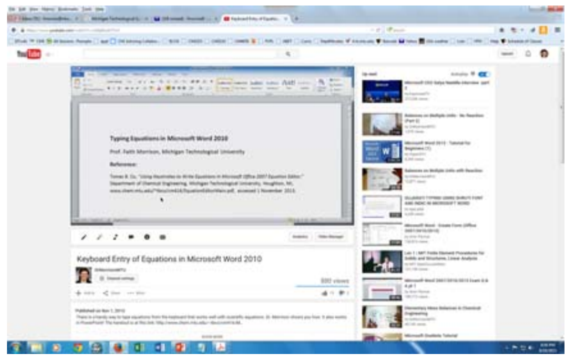
CM3215
Fundamentals of Chemical Engineering Laboratory

MichiganTech

# Typing Equations in MS Word 2010



https://www.youtube.com/watch?v=ceNp9meHTmY

*Professor Faith Morrison*
Department of Chemical Engineering
Michigan Technological University

1



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## Where are we in our discussion of error analysis?

Let's revisit:

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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

2

From Lecture 4—Error Propagation:

## 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 *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* $e_s = \text{max error}/2$
- Standard error $e_f$ for derived quantities (arrived at from equations), is obtained at through **error propagation,** which is a combination of *variances*.

3



From Lecture 4—Error Propagation:

## 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 $\sigma_f^2$:

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

4

From Lecture 4—Error Propagation:

## 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 $\sigma_f^2$:

**neglect**

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

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

5



From Lecture 4—Error Propagation:

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**Error Propagation Worksheet**
CM3215 Fundamentals of Chemical Engineering Lab
Prof. Faith Morrison

This worksheet guides the user through the determination of the standard error $e_{s_f}$ of a quantity $f(x_1, x_2, x_3, x_4, x_5)$ that is calculated from measured quantities $x_1, x_2, x_3, x_4$ and $x_5$. The $x_i$ are subject to random errors. The replicate standard deviations $\sigma_i$ or the reading errors $e_{R_i}$ for each variable $x_i$ must be determined first, and these uncertainties are propagated to determine $e_{s_f}$ using the relationship given below. Note: if standard error $e_{x_i}$ estimates via both replicates and reading error are available, use the larger of the two.

| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: | Representative value of $f$: (include units) | 95% C.I. of $f$: $(f \pm 2e_{s_f})$ (include units) |
|---|---|---|---|
| | | | |

| Measured quantities, $x_i$ | | | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{\sigma_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_s$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
|---|---|---|---|---|---|
| $x_i$ | Symbol | Representative value | | | |
| $x_1$ | | | | | |
| $x_2$ | | | | | |
| $x_3$ | | | | | |
| $x_4$ | | | | | |
| $x_5$ | | | | | |

$$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{s_f}^2 =$

$e_{s_f} =$ units

Standard error of calculated quantity $f$

Note: For some quantities, you will look up the uncertainty; for example the volume of a volumetric flask may be given as $100.00 \pm 0.04ml$. In these circumstances it is reasonable to assume that the reported uncertainty is $\pm 1.96e_s$. For example, if volume is given as $100.00 \pm 0.04ml$, then $1.96e_s \approx 2e_s = 0.04$. Reference: page 564 of Fritz and Schenk, *Quantitative Analytical Chemistry*, Allyn and Bacon, Boston, 1987.

**Worksheet for error propagation**

www.chem.mtu.edu/~fmorriso/cm3215/ErrorPropagationWorksheet.pdf

6

From Lecture 4—Error Propagation:

## Example 1:

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

**Error Propagation Worksheet**
CM3215 Fundamentals of Chemical Engineering Lab
Prof. Faith Morrison

| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: $\rho_{BF} = \frac{M_F - M_E}{V_{pyc}}$ | Representative value of $f$: (include units) $1.739\ g/ml$ | 95% C.I. of $f$: $(f \pm 2e_{sf})$ (include units) $1.739 \pm 0.007\ g/ml$ |
|---|---|---|---|

| Measured quantities, $x_i$ | | | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_{s_i}$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
|---|---|---|---|---|---|
| $x_i$ | Symbol | Representative value | | | |
| $x_1$ | $M_F$ | $30.800\ g$ | $1/V_{pyc}$ | $5.8 \times 10^{-5} g$ | $3.3 \times 10^{-11}\ g^2/ml^2$ |
| $x_2$ | $M_E$ | $13.410\ g$ | $-1/V_{pyc}$ | $5.8 \times 10^{-5} g$ | $3.3 \times 10^{-11}\ g^2/ml^2$ |
| $x_3$ | $V_{pyc}$ | $10.00\ ml$ | $-(M_F - M_E)/V_{pyc}^2$ | $0.02\ ml$ | $1.21 \times 10^{-5}\ g^2/ml^2$ |
| $x_4$ | | | | | |
| $x_5$ | | | | | |

Review

$$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{s_f}^2 = 1.21 \times 10^{-5}\ g^2/ml^2$

$e_{s_f} = 0.0035$ units $g/ml$ — Standard error of calculated quantity, $f$

7



From Lecture 4—Error Propagation:

## Example 1:

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

**Excel is an excellent tool for error propagation**

Review

| Error propagation Worksheet | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | |
| $f(x_1,x_2,x_3)$ | | | $f$ | $\rho_{BF}$ | 1.739 | g/ml | $2e_s$ | 0.007 | g/ml |
| | | | | | | | | | |
| | $x_i$ | value | | $df/dx_i$ | $(df/dx_i)^2$ | $e_{xi}$ | $e_{xi}^2$ | $(df/dx_i)^2 e_{xi}^2$ | |
| $x_1$ | $M_F$ | 30.800 | g | 0.10 | 0.010 | 5.8E-05 | 3.3E-09 | 3.33E-11 | $g^2/ml^2$ |
| $x_2$ | $M_E$ | 13.410 | g | -0.10 | 0.010 | 5.8E-05 | 3.3E-09 | 3.33E-11 | $g^2/ml^2$ |
| $x_3$ | $V_{pyc}$ | 10.000 | ml | -0.174 | 0.0302 | 0.02 | 4.0E-04 | 1.210E-05 | $g^2/ml^2$ |
| | | | | | | | | | |
| | | | | | | | $e_s^2$ | 1.21E-05 | $g^2/ml^2$ |
| | | | | | | | $e_s$ | 0.0035 | g/ml |

8

From Lecture 4—Error Propagation:

# Review

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Fundamentals of Chemical Engineering Laboratory

**Error Analysis for Laboratory Data**

1. Quick start—Replicate error
2. Reading Error
3. Calibration Error
4. Error Propagation

## 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 sum, in quadrature, of:
  - $e_s$ determined by *replicates* $e_s = s/\sqrt{n}$
  - $e_s$ by estimate of *reading error* $e_s = e_R/\sqrt{3}$
  - $e_s$ by estimate of *calibration error* $e_s = \text{error limits}/2$
- Standard error $e_f$ for derived quantities (arrived at from equations), is obtained through **error propagation,** which is a combination of *variances*.
- Replication improves the **estimation of the mean.** — The answer from replicates is more reliable than single values (if no systematic errors).
- The **prediction interval of the next value of x** should encompass 95% of all measured values. — 95% PI: $\bar{x} \pm 2s$ 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.

