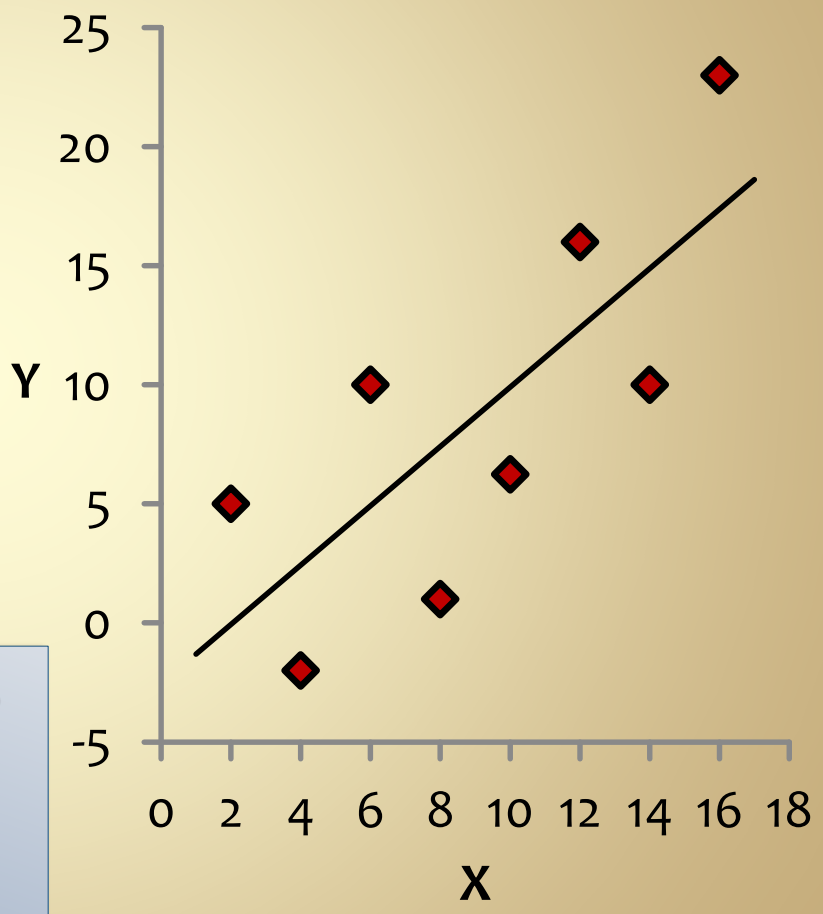
Regression Statistics

2020

Engineers and Regression

Engineers often:

- Regress data
  - Analysis
  - Fit to theory
  - Data reduction
- Use the regression of others
  - Antoine Equation
  - DIPPR



We need to be able to report uncertainties associated with regression.

- Do the data fit the model?
- What are the errors in the prediction?
- What are the errors in the parameters?

Linear Regression

- There are two classes of regressions
  - Linear
  - Non-linear
- “Linear” refers to the parameters, not the functional dependence of the independent variable
- What is the Python command to fit a linear equation?

Linear Regression

Quiz

1. $y = ax^2 + bx + c$
2. $y = ae^{bx}$
3. $y = a + \frac{b}{T} + \frac{c}{T^3} + \frac{d}{T^4} + \frac{e}{T^5}$
4. $y = \exp\left(A - \frac{B}{T + C}\right)$
5. $y = mx + b$

Straight Line Model

$$Y_i = b_0 + b_1 X_i + e_i$$

slope

Intercept

"X" data

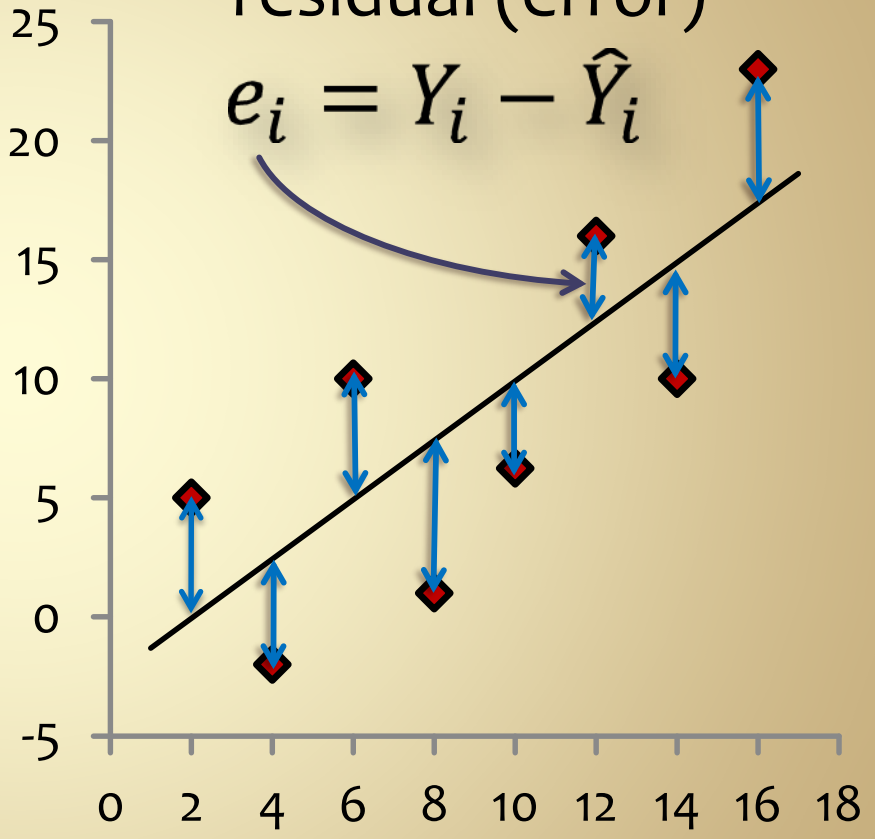
"Y" Measured

"Y" Predicted

$$\hat{Y}_i = b_0 + b_1 X_i$$

residual (error)

