STAT 500

Simple Linear Regression: ANOVA Table and \mathbb{R}^2

- ullet Write the deviation from the overall sample mean as $Y_i ar{Y} = (Y_i \hat{Y}_i) + (\hat{Y}_i ar{Y})$ where $\hat{Y}_i = b_o + b_1 X_i$
- Partition the corrected total sums of squares

$$egin{aligned} SS_{corrected\ total} &= \sum\limits_{i} (Y_i - ar{Y})^2 = \sum\limits_{i} (Y_i - \hat{Y}_i + \hat{Y}_i - ar{Y})^2 \ &= \sum\limits_{i} (Y_i - \hat{Y}_i)^2 + \sum\limits_{i} (\hat{Y}_i - ar{Y})^2 \ &+ 2\sum\limits_{i} (Y_i - \hat{Y}_i) (\hat{Y}_i - ar{Y}) \ &= \sum\limits_{i} (Y_i - \hat{Y}_i)^2 + \sum\limits_{i} (\hat{Y}_i - ar{Y})^2 \ &= SS_{residuals} + SS_{model} \end{aligned}$$

Cross product term is

$$2\sum\limits_i (Y_i-\hat{Y}_i)(\hat{Y}_i-ar{Y}) \ = \ 2\sum\limits_i e_i(b_o+b_1x_i-ar{Y})$$

$$= \ 2(b_o-ar{Y})\sum\limits_i e_i+2b_1\sum\limits_i e_ix_i$$

$$= \ 0 \quad ext{because} \ \sum\limits_i e_i=\sum\limits_i e_ix_i=0$$

Note that

$$egin{array}{lll} SS_{model} &=& \sum\limits_{i}(\hat{Y}_{i}-ar{Y})^{2} = \sum\limits_{i}(b_{o}+b_{1}x_{i}-ar{Y})^{2} \ &=& b_{1}^{2}\sum\limits_{i=1}^{n}(x_{i}-ar{x})^{2} \end{array}$$

$$egin{aligned} ullet SS_{model} &= SS_{total} - SS_{error} \ &= \Sigma_i (\hat{Y}_i - ar{Y})^2 \ &= \Sigma_i (b_o + b_1 x_i - ar{Y})^2 \ &= b_1^2 \sum\limits_{i=1}^n (x_i - ar{x})^2 \end{aligned}$$

- ullet SS_{model} is also denoted by $SS_{regression}$
- ullet SS_{error} is also denoted by $SS_{residuals}$ or SSE

 SS_{error} has n-2 degrees of freedom because

- ullet Two parameters must be estimated to calculate \hat{Y}_i
- The residuals satisfy two constraints

$$\sum e_i = 0$$
 and $\sum e_i x_i = 0$

ANOVA Table

Source	df	Sums of Squares	
Model	1	$SS_{model} = \Sigma_{i=1}^n (\hat{Y}_i - ar{Y})^2$	
Error	n-2	SS error $= \Sigma_{i=1}^n (Y_i - \hat{Y}_i)^2$	
Total	n-1	$SS_{Total} = \scriptscriptstyle{\Sigma}_{i=1}^n (Y_i - ar{Y})^2$	

ANOVA Table: Example

Source	df	SS	MS	F	p-value
Model	1	0.22573	0.22573	2961.55	< 0.0001
Error	15	0.00114	0.00007622		
Total	16	0.22688			

Mean Squares

• MSerror

$$-\hat{\sigma}^2 = MS_{ ext{error}} = SS_{ ext{error}}/(n-2)$$

- $\hat{\sigma}^2$ is an unbiased estimate of σ^2

$$E(MS_{ ext{error}}) = \sigma^2$$

ullet MS_{model}

$$-E(MS_{\mathsf{model}}) = \sigma^2 + eta_1^2 \Sigma_{i=1}^n (x_i - \bar{x})^2$$

- When eta_1 =0, $E(MS_{ ext{model}}) = \sigma^2$. Otherwise, $E(MS_{ ext{model}}) > \sigma^2$.