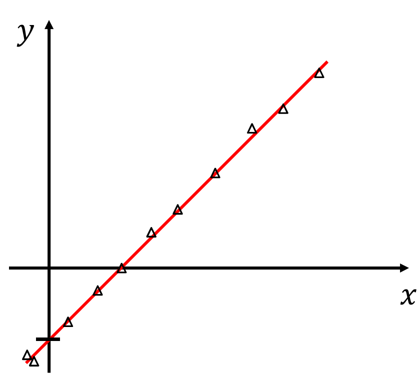
68

9



**Now,** how do we determine ***uncertainty*** from numbers that we obtain as parameters in a curve-fit?

| $i$ | $x_i$ | $y_i$ |
|---|---|---|
| 1 | $x_1$ | $y_1$ |
| 2 | $x_2$ | $y_2$ |
| ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ |




$$y = mx + b$$

10

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# Uncertainty in Least Squares Curve Fitting: Excel's LINEST

***Professor Faith Morrison***

Department of Chemical Engineering
Michigan Technological University

Reference:
- www.chem.mtu.edu/~fmorriso/cm3215/UncertaintySlopeInterceptOfLeastSquaresFit.pdf

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

11

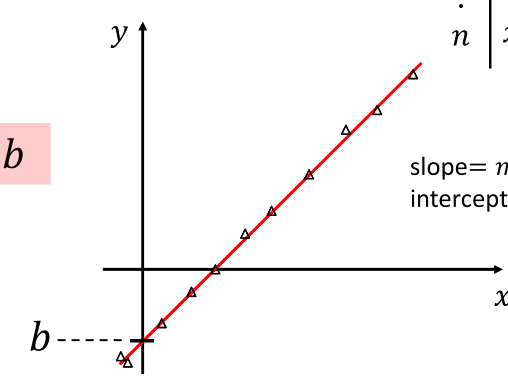


## Ordinary, *Least Squares*, Linear Regression

*Question*: For a dataset of $n$ data pairs $x_i, y_i$ that is expected to show a linear relationship between $y$ and $x$, what are the parameters $m$ and $b$ of the equation for the line?

| $i$ | $x_i$ | $y_i$ |
|---|---|---|
| 1 | $x_1$ | $y_1$ |
| 2 | $x_2$ | $y_2$ |
| ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ |

$$y = mx + b$$



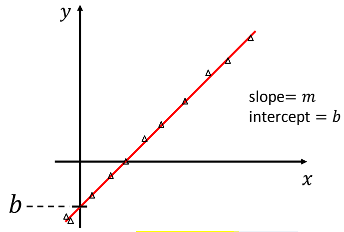

slope$= m$
intercept $= b$

12

## Ordinary, *Least Squares*, Linear Regression

*Solution*:

- Assume you know the $x_i$ with certainty (*"ordinary"* **least squares**)
- Guess a line, $\hat{y} = mx + b$
- Create a measure of the error between the *guess* and the *data* (**error measure should always be positive, so *square* it**)
- Add these individual error measures to calculate a *sum of squared errors*, $SS_E$
- Use *calculus* (derivatives) to find the values of $m$ and $b$ that result in the **least** sum of squared error.




| | data | | line |
|---|---|---|---|
| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

$$\hat{y}_i = mx_i + b$$

$$SS_E \equiv \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

13

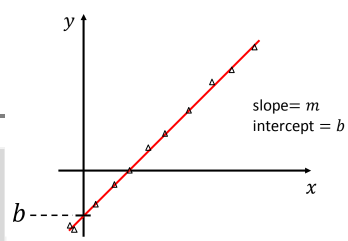


## Ordinary, *Least Squares*, Linear Regression

*Result:*

$$\hat{m} = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\hat{b} = \frac{\left(\sum_{i=1}^{n} x_i\right)^2\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i y_i\right)\left(\sum_{i=1}^{n} x_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

$$y = \hat{m}x + \hat{b}$$

Least squares slope $= \hat{m}$
Least squares intercept $= \hat{b}$

In Excel:
$\hat{m}$ = SLOPE(y-range, x-range)
$\hat{b}$ =INTERCEPT(y-range,x-range)

14

## Ordinary, *Least Squares*, Linear Regression

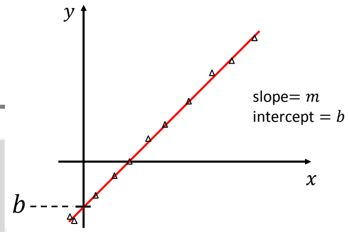
These are the formulas used in Excel trendlines.

*Result:*

$$\hat{m} = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\hat{b} = \frac{\left(\sum_{i=1}^{n} x_i\right)^2\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i y_i\right)\left(\sum_{i=1}^{n} x_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$\hat{m}$ and $\hat{b}$ are calculated from the $x_i, y_i$




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

$$y = \hat{m}x + \hat{b}$$

In Excel:
$\hat{m}$ = SLOPE(y-range, x-range)
$\hat{b}$ =INTERCEPT(y-range,x-range)

Least squares slope = $\hat{m}$
Least squares intercept = $\hat{b}$

15

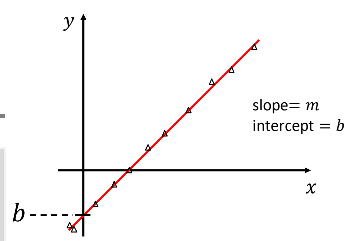


## Ordinary, *Least Squares*, Linear Regression

*Result:*

$$\hat{m} = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\hat{b} = \frac{\left(\sum_{i=1}^{n} x_i\right)^2\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i y_i\right)\left(\sum_{i=1}^{n} x_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$