$$e_i = Y_i - \hat{Y}_i$$



Straight Line Model

$$\hat{Y}_i = b_0 + b_1 X_i$$

intercept	0.92291455	slope	0.516173934

	X_i	Y_i	$\hat{Y}_i$	e_i
1		2.749032178	1.439088483	1.309943694
2		3.719910224	2.362003033	1.357907192
3		0.925995017	3.284917582	-2.35892257
4		2.623482686	4.207832132	-1.58434945
5		6.539797342	5.130746681	1.409050661
6		6.779909177	6.053661231	0.726247946
7		4.946150401	6.976575781	-2.03042538
8		9.674178069	7.89949033	1.774687739
9		7.61959821	8.82240488	-1.20280667
10		7.650020996	9.745319429	-2.09529843
11		11.514	10.66823398	0.845766021
12		13.18285068	11.59114853	1.591702152
13		13.28173635	12.51406308	0.767673275
14		13.60444592	13.43697763	0.16746829
15		12.79535218	14.35989218	-1.56454
16		17.82374778	15.28280673	2.540941056
17		14.55068379	16.20572128	-1.65503748

42.76608602	SS_E

$$e_i = Y_i - \hat{Y}_i$$

residual (error)

"X" data

"Y" data

"Y" predicted

sum squared error

$$SS_E = \sum_{i=1}^{n} e_i^2$$

mean squared error

$$MS_E = \hat{\sigma}^2 = \frac{SS_E}{n-2}$$

Number of fitted parameters:
2 for a two-parameter model

The R^2 Statistic

$$R^2 = \frac{SS\ due\ to\ regression}{(Total\ SS, corrected\ for\ the\ mean\ \bar{Y})}$$

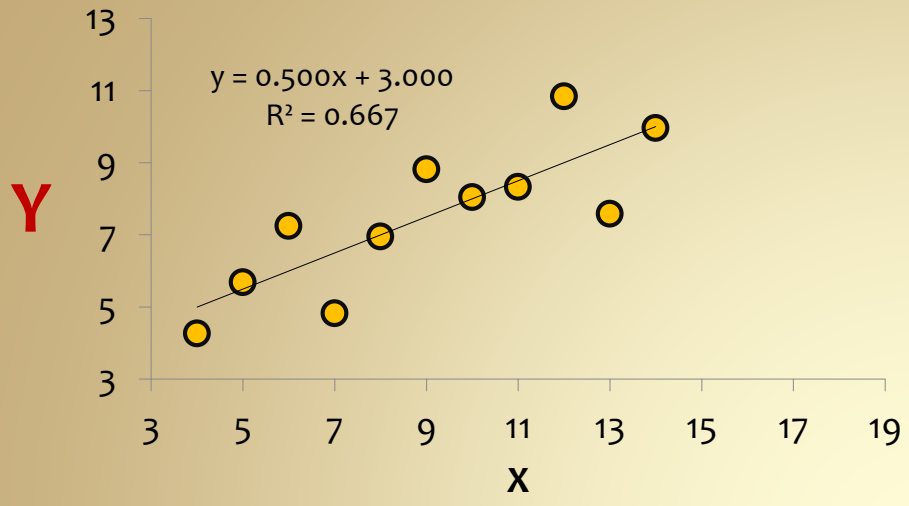
$$= \frac{SS_R}{SS_T}$$

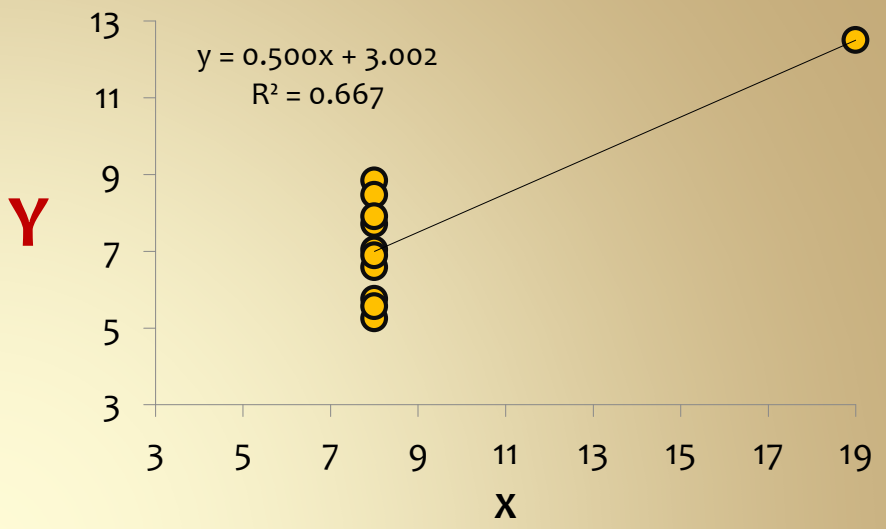
$$= \frac{\sum_{i=1}^{n}\left(\hat{Y}_i - \bar{Y}\right)^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}$$