F-test for Significance of Model

$$\bullet \ H_0: \beta_1 = 0 \to Y_i = \beta_0 + \epsilon_i$$

•
$$H_a: \beta_1 \neq 0 \rightarrow Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

• Test Statistic:

$$F = rac{MS_{\mathsf{model}}}{MS_{\mathsf{error}}}$$

ullet Reject H_0 if

$$F = rac{MS_{\mathsf{model}}}{MS_{\mathsf{error}}} > F_{1,n-2,1-lpha}$$

F-test: Example

- $H_0: \beta_1 = 0$
- $H_a: \beta_1 \neq 0$
- F = 2961.55 with p-value < 0.0001.
- ullet Reject H_0 and conclude there is a significant linear relationship between boiling point of water and log of barometric pressure.

Coefficient of Determination (R^2)

$$R^2 = rac{SS_{\mathsf{model}}}{SS_{\mathsf{Total}}}$$

- ullet Fraction of variation in the response variable that can be explained by the linear regression model with the explanatory variable x.
- ullet Expressed as percentage: $0\% \le R^2 \le 100\%$
- ullet Large values of R^2 indicate better model fit.

R^2 : Example

$$R^2 = rac{SS_{ ext{model}}}{SS_{ ext{Total}}} = rac{0.22573}{0.22688} = 0.9950$$

99.50% of the variation in log(barometric pressure) can be explained by the linear regression model with boiling point of water.

STAT 500

Simple Linear Regression: Inference for Parameters and Prediction Intervals

Inference for Model Parameters

- ullet Population Slope eta_1
- ullet Population Intercept eta_0
- ullet Conditional Mean $\mu_{Y|x}$

Inference for the Slope (β_1)

ullet Discuss inference for eta_1 in detail (then summarize the rest)

$$b_1 = rac{\Sigma_{i=1}^n (x_i - ar{x})(Y_i - ar{Y})}{\Sigma_{i=1}^n (x_i - ar{x})^2} = rac{\Sigma_{i=1}^n (x_i - ar{x})Y_i}{\Sigma_{i=1}^n (x_i - ar{x})^2}$$

ullet b_1 is a linear combination of normal random variables (the Y_i 's) so b_1 is normally distributed with

$$E(b_1)=eta_1 \qquad extstyle ext{Var}(b_1)=rac{\sigma^2}{\Sigma_{i=1}^n(x_i-ar{x})^2}$$

$$ullet \ b_1 \sim N\left(eta_1, rac{\sigma^2}{\sum_{i=1}^n (x_i - ar{x})^2}
ight)$$

Inference for the Slope (β_1)

Examine

$$\mathsf{Var}(b_1) = rac{\sigma^2}{\Sigma_{i=1}^n (x_i - ar{x})^2}$$

A more precise estimate of eta_1 can be obtained by :

- ullet Spreading out the X values
- ullet Getting a larger sample i.e. more (X,Y) pairs
- Making the error variance smaller

Inference for the Slope (β_1)

- ullet Use MS_{error} to estimate σ^2 $(ext{Note that } MS_{error} \sim rac{\sigma^2 \chi_{n-2}^2}{n-2} \;)$
- ullet Standard error of b_1 is $S_{b_1} = \sqrt{M S_{error} / \sum\limits_{i=1}^n (x_i ar{x})^2}$
- ullet $(b_1-eta_1)/S_{b_1}$ has a t-distribution with n-2 d.f.

Hypothesis Test for β_1

Null and Alternative Hypotheses

$$H_0: \beta_1 = 0$$
 $H_a: \beta_1 \neq 0$

Test Statistic

$$T=rac{b_1-0}{S_{b_1}}$$

- ullet Reject H_0 if $|T|>t_{n-2,1-lpha/2}$
- ullet Note that $T^2=F$, this t-test for eta_1 is the same as the F-test for significance of model from ANOVA Table.
- ullet One-sided alternative hypothesis is possible for the t-test: $H_a:eta_1>0$ or $H_a:eta_1<0$

CI for β_1

• $100(1-\alpha)\%$ confidence interval for β_1 :

$$b_1\pm t_{n-2,1-lpha/2}S_{b_1}$$

Forbes Data

Weisberg, Sanford, Applied Linear Regression, Wiley, 1980.