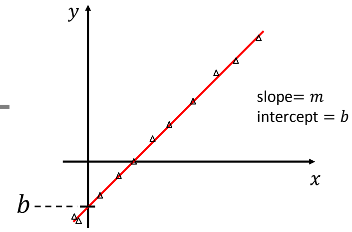

**But, what are the error limits on $\hat{m}$ and $\hat{b}$?**

$$y = \hat{m}x + \hat{b}$$

Least squares slope = $\hat{m}$
Least squares intercept = $\hat{b}$

16

**Ordinary, *Least Squares*, Linear Regression**




$$y = \hat{m}x + \hat{b}$$

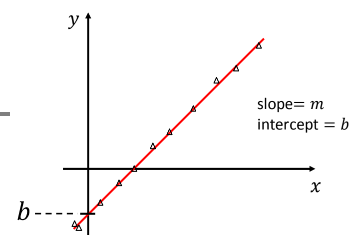
$$\text{slope} = \hat{m} \pm ?$$
$$\text{Intercept} = \hat{b} \pm ?$$

**But, what are the error limits on $\hat{m}$ and $\hat{b}$?**

17



**Ordinary, *Least Squares*, Linear Regression**




$$y = \hat{m}x + \hat{b}$$

$$\text{slope} = \hat{m} \pm ?$$
$$\text{Intercept} = \hat{b} \pm ?$$

**But, what are the error limits on $\hat{m}$ and $\hat{b}$?**

*Answer:*

$$\text{slope} = \hat{m} \pm 2e_s$$
$$\text{Intercept} = \hat{b} \pm 2e_s$$

*But what is $e_s$?*

18

(Later we will correct the "2" for small $n$)

## Ordinary, *Least Squares*, Linear Regression

*Answer:* $e_s = e_{sf}$

**Michigan Tech**
Michigan Technological University
Department of Chemical Engineering

**Error Propagation Worksheet**
CM3215 Fundamentals of Chemical Engineering Lab
Prof. Faith Morrison

This worksheet guides the user through the determination of the standard error $e_{sf}$ of a quantity $f(x_1, x_2, x_3, x_4, x_5)$ that is calculated from measured quantities $x_1, x_2, x_3, x_4$ and $x_5$. The $x_i$ are subject to random errors. The replicate standard deviations $\sigma_i$ or the reading errors $e_{R_i}$ for each variable $x_i$ must be determined first, and these uncertainties are propagated to determine $e_{sf}$ using the relationship given below. Note: If standard error $e_{x_i}$ estimates via both replicates and reading error are available, use the larger of the two.

| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: | Representative value of $f$: (include units) | 95% C.I. of $f$: $(f \pm 2e_{sf})$ (include units) |
|---|---|---|---|
| | | | |

| Measured quantities, $x_i$ | | | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{\sigma_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_s$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
|---|---|---|---|---|---|
| $x_i$ | Symbol | Representative value | | | |
| $x_1$ | | | | | |
| $x_2$ | | | | | |
| $x_3$ | | | | | |
| $x_4$ | | | | | |
| $x_5$ | | | | | |

$$e_{sf}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{sf}^2 =$

$e_{sf} =$ units

Standard error of calculated quantity $f$

Note: For some quantities, you will look up the uncertainty; for example the volume of a volumetric flask may be given as $100.00 \pm 0.04 ml$. In these circumstances it is reasonable to assume that the reported uncertainty is $\pm 1.96 e_s$. For example, if volume is given as $100.00 \pm 0.04 ml$, then $1.96 e_s \approx 2e_s = 0.04$. Reference: page 564 of Fritz and Schenk, *Quantitative Analytical Chemistry*, Allyn and Bacon, Boston, 1987.

19



## Error limits on $\hat{m}$

### Ordinary, *Least Squares*, Linear Regression

*Answer:* $e_s = e_{sf}$

**Error Propagation Worksheet**
CM3215 Fundamentals of Chemical Engineering Lab
Prof. Faith Morrison

| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: | Representative value of $f$: (include units) | 95% C.I. of $f$: $(f \pm 2e_{sf})$ (include units) |
|---|---|---|---|
| | $\hat{m} = \frac{n\sum_{i=1}^n x_i y_i - (\sum_{i=1}^n x_i)(\sum_{i=1}^n y_i)}{n\sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2}$ | $\hat{m} =$ | $\hat{m} = \pm(2)(s_m)$ |

| Measured quantities, $x_i$ | | | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_{s_i}$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
|---|---|---|---|---|---|
| $x_i$ | Symbol | Representative value | | | |
| $x_1$ | $y_1$ | | $\frac{\partial \hat{m}}{\partial y_1}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_1}\right)^2 s_{y,x}^2$ |
| $x_2$ | $y_2$ | | $\frac{\partial \hat{m}}{\partial y_2}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_2}\right)^2 s_{y,x}^2$ |
| $x_3$ | $y_3$ | | $\frac{\partial \hat{m}}{\partial y_3}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_3}\right)^2 s_{y,x}^2$ |
| $x_4$ | $y_4$ | | $\frac{\partial \hat{m}}{\partial y_4}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_4}\right)^2 s_{y,x}^2$ |
| $x_5$ | $\vdots$ | | $\vdots$ | $\vdots$ | $\vdots$ |

$$e_{sf}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{sf}^2 = s_m^2$

$e_{sf} = s_m$ units

## Error limits on $\hat{m}$

**Ordinary, *Least Squares*, Linear Regression**

Error Propagation Worksheet
CM3215 Fundamentals of Chemical Engineering Lab
Prof. Faith Morrison

*Answer:* $e_s = e_{sf}$

| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: $\hat{m} = \frac{n\sum_{i=1}^{n} x_i y_i - (\sum_{i=1}^{n} x_i)(\sum_{i=1}^{n} y_i)}{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}$ | Representative value of $f$: (include units) $\hat{m} =$ | 95% C.I. of $f$: $(f \pm 2e_{sf})$ (include units) $\hat{m} = \pm(2)(s_m)$ |
|---|---|---|---|

Only the $y_i$ are variables; we assumed we knew the $x_i$ with certainty

| $x_i$ | Symbol | Representative value | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_{s_i}$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
|---|---|---|---|---|---|
| $x_1$ | $y_1$ | | $\frac{\partial \hat{m}}{\partial y_1}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_1}\right)^2 s_{y,x}^2$ |
| $x_2$ | $y_2$ | | $\frac{\partial \hat{m}}{\partial y_2}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_2}\right)^2 s_{y,x}^2$ |
| $x_3$ | $y_3$ | | $\frac{\partial \hat{m}}{\partial y_3}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_3}\right)^2 s_{y,x}^2$ |
| $x_4$ | $y_4$ | | $\frac{\partial \hat{m}}{\partial y_4}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_4}\right)^2 s_{y,x}^2$ |
| $x_5$ | $\vdots$ | | $\vdots$ | $\vdots$ | $\vdots$ |

$$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{s_f}^2 = s_m^2$

$e_{s_f} = s_m$ units



## Error limits on $\hat{m}$

**Ordinary, *Least Squares*, Linear Regression**

Error Propagation Worksheet
CM3215 Fundamentals of Chemical Engineering Lab
Prof. Faith Morrison