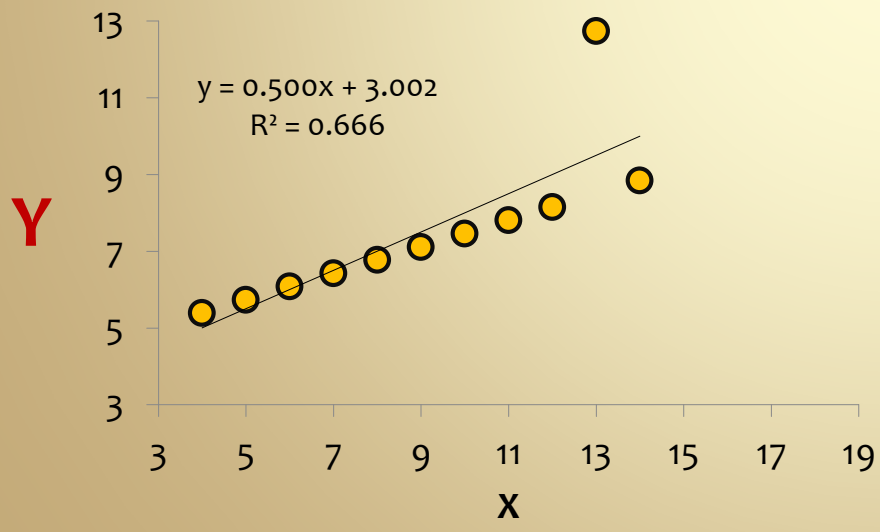
- A *useful* statistic but not definitive
- Tells you how well the data fit the model.
- It does *not* tell you if the model is correct.

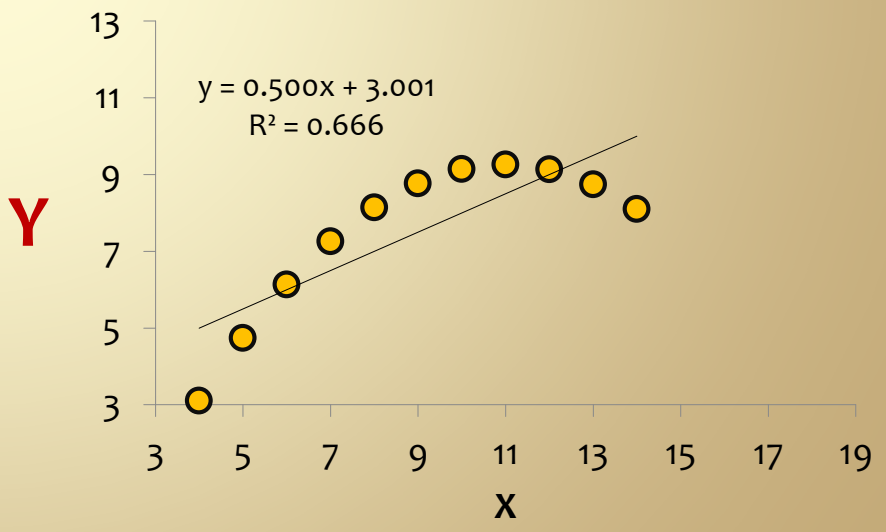
How much of the distribution of the data *about the mean* is described by the model.