- James D. Forbes collected data in the mountains of Scotland
- n=17 locations (at different altitudes)
- Objective: Predict barometric pressure (in inches of mercury) from boiling point of water (X) in ${}^{o}F$.
- Use Y=log(barometric pressure)
- Motivation: Fragile barometers of the 1840's were difficult to transport

- ullet Test $H_o:eta_1=0$ $(Y_i=eta_0+\epsilon_i)$ versus $H_a:eta_1
 eq 0$ $(Y_i=eta_0+eta_1x_i+\epsilon_i)$
- Evaluate

$$t = \frac{b_1 - 0}{S_{b_1}} = \frac{.020623 - 0}{0.000379} = 54.42$$

- The least squares estimate of the slope is 54 standard errors away from zero (p-value << .0001).
 - It is extremely unlikely that an estimate that far from zero could occur simply because of random errors when eta_1 is actually zero.
 - Consequently, reject the null hypothesis and conclude that the slope is positive.

• A 95% confidence interval for the slope indicates that the slope is "very well" estimated from these data

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b_1 \pm t_{15,.975} S_{b_1}
\Rightarrow 0.020623 \pm (2.131)(0.00037895)
\Rightarrow (0.0198, 0.0214)
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Inference for the Intercept (β_0)

$$ullet \ b_o = ar{Y} - b_1ar{x} \sim N(eta_o, \sigma^2(rac{1}{n} + rac{ar{x}^2}{\Sigma_i(x_i - ar{x})^2}))$$

$$ullet$$
 $ullet b_o$ has standard error $S_{b_o} = \left| MS_{error} \left(rac{1}{n} + rac{ar{x}^2}{\sum\limits_{i=1}^n (x_i - ar{x})^2}
ight)
ight.$

$$ullet$$
 Reject $H_o:eta_o=0$ if $|t|=\left|rac{b_o-0}{S_{b_o}}
ight|>t_{n-2,1-lpha/2}$

• $100(1-\alpha)\%$ confidence interval for β_o is

$$b_0 \pm t_{n-2,1-lpha/2} \ S_{b_0}$$

Inference for the Intercept (β_0)

- Rarely considered
- ullet Values of x must be near 0 for meaningful interpretations
- Would be most likely to use confidence interval

- ullet Test $H_o:eta_0=0$ $(Y_i=eta_1x_i+\epsilon_i)$ versus $H_a:eta_0
 eq 0$ $(Y_i=eta_0+eta_1x_i+\epsilon_i)$
- ullet Evaluate $t=rac{b_0-0}{S_{b_0}}=rac{-0.971-0}{0.0769}=-12.6$
- The least squares estimate of the intercept is 12.6 standard errors away from zero (p-value << .0001). Reject the null hypothesis and conclude that the intercept is negative. (No practical motivation)
- A 95% confidence interval for the intercept is

$$b_0 \pm t_{15,.975} S_{b_0} \Rightarrow -0.971 \pm (2.131)(0.0769) \Rightarrow (-1.135, -0.807)$$

Inference for Conditional Means

Inference for $\mu_{Y|x} = E(Y|X=x) = eta_o + eta_1 x$

- ullet Estimate is $\hat{\mu}_{Y|x} = b_o + b_1 x$
- ullet $\hat{\mu}_{Y|x}$ is a linear function of two normally distributed random variables $(b_0$ and b_1 , not independent)

$$ullet \hat{\mu}_{Y|x}$$
 is $N\left(eta_o + eta_1 x, \sigma^2\left(rac{1}{n} + rac{(x-ar{x})^2}{\Sigma_{i=1}^n(x_i-ar{x})^2}
ight)
ight)$

ullet Note: value of x does not need to be present in sample.