*Answer:* $e_s = e_{sf}$

Assume that the variances of the $y_i$ are the same for all $y_i$.

| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: $\hat{m} = \frac{n\sum_{i=1}^{n} x_i y_i - (\sum_{i=}^{n}}{n\sum_{i=1}^{n} x_i^2 - (}$ | 95% C.I. of $f$: $(f \pm 2e_{sf})$ (include units) $\hat{m} = \pm(2)(s_m)$ |
|---|---|---|

| Measured quantities, $x_i$ | | | | | |
|---|---|---|---|---|---|
| $x_i$ | Symbol | Representative value | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_{s_i}$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
| $x_1$ | $y_1$ | | $\frac{\partial \hat{m}}{\partial y_1}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_1}\right)^2 s_{y,x}^2$ |
| $x_2$ | $y_2$ | | $\frac{\partial \hat{m}}{\partial y_2}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_2}\right)^2 s_{y,x}^2$ |
| $x_3$ | $y_3$ | | $\frac{\partial \hat{m}}{\partial y_3}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_3}\right)^2 s_{y,x}^2$ |
| $x_4$ | $y_4$ | | $\frac{\partial \hat{m}}{\partial}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{m}}{\partial y_4}\right)^2 s_{y,x}^2$ |
| $x_5$ | $\vdots$ | | | $\vdots$ | $\vdots$ |

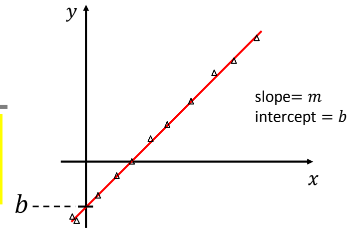
($s_{y,x}$ is the standard deviation of $y$ at a given value of $x$)

$$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{s_f}^2 = s_m^2$

$e_{s_f} = s_m$ units

## Ordinary, *Least Squares*, Linear Regression




$s^2_{y,x}$

($s_{y,x}$ is the standard deviation of $y$ at a given value of $x$; ordinary least squares assumes it is constant)

The variance of $y$, given $x$

$$s^2_{y,x} \equiv \left(\frac{1}{n-2}\right)\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

(This formula comes from the *definition* of variance)

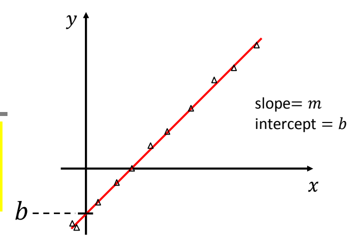
The variance of the mean value of $y$ at a given $x$

In Excel:
- $s_{y,x}$ = STEYX(y-range, x-range), or
- use LINEST

23



## Ordinary, *Least Squares*, Linear Regression




$s^2_{y,x}$

($s_{y,x}$ is the standard deviation of $y$ at a given value of $x$; ordinary least squares assumes it is constant)

The variance of $y$, given $x$

$$s^2_{y,x} \equiv \left(\frac{1}{n-2}\right)\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Best value of $y$ at a given $x$

(This formula comes from the *definition* of variance)

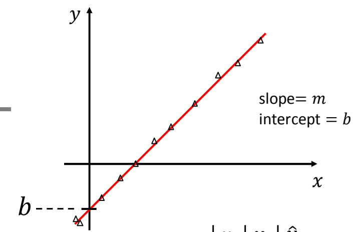
The variance of the mean value of $y$ at a given $x$

$s^2_{y,x}$ is calculated from the $x_i, y_i$

In Excel:
- $s_{y,x}$ = STEYX(y-range, x-range), or
- use LINEST

24

## Ordinary, *Least Squares*, Linear Regression




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

What are the error limits on $\hat{m}$?

*Answer:*

$$\text{slope} = \hat{m} \pm 2s_m$$

$$s_m^2 = \frac{s_{y,x}^2}{SS_{xx}}$$

(This is the final result of the algebra indicated on the error propagation slide)

for $n-2 \leq 6$:
slope $= \hat{m} \pm t_{0.025,n-2} s_m$

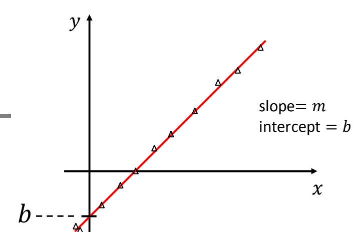
In Excel:

- $s_m^2 = \frac{(\text{STEYX(y–range, x–range)})^2}{(\text{DEVSQ(x–range)})}$, or
- use LINEST

25



## Ordinary, *Least Squares*, Linear Regression




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

What are the error limits on $\hat{b}$?

*Answer:*

$$\text{intercept} = \hat{b} \pm 2e_s$$

?

Solve the same way, error propagation on the formula for $\hat{b}$

26

# Error limits on $\hat{b}$

**Ordinary, *Least Squares*, Linear Regression**

*Answer:* $e_s = e_{sf}$

**Error Propagation Worksheet**
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Prof. Faith Morrison

| $f(x_1, x_2, x_3, x_4, x_5)$: | **Formula for $f$:** $\hat{b} = \frac{(\sum_{i=1}^n x_i)^2(\sum_{i=1}^n y_i) - (\sum_{i=1}^n x_i y_i)(\sum_{i=1}^n x_i)}{n\sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2}$ | **Representative value of $f$:** (include units) $\hat{b} =$ | **95% C.I. of $f$: $(f \pm 2e_{sf})$** (include units) $\hat{b} = \pm(2)(s_b)$ |
|---|---|---|---|

| Measured quantities, $x_i$ | | | | | |
|---|---|---|---|---|---|
| $x_i$ | Symbol | Representative value | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_{s_i}$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
| $x_1$ | $y_1$ | | $\frac{\partial \hat{b}}{\partial y_1}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{b}}{\partial y_1}\right)^2 s_{y,x}^2$ |
| $x_2$ | $y_2$ | | $\frac{\partial \hat{b}}{\partial y_2}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{b}}{\partial y_2}\right)^2 s_{y,x}^2$ |
| $x_3$ | $y_3$ | | $\frac{\partial \hat{b}}{\partial y_3}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{b}}{\partial y_3}\right)^2 s_{y,x}^2$ |
| $x_4$ | $y_4$ | | $\frac{\partial \hat{b}}{\partial y_4}$ | $s_{y,x}$ | $\left(\frac{\partial \hat{b}}{\partial y_4}\right)^2 s_{y,x}^2$ |
| $x_5$ | ⋮ | | ⋮ | ⋮ | ⋮ |

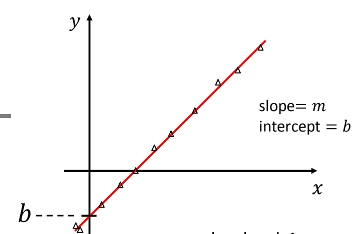
$$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{s_f}^2 = s_b^2$

$e_{s_f} = s_b$ units



**Ordinary, *Least Squares*, Linear Regression**




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

What are the error limits on $\hat{b}$?