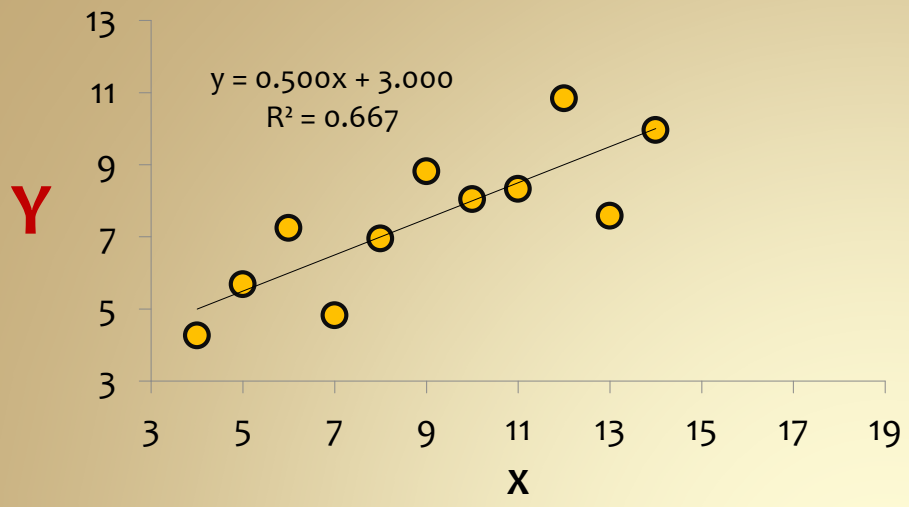
Problems with R^2

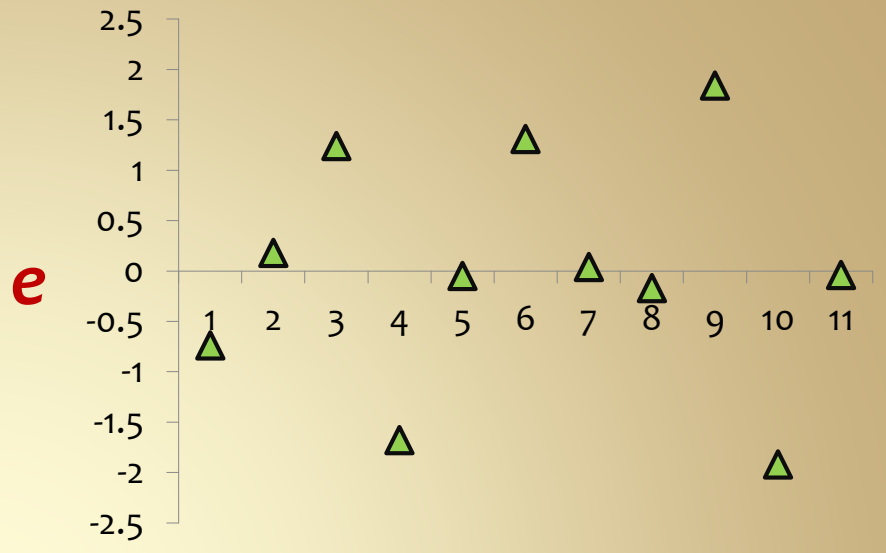




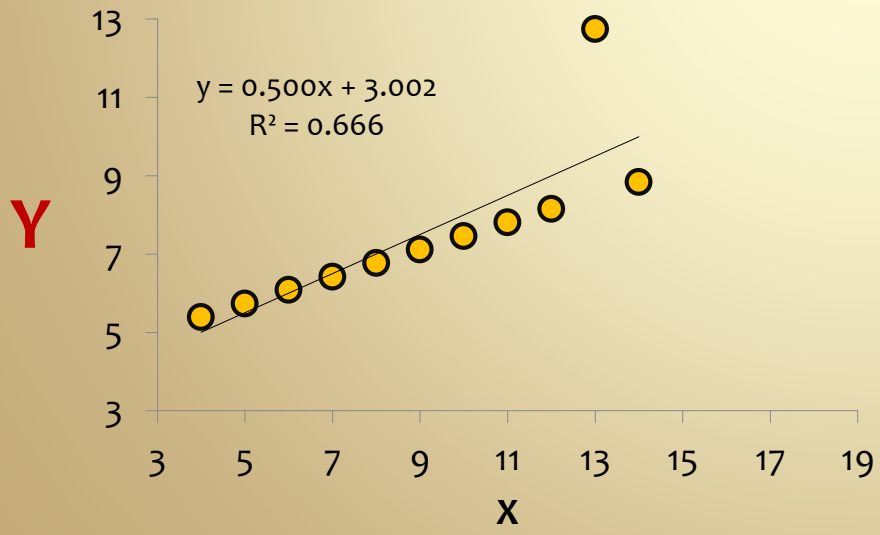


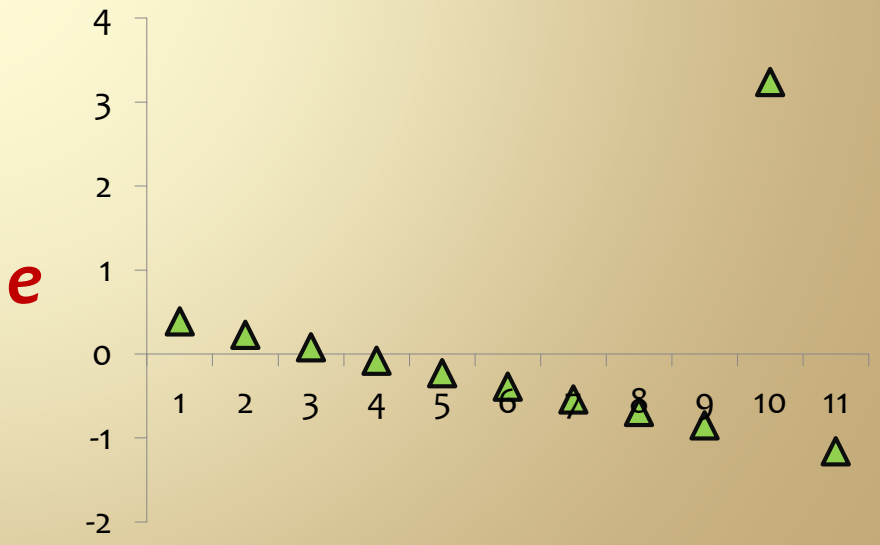


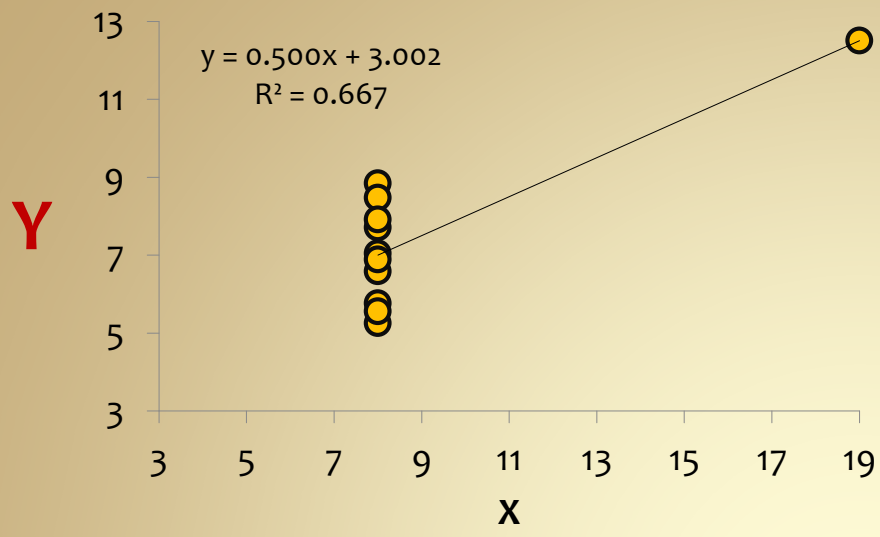


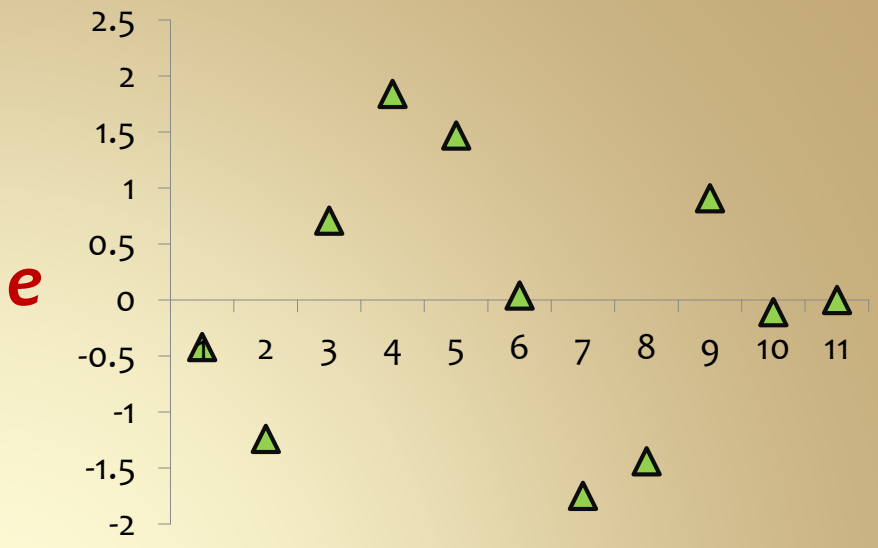


Residuals (e_i) should be normally distributed

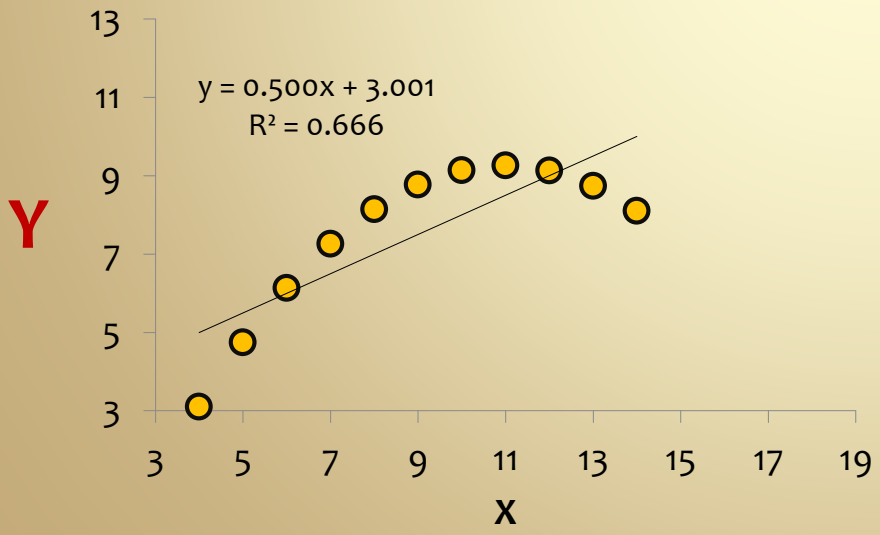


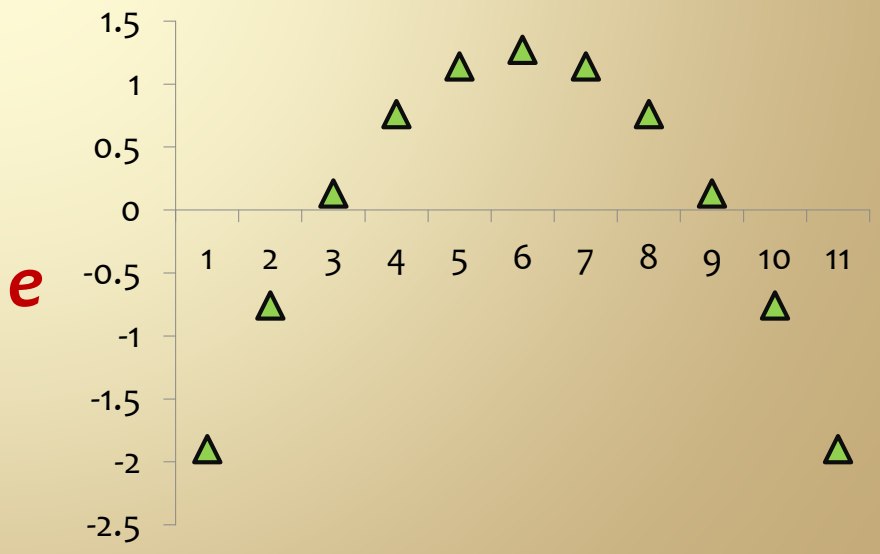






Residuals (e_i) should be normally distributed

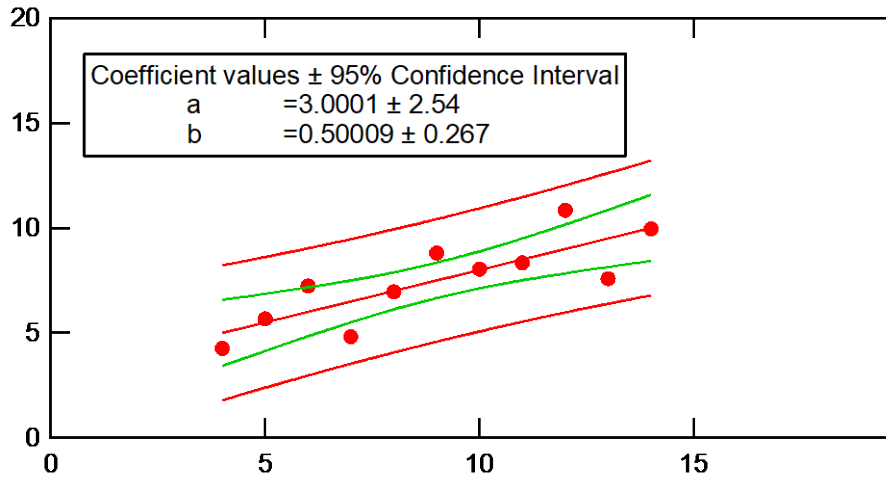


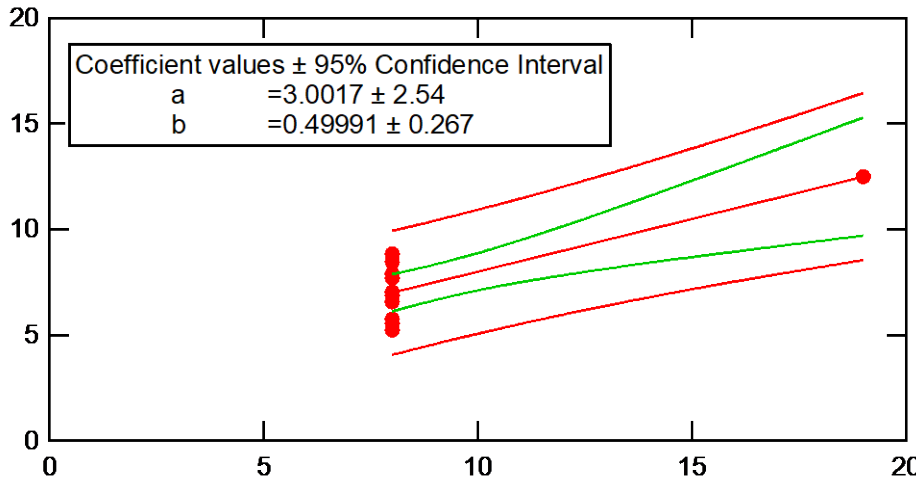