Inference for Conditional Means

standard error is

$$S_{\hat{\mu}_{Y|x}} = S_{b_o+b_1x} = \left| MS_{error} \left(rac{1}{n} + rac{(x-ar{x})^2}{\Sigma_{i=1}^n (x_i - ar{x})^2}
ight)
ight|$$

ullet 100(1-lpha)% confidence interval for eta_o+eta_1x is

$$(b_o + b_1 x) \pm t_{n-2,1-lpha/2} \; S_{\hat{\mu}_{Y|x}}$$

Confidence Region for a Line Segment

Use the Scheffe' procedure to get simultaneous confidence intervals for every x in an entire line segment:

$$(b_o + b_1 x) \pm \sqrt{2F_{2,n-2,1-lpha}} \ S_{b_o + b_1 x}$$

for
$$a \le x \le b$$

Prediction

Predict the value for Y at given x:

$$Y_{new} = \beta_o + \beta_1 x + \epsilon$$

- ullet Estimate is still $\hat{Y}=b_o+b_1x$
- Standard error is

$$S_{pred} = \left| MS_{error} \left(1 + rac{1}{n} + rac{(x - ar{x})^2}{\Sigma_{i=1}^n (x_i - ar{x})^2}
ight)
ight|$$

• $100(1-\alpha)\%$ prediction interval:

$$(b_o + b_1 x) \pm t_{n-2,1-\alpha/2} \ S_{pred}$$

Comparison

- ullet Confidence Interval for Condition Mean $\mu_{Y|x}$
 - Inference for a point on the population regression line given value of $oldsymbol{x}$
 - Source of inference is estimating regression line
- ullet Prediction Interval for Y
 - Inference for a point in the scatterplot of all population values given value of x.
 - Sources of inference are estimating regression line AND predicting $oldsymbol{Y}$ given the regression line.

- Construct a 95% confidence interval for the mean of possible log-pressure measurements when the boiling point of water is x=209 ^{o}F
- Estimated mean is

$$\hat{\mu}_{Y|x} = b_0 + b_1 x = -0.9710 + (.0206)(209) = 3.339$$

• Evaluate the standard error of this estimate

$$S_{\hat{\mu}_{Y|x}} = \sqrt{.0000762 \left(rac{1}{17} + rac{(209 - 202.953)^2}{530.78}
ight)} = 0.00312$$

A 95% confidence interval is

$$\hat{\mu}_{Y|x} \pm t_{15,.975} S_{\hat{\mu}_{Y|x}} \Rightarrow 3.339 \pm (2.131)(0.00312) \Rightarrow (3.333, 3.346)$$

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• Apply the exponential function to the end points to get an approximate confidence interval for the mean pressure

(28.02, 28.39) inches of Hg

 This could be computed with either the REG procedure or the GLM procedure in SAS by adding an additional line to the data file with X=209 and a missing value for Y

Scheffe procedure for constructing a 95% confidence region for a segment of the true regression line

Evaluate
$$(b_0+b_1x)\pm\sqrt{2F_{(2,n-2),1-\alpha}}S_{b_0+b_1x}$$
 $\Rightarrow (b_0+b_1x)\pm\sqrt{2F_{(2,15),0.95}}S_{b_0+b_1x}$ $\Rightarrow (b_0+b_1x)\pm(2.713)\sqrt{.0000762\left(\frac{1}{17}+\frac{(x-202.953)^2}{530.78}\right)}$

- Construct a 95% prediction interval for a log-pressure value when the boiling point of water is x=209 ^{o}F
- Prediction is the estimated mean

$$\hat{Y} = b_0 + b_1 x + error = -0.9710 + (.0206)(209) + 0 = 3.339$$

ullet Evaluate the standard error of the prediction (include the variation of the associated random error, estimated as $MS_{error}=.0000762)$

$$S_{pred} = \sqrt{.0000762 \left(1 + rac{1}{17} + rac{(209 - 202.953)^2}{530.78}
ight)} = 0.00927$$

A 95% prediction interval is

$$\hat{y} \pm t_{15,.975} S_{pred} \implies 3.339 \pm (2.131)(0.00927)$$

$$\Rightarrow (3.319, 3.359)$$

- Apply the exponential function to the end points to get an approximate prediction interval for barometric pressure: (27.63, 28.76) inches of Hg
- This could be computed with either the REG or GLM procedure in SAS by adding an additional line to the data file with X=209 and a missing value for Y