*Answer:*

$$\text{intercept} = \hat{b} \pm 2s_b$$

$$s_b^2 = s_{y,x}^2\left(\frac{1}{n} + \frac{\bar{x}^2}{SS_{xx}}\right)$$

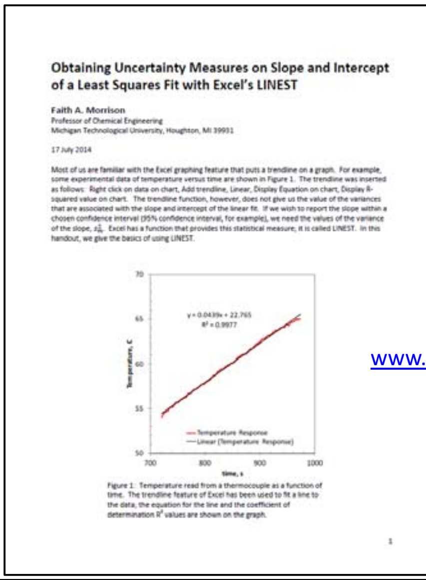
(This is the final result of the algebra indicated on the error propagation slide)

for $n - 2 \leq 6$:
intercept $= \hat{b} \pm t_{0.025,n-2}s_b$

In Excel:
- Calculate $s_b^2$ from STEYX(y–range, x–range) and DEVSQ(x–range) and the formula above, or
- use LINEST

28

## Ordinary, *Least Squares*, Linear Regression



**Obtaining Uncertainty Measures on Slope and Intercept of a Least Squares Fit with Excel's LINEST**

Faith A. Morrison
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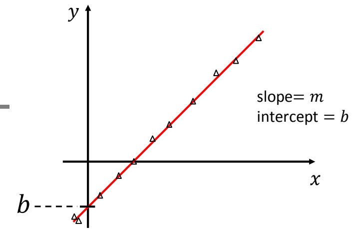
17 July 2014

Most of us are familiar with the Excel graphing feature that puts a trendline on a graph. For example, some experimental data of temperature versus time are shown in Figure 1. The trendline was inserted as follows: Right click on data on chart, Add trendline, Linear, Display Equation on chart, Display R-squared value on chart. The trendline function, however, does not give us the value of the variances that are associated with the slope and intercept of the linear fit. If we wish to report the slope within a chosen confidence interval (95% confidence interval, for example), we need the values of the variance of the slope, $s_m^2$. Excel has a function that provides this statistical measure; it is called LINEST. In this handout, we give the basics of using LINEST.



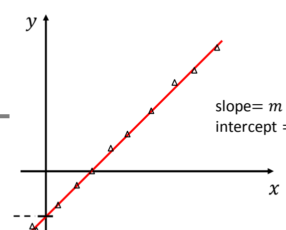

For instructions on how to use Microsoft Excel's LINEST function, see the handout on the web:

www.chem.mtu.edu/~fmorriso/cm3215/UncertaintySlopeInterceptOfLeastSquaresFit.pdf

(the appendix has some derivations, if you're interested)




## Ordinary, *Least Squares*, Linear Regression




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

**What are the error limits on a value of $y$ obtained from the equation $y = \hat{m}x + \hat{b}$?**

At a chosen $x_p$,

$$y_p = \left(\hat{m}x_p + \hat{b}\right) \pm 2e_s$$

?

# Error limits on $y_p = \hat{m}x_p + \hat{b}$

**Ordinary, *Least Squares*, Linear Regression**

*Answer:* $e_s = e_{sf}$

**Error Propagation Worksheet**
CM3215 Fundamentals of Chemical Engineering Lab
Prof. Faith Morrison

| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: $y_p = \hat{m}x_p + \hat{b}$ | Representative value of $f$: (include units) $y_p =$ | 95% C.I. of $f$: $(f \pm 2e_{s_f})$ (include units) $y_p = \pm(2)(s_{y_p})$ |
|---|---|---|---|

| Measured quantities, $x_i$ | | | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_{s_i}$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
|---|---|---|---|---|---|
| $x_i$ | Symbol | Representative value | | | |
| $x_1$ | $\hat{m}$ | | $\frac{\partial y_p}{\partial \hat{m}} = x_p$ | $s_m$ | $(x_p s_m)^2$ |
| $x_2$ | $x_p$ | | $\frac{\partial y_p}{\partial x_p} = \hat{m}$ | 0 | 0 |
| $x_3$ | $\hat{b}$ | | $\frac{\partial y_p}{\partial \hat{b}} = 1$ | $s_b$ | $s_b^2$ |
| $x_4$ | | | | | |
| $x_5$ | | | | | |

$$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{s_f}^2 = s_{y_p}^2$

$e_{s_f} = s_{y_p}$ units




# Error limits on $y_p = \hat{m}x_p + \hat{b}$

**Ordinary, *Least Squares*, Linear Regression**

*Answer:* $e_s = e_{sf}$

**Error Propagation Worksheet**
CM3215 Fundamentals of Chemical Engineering Lab
Prof. Faith Morrison

| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: $y_p = \hat{m}x_p + \hat{b}$ | Representative value of $f$: (include units) $y_p =$ | 95% C.I. of $f$: $(f \pm 2e_{s_f})$ (include units) $y_p = \pm(2)(s_{y_p})$ |
|---|---|---|---|

| Measured quantities, $x_i$ | | | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_{s_i}$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
|---|---|---|---|---|---|
| $x_i$ | Symbol | Representative value | | | |
| $x_1$ | $\hat{m}$ | | $\frac{\partial y_p}{\partial \hat{m}} = x_p$ | $s_m$ | $(x_p s_m)^2$ |
| $x_2$ | $x_p$ | | $\frac{\partial y_p}{\partial x_p} = \hat{m}$ | 0 | 0 |
| $x_3$ | $\hat{b}$ | | $\frac{\partial y_p}{\partial \hat{b}} = 1$ | $s_b$ | $s_b^2$ |
| $x_4$ | | | | | |
| $x_5$ | | | | | |


But, $\hat{m}$ and $\hat{b}$ are not **independent** (both are calculated from the $y_i$).