Other Questions About Fit

- How well does the line fit the data at each point (not just the mean)?
- In what range should the data lie (are there outliers)?
- What are the confidence intervals on the slope and intercept?

Confidence Intervals from Example





Green is confidence interval

How well does the model fit the data?

Red is the prediction band

Where should the data fall? Can I throw out any points?

Statistics on the Slope/Intercept

When you fit data to a straight line, the slope and intercept are only *estimates* of the *true* slope and intercept.

(1-α)100% Confidence Intervals

$$b_0 \pm S_{b_0} t_{n-2,1-\frac{\alpha}{2}}$$

(slope)

$$b_1 \pm S_{b_1} t_{n-2,1-\frac{\alpha}{2}}$$

(intercept)

Standard Errors

$$S_{b_0} = \left(\frac{\sum_{i=1}^{n} X_i^2}{n \sum_{i=1}^{n} (X_i - \bar{X})^2} \right)^{0.5} \hat{\sigma}$$

$$S_{b_1} = \left(\frac{1}{\sum_{i=1}^{n} (X_i - \bar{X})^2} \right)^{0.5} \hat{\sigma}$$

Confidence Interval on the Prediction & Prediction Band of Data

Confidence Interval on the Prediction

Given a specific value for x, X_0, what is the error in $\hat{Y}_0$?

