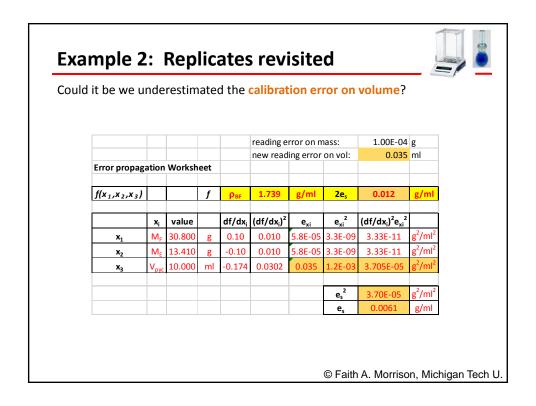


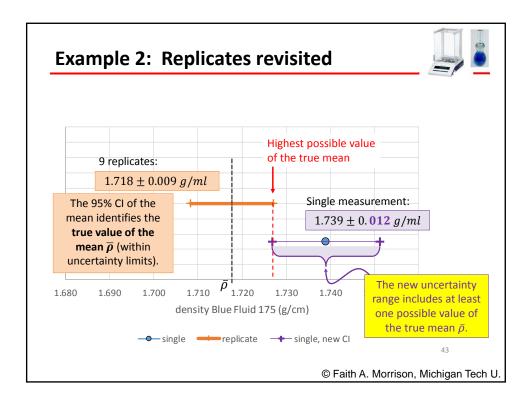












Summary: Error Analysis with Real Numbers

- To understand the accuracy of our numbers, we need to determine a confidence interval. $\bar{x}\pm 2e_s$ with 95.0% confidence For replicate data with n<7, replace "2" with $t_{0.025,n-1}$
- The Standard error e_s for a measured quantity is the largest of:
 - e_s determined by <u>replicates</u> $e_s = s/\sqrt{n}$ or
 - e_s by estimate of <u>reading error</u> $e_s = e_R/\sqrt{3}$ or

Replication always improves the estimation of the mean.

- $e_{\scriptscriptstyle S}$ by estimate of $\underline{calibration\ error}\ e_{\scriptscriptstyle S} = \max \, {\rm error}/2$
- Standard error e_f for derived quantities (arrived at from equations), is obtained through
 error propagation, which is a combination of variances.
- error propagation, which is a combination of *variances*.

 The answer from replicates is
- The prediction interval of the next value of x should 95% PI: $\bar{x} \pm 2s$
- encompass 95% of all measured values. or $\bar{x} \pm t_{0.025,n-1} s$ if n < 7• The weighting values $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ indicate the impact of individual errors on the final value.
- Estimates for e_s (particularly those obtained through e_R) may need to be re-evaluated, if unreasonably narrow confidence intervals are identified.

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more reliable than single values.