$$e_{s_f}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{s_f}^2 = s_{y_p}^2$

$e_{s_f} = s_{y_p}$ units

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# Error limits on $y_p = \hat{m}x_p + \hat{b}$

**Ordinary, *Least Squares*, Linear Regression**

*Answer:* $e_s = e_{sf}$

**Error Propagation Worksheet**
CM3215 Fundamentals of Chemical Engineering Lab
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| $f(x_1, x_2, x_3, x_4, x_5)$: | Formula for $f$: $y_p = \hat{m}x_p + \hat{b}$ | Representative value of $f$: (include units) $y_p =$ | 95% C.I. of $f$: $(f \pm 2e_{sf})$ (include units) $y_p = \pm(2)(s_{y_p})$ |
|---|---|---|---|

| $x_i$ | Symbol | Representative value | $\frac{\partial f}{\partial x_i}$ | $e_{x_i} = \frac{s_i}{\sqrt{N}}$ or $\frac{e_{R_i}}{\sqrt{3}}$ or $e_{s_i}$ | $\left(\frac{\partial f}{\partial x_i}\right)^2 e_{x_i}^2$ |
|---|---|---|---|---|---|
| $x_1$ | $\hat{m}$ | | $\frac{\partial y_p}{\partial \hat{m}} = x_p$ | $s_m$ | $(x_p s_m)^2$ |
| $x_2$ | $x_p$ | | $\frac{\partial y_p}{\partial x_p} = \hat{m}$ | 0 | 0 |
| $x_3$ | $\hat{b}$ | | $\frac{\partial y_p}{\partial \hat{b}} = 1$ | $s_b$ | $s_b^2$ |
| $x_4$ | | | | | |
| $x_5$ | | | | | |

$$+2\left(\frac{\partial y_p}{\partial \hat{m}}\right)\left(\frac{\partial y_p}{\partial \hat{b}}\right)\mathrm{Cov}(\hat{m}, \hat{b})$$

$$e_{sf}^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 e_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 e_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 e_{x_3}^2 + \left(\frac{\partial f}{\partial x_4}\right)^2 e_{x_4}^2 + \left(\frac{\partial f}{\partial x_5}\right)^2 e_{x_5}^2$$

$e_{sf}^2 = s_{y_p}^2$

$e_{sf} = s_{y_p}$ units

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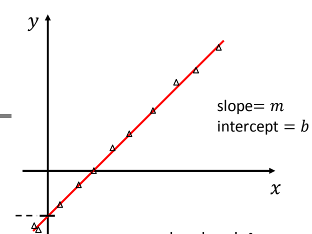
## Ordinary, *Least Squares*, Linear Regression




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

**What are the error limits on a value of $y$ obtained from the equation $y = \hat{m}x + \hat{b}$?**

*Answer:*

at $x_p$, $y_p = (\hat{m}x_p + \hat{b}) \pm 2s_{y_p}$

$$s_{y_p}^2 = s_{y,x}^2\left(\frac{1}{n} + \frac{(x_p - \bar{x})^2}{SS_{xx}}\right)$$

for $n - 2 \leq 6$,
replace "2" with $t_{0.025,n-2}$

(This is the final result of the algebra indicated on previous slide; see Appendix B of the handout.)

Use this for error limits on values obtained from the fit.

In Excel:
- $s_{y,x}$ = STEYX(y-range,x-range)
- $SS_{xx}$ = DEVSQ(x-range)
- $\bar{x}$ = AVERAGE(x-range)

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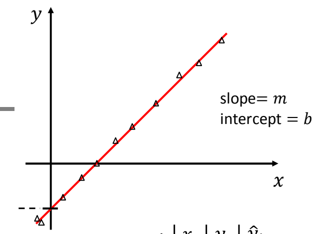
## Ordinary, *Least Squares*, Linear Regression




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

**What are the error limits on a predicted next experimental value of $y$?**

*Answer:*

at $x_p$, we predict a new measurement of $y_{\hat{p}}$ will fall in the prediction interval:

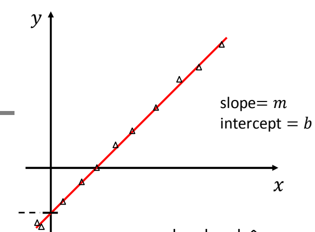
$$y_{\hat{p}} = \left(\hat{m}x_p + \hat{b}\right) \pm 2e_s$$

**?**

35



## Ordinary, *Least Squares*, Linear Regression

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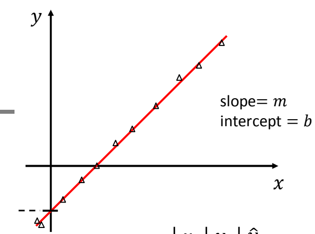
**?**

Solve with same approach as we have been using: write the equation to calculate the quantity, then propagate the error.

(See Appendix B of the handout.)

36

## Ordinary, *Least Squares*, Linear Regression




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
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**What are the error limits on a predicted next experimental value of $y$?**

*Answer:*

at $x_p$, we predict a new measurement of $y_{\hat{p}}$ will fall in the prediction interval:

$$y_{\hat{p}} = \left(\hat{m}x_p + \hat{b}\right) \pm 2s_{y_{\hat{p}}}$$

$$s^2_{y_{\hat{p}}} = s^2_{y,x}\left(1 + \frac{1}{n} + \frac{\left(x_p - \bar{x}\right)^2}{SS_{xx}}\right)$$

(See Appendix B of the handout.)

for $n - 2 \leq 6$, replace "2" with $t_{0.025,n-2}$

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## Ordinary, *Least Squares*, Linear Regression

**Confidence interval for values from the fit:**

$$y_p = \left(\hat{m}x_p + \hat{b}\right) \pm 2s_{y_p}$$

$$s^2_{y_p} = s^2_{y,x}\left(\frac{1}{n} + \frac{\left(x_p - \bar{x}\right)^2}{SS_{xx}}\right)$$

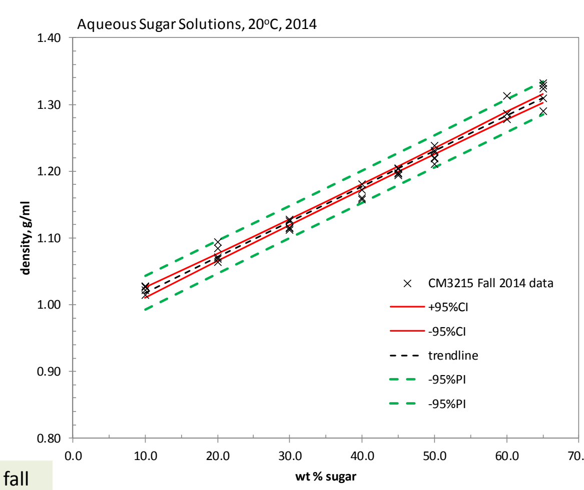
(for large $n$, the values of $y$ at each $x$ are well predicted (CI is narrow))

**Prediction interval of data:**

$$y_{\hat{p}} = \left(\hat{m}x_p + \hat{b}\right) \pm 2s_{y_{\hat{p}}}$$

$$s^2_{y_{\hat{p}}} = s^2_{y,x}\left(1 + \frac{1}{n} + \frac{\left(x_p - \bar{x}\right)^2}{SS_{xx}}\right)$$

(Notice that ≈ 95% of the data points fall within the PI; that's what it means to be a PI. The next data point likely will fall here too.)