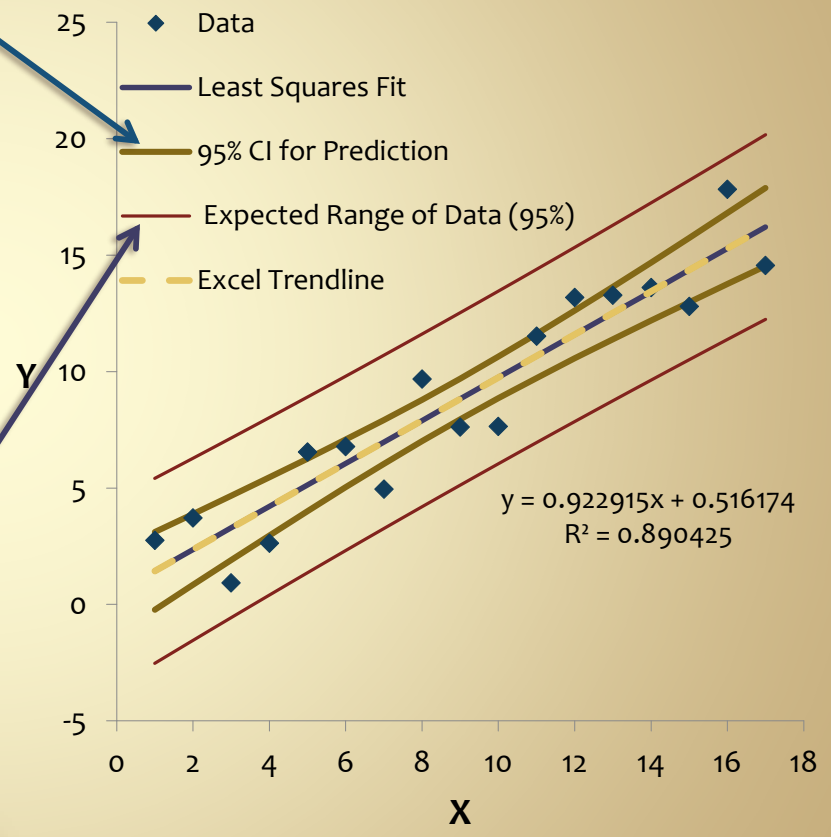
$$\hat{Y}_0 \pm S_{\hat{Y}} t_{n-2,1-\frac{\alpha}{2}}$$

$$S_{\hat{Y}} = \left(\frac{1}{n} + \frac{(X_0 - \bar{X})^2}{\sum_{i=1}^{n} (X_i - \bar{X})^2} \right)^{0.5} \hat{\sigma}$$

Prediction Band: Expected Range of Data

If I take more data, where will the data fall? (Where will Y_0 be found if measured at X_0?)

$$Y_0 = \hat{Y}_0 \pm t_{n-2,1-\frac{\alpha}{2}} \left(1 + \frac{1}{n} + \frac{(X_0 - \bar{X})^2}{\sum_{i=1}^{n} (X_i - \bar{X})^2} \right)^{0.5} \hat{\sigma}$$



3. Linear Regression
(Confidence Interval)

- Confidence Interval for each $(X_0, \hat{Y}_0)$

$$\hat{Y}_0 \pm S_{\hat{Y}} t_{n-2,1-\alpha} \qquad \text{(using 2-tailed t table)}$$

$$S_{\hat{Y}} = \left(\frac{1}{n} + \frac{(X_0 - \bar{X})^2}{\sum_{i=1}^{n} (X_i - \bar{X})^2} \right)^{0.5} s_{yx}$$

$$s_{yx} = \left(\frac{1}{n-2} \left[\sum_{i=1}^{n} (Y_i - \bar{Y})^2 - \frac{[\sum_{i=1}^{n} (X_i - \bar{X})(Y_i - \bar{Y})]^2}{\sum_{i=1}^{n} (X_i - \bar{X})^2} \right] \right)^{0.5}$$

- Prediction Band for each $(X_0, \hat{Y}_0)$

$$Y_0 = \hat{Y}_0 \pm t_{n-2,1-\alpha} \left(1 + \frac{1}{n} + \frac{(X_0 - \bar{X})^2}{\sum_{i=1}^{n} (X_i - \bar{X})^2} \right)^{0.5} s_{yx}$$

- In Excel, s_{yx} can be solved using
  =STEYX(Ydata,Xdata)
- In Excel, $\sum_{i=1}^{n} (X_i - \bar{X})^2$ can be solved using
  =DEVSQ(Xdata)
- For 95% confidence interval with 15 data points, get t from
  =T.INV.2T(.05,13)

Confidence Interval vs. Prediction Band

Confidence Interval

- Shows possible errors in where the line will go
- Interval narrows with increasing number of data points
  - See equation on previous slide

Prediction Band

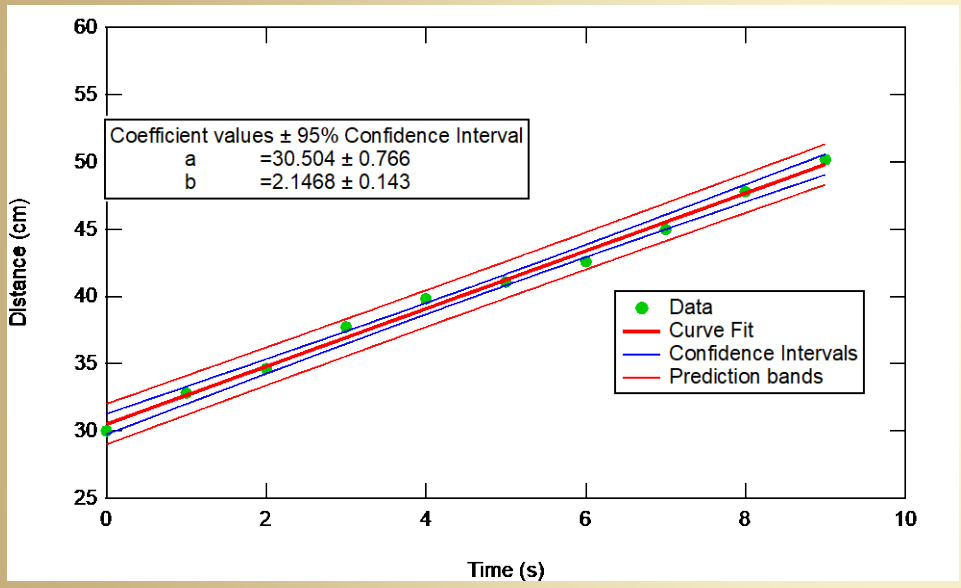
- Shows where the data should lie
- Interval does not narrow much with increasing number of data points
  - See equation on previous slide