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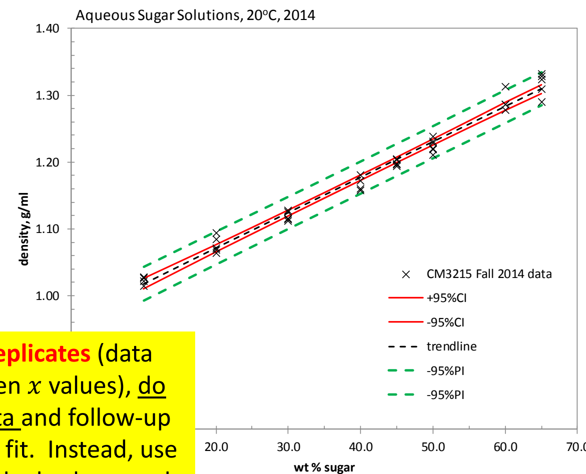
## Ordinary, *Least Squares*, Linear Regression



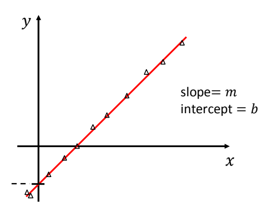

Note: if your data are **replicates** (data taken repeatedly at chosen $x$ values), <u>do not pre-average the $y$-data</u> and follow-up with a least-squares curve fit. Instead, use <u>all</u> the replicates as individual values, and let LINEST find the least squared error.

39



## Summary:
## Uncertainty Ordinary, *Least Squares*, Linear Regression

- The **Ordinary *Least Squares* Linear Regression** method provides the equations needed to obtain model parameters ***slope*** and ***intercept***.
- The equations for the parameters may be used with error propagation to obtain the variances associated with the parameters $m$ and $b$.
  - ✓ 95% confidence intervals on the parameters are constructed with $\pm 2e_s$ for large $n$
  - ✓ For $n-2 \leq 6$, the 95% CI is constructed as $\pm\, t_{0.025,n-2}e_s$
- We can construct 95% CI on the best values of $y$ at a chosen $x$. These CI are used for **error range** on the fit.
- We can construct 95% prediction intervals (PI) on a next value of $y$ at a chosen $x$; use to evaluate next experimental point acquired.




| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
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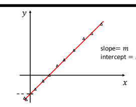
| ⋮ | ⋮ | ⋮ | ⋮ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |

40

| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |



## Excel Summary:
## Uncertainty Ordinary, *Least Squares*, Linear Regression

- $\bar{x}$ = AVERAGE(range)
- $s^2$ = VAR.S(range)
- $s$ = STDEV.S(range)
- $n$ = COUNT(range)
- $SS_{xx}$ = DEVSQ(x-range)
- $\hat{m}$ = SLOPE(y-range, x-range)
- $\hat{b}$ =INTERCEPT(y-range,x-range)
- $s_{y,x}$ = STEYX(y-range, x-range)
- LINEST (see handout)
- LOGEST (look it up)

- $s_m^2 = \frac{s_{y,x}^2}{SS_{xx}}$
- $s_b^2 = s_{y,x}^2\left(\frac{1}{n} + \frac{\bar{x}^2}{SS_{xx}}\right)$
- $s_{\hat{y}_p}^2 = s_{y,x}^2\left(\frac{1}{n} + \frac{(x_p-\bar{x})^2}{SS_{xx}}\right)$ — Use for CI error bars on $y$-values obtained from a fit
- $s_{y_{\tilde{p}}}^2 = s_{y,x}^2\left(1 + \frac{1}{n} + \frac{(x_p-\bar{x})^2}{SS_{xx}}\right)$ — Use for PI of next measured value of $y$





| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
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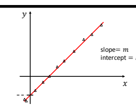
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $n$ | $x_n$ | $y_n$ | $\hat{y}_n$ |



## Excel Handy List:
## Uncertainty Ordinary, *Least Squares*, Linear Regression

- $\hat{y}(x_p)$ = TREND(known-y's, known-x's,$x_p$) for $y$ and $x$ related by $y = mx + b$
- $\hat{y}(x_p)$ = GROWTH(known-y's, known-x's, $x_p$) for $y$ and $x$ related by $y = ae^{bx}$

| $i$ | $x_i$ | $y_i$ | $\hat{y}_i$ |
|---|---|---|---|
| 1 | $x_1$ | $y_1$ | $\hat{y}_1$ |
| 2 | $x_2$ | $y_2$ | $\hat{y}_2$ |
| ⋮ | ⋮ | ⋮ | ⋮ |
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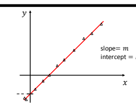



## One final piece of advice:

Uncertainty Ordinary, *Least Squares*, Linear Regression

Often, you can **transform** your data to make it linear, allowing you to use linear regression. For example, if you know the $y$-data vary as the square root of the $x$-data, then

$$y \text{ versus } \sqrt{x}$$

will be linear. If data plotted with log-log scaling (using scatterplot) look quadratic, then

$$\log y \text{ versus } \log x$$

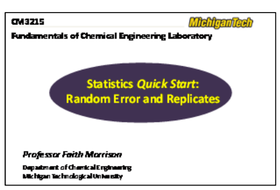
will be quadratic, and we can use trendline to obtain a fit:

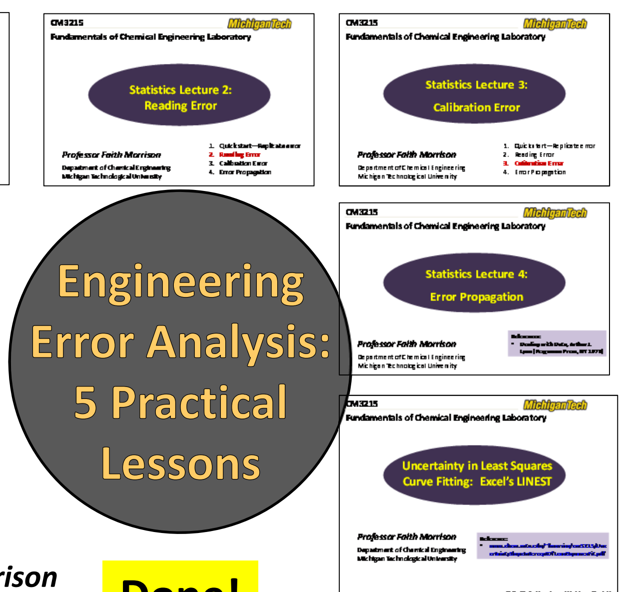
$$\log y = a(\log x)^2 + b(\log x) + c$$

Transforming data can greatly broaden our ability to fit empirical models to data.