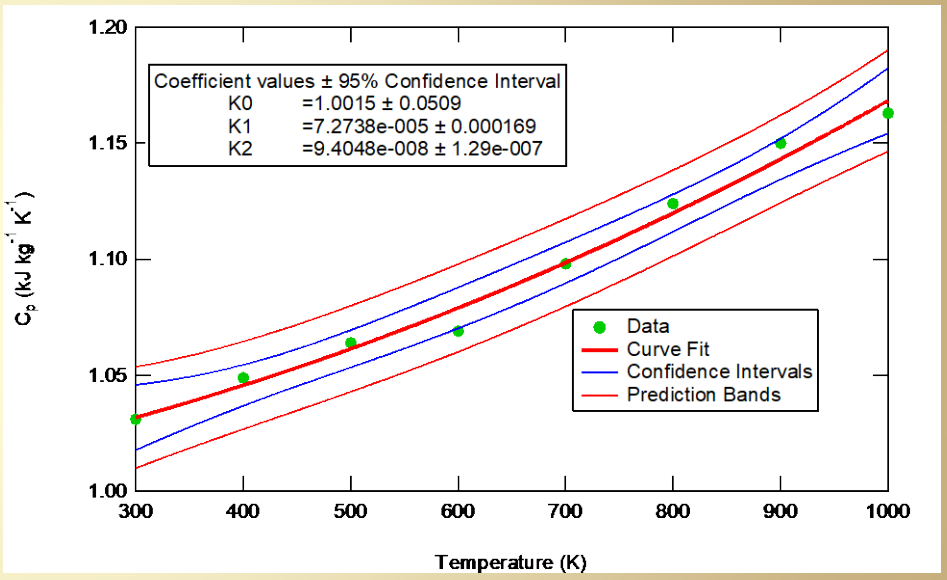
Good News: IGOR!

- Igor has the equations already programmed and will
  - Plot the confidence intervals
  - Plot the prediction bands
  - Print the ± confidence intervals on the slope and intercept

In-Class Assignment

Answers


Coefficient values ± 95% Confidence Interval
a =30.504 ± 0.766
b =2.1468 ± 0.143
Data
Curve Fit
Confidence Intervals
Prediction bands
Distance (cm)
Time (s)
60
55
50
45
40
35
30
25
0
2
4
6
8
10


Coefficient values ± 95% Confidence Interval
K0 =1.0015 ± 0.0509
K1 =7.2738e-005 ± 0.000169
K2 =9.4048e-008 ± 1.29e-007
Data
Curve Fit
Confidence Intervals
Prediction Bands
Cp (kJ kg-1 K-1)
Temperature (K)
1.20
1.15
1.10
1.05
1.00
300
400
500
600
700
800
900
1000

Example Using Excel

- In Analysis Toolpak, use “Regression”
- Gives confidence intervals on slope and intercept
- Does not give
  - Confidence interval on the line
  - Prediction band

Generalized Linear Regression

- Linear regression can be written in matrix form.

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{b} + \boldsymbol{e}$$

X	Y
21	186
24	214
32	288
47	425
50	455
59	539
68	622
74	675
62	562
50	453
41	370
30	274

Straight Line Model

$$\hat{Y}_i = b_0 + b_1 X_i + e_i$$

$$\boldsymbol{X} = \begin{bmatrix} 1 & 21 \\ 1 & 24 \\ \vdots & \vdots \\ 1 & 41 \\ 1 & 30 \end{bmatrix} \quad \boldsymbol{Y} = \begin{bmatrix} 186 \\ 214 \\ \vdots \\ 370 \\ 274 \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix} \quad \boldsymbol{e} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_{n-1} \\ e_n \end{bmatrix}$$

Quadratic Model

$$\hat{Y}_i = b_0 + b_1 X_i + b_2 X_i^2 + e_i$$

$$\boldsymbol{X} = \begin{bmatrix} 1 & 21 & 441 \\ 1 & 24 & 576 \\ \vdots & \vdots & \vdots \\ 1 & 41 & 1681 \\ 1 & 30 & 900 \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix}$$

$$\boldsymbol{b} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{Y}$$

Statistics with Matrices

$$SS_E = \boldsymbol{Y^T Y} - \boldsymbol{b^T X^T Y}$$

$$MS_E = \hat{\sigma}^2 = \frac{SS_E}{n-p}$$

Parameter Confidence Intervals

$$b_i \pm S_{b_i} t_{n-p,1-\frac{\alpha}{2}}$$

Standard Error of b_i is the square root of the i-th diagonal term of the matrix

$$\left(\boldsymbol{X^T X}\right)^{-1} \hat{\sigma}^2$$

Predicted Variable Confidence Intervals

$$\hat{Y}_0 \pm S_{\hat{Y}} t_{n-p,1-\frac{\alpha}{2}}$$

$$S_{\hat{Y}} = \left(\boldsymbol{X_0^T}\left(\boldsymbol{X^T X}\right)^{-1}\boldsymbol{X_0}\right)^{0.5} \hat{\sigma}$$