43








MichiganTech

***Professor Faith Morrison***

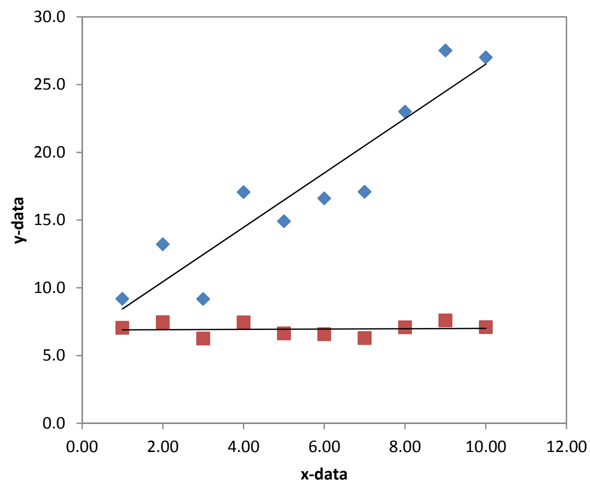
Department of Chemical Engineering
Michigan Technological University

**Done!**

44

## Comment on Curve Fitting: *Coefficient of Determination, $R^2$*

Which data set has a larger $R^2$?




45



## Comment on Curve Fitting: *Coefficient of Determination, $R^2$*

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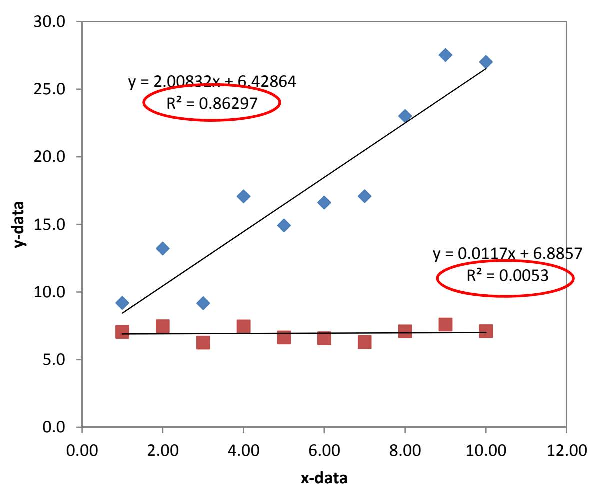
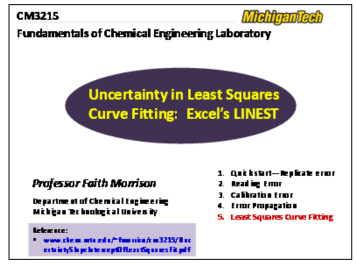



46

## Comment on Curve Fitting: *Coefficient of Determination*, $R^2$

$R^2$ is a measure of the comparison of the hypothesized linear relationship $y = mx + b$ and the relationship $y =$ constant (horizontal line). So, if it ***is*** a horizontal line, $R^2$ will be zero.




From page 6:

9. $R^2$ Coefficient of Determination—fraction of the variability of the $y_i$ accounted for by the linear model:

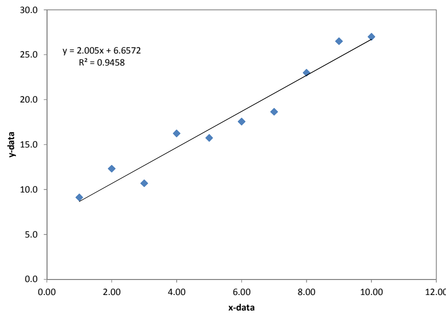
$$R^2 = \frac{\text{explained error}}{\text{total error}} = \frac{SS_R}{SS_T} = \frac{SS_T - SS_E}{SS_T} \qquad (20)$$

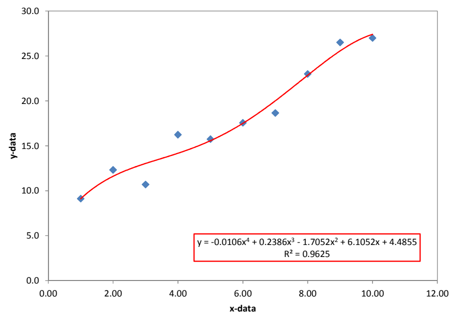
When the model is a very good fit, there is little deviation between the data and the model; then, $SS_E \to 0$ and $R^2 = 1$. Note, however, that if the model is a horizontal line, the model is $\hat{y} = \bar{y}$, and $SS_T$ is equal to $SS_E$, and $R^2$ is zero. The coefficient of determination is a measure of goodness of fit except when the data are nearly constant.

47



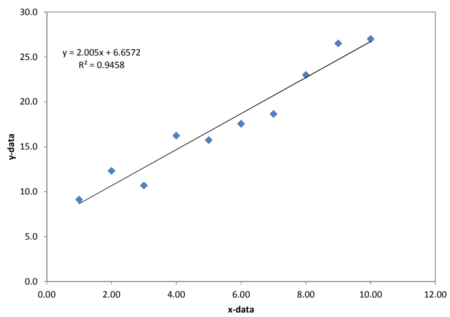
## Which is the correct fit?

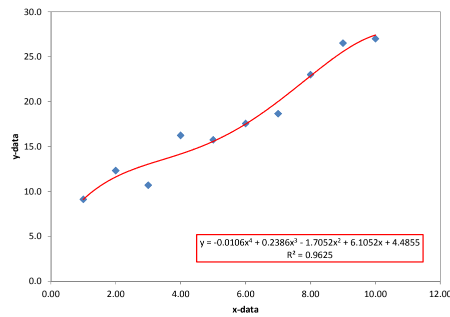



48

## Which is the correct fit?




- (it depends on the error bars)
- Likely that the linear fit is a “truer” relationship to be used for interpolation

49