STAT 305: Chapter 9

Inference for curve and surface fitting

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Chapter 9:

Inference for curve and surface fitting

Inference for curve and surface fitting

> Previously, we have discussed how to describe relationships between variables (Ch. 4). We now move into formal inference for these relationships starting with relationships between two variables and moving on to more.

Simple linear regression

Recall, in Ch. 4, we wanted an equation to describe how a dependent (response) variable, y, changes in response to a change in one or more independent (experimental) variable(s), x.

We used the notation

$$y = \beta_0 + \beta_1 x + \epsilon$$

Simple Linear Regression

where β_0 is the intercept.

> It is the expected value for y when $x = 0$.

β_1 is the slope.

> It is the expected increase (decrease) in y for every **one** unit change in x

ϵ is some error. In fact,

$$\epsilon \sim^{\text{iid}} N(0, \sigma^2)$$

Recall:

> Cheking if residuals are normally distributed is one of our model assessment technique.

Goal: We want to use inference to get interval estimates for our slope and predicted values and significance tests that the slope is not equal to zero.

Variance Estimation

Variance estimation

In the simple linear regression $y = \beta_0 + \beta_1 x + \epsilon$, the parameters are β_0, β_1 and σ^2.

We already know how to estimate β_0 and β_1 using least squares.

We need an estimate for σ^2 in a *regression*, or "*line-fitting*" context.

Definition:

For a set of data pairs $(x_1, y_1), \ldots, (x_n, y_n)$ where least squares fitting of a line produces fitted values $\hat{y}_i = b_0 + b_1 x_i$ and residuals $e_i = y_i - \hat{y}_i$,

$$s_{LF}^2 = \frac{1}{n-2} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \frac{1}{n-2} \sum_{i=1}^{n} e_i^2$$

is the line-fitting sample variance.

Simple Linear Regression

Variance Estimation

MSE

Variance estimation

Associated with s^2_{LF} are $\nu = n - 2$ degrees of freedom and an estimated standard deviation of response $s_{LF} = \sqrt{s^2_{LF}}$.

> This is also called **Mean Square Error (MSE)** and can be found in *JMP* output.
>
> It has $\nu = n - 2$ degrees of freedom because we must estimate 2 quantities β_0 and β_1 to calculate it.
>
> s^2_{LF} estimates the level of basic background variation σ^2, whenever the model is an adequate description of the data.

Inference for Parameters β_0 and β_1

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for parameters

Inference for β_1:

We are often interested in testing if $\beta_1 = 0$. This tests whether or not there is a *significant linear relationship* between x and y. We can do this using

> 1. 100* $(1-\alpha)$ % confidence interval
>
> 2.Formal hypothesis tests

Both of these require

> 1. An estimate for β_1 and
>
> 2. a **standard error** for β_1

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for β_1:

It can be shown that since $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$ and $\epsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2)$, then

$$b_1 \sim N\left(\beta_1, \frac{\sigma^2}{\sum(x-\bar{x})^2}\right)$$

Note that we never know σ^2, so we must estimate it using $\sqrt{\text{MSE}} = S_{LF}$.

So, a $(1-\alpha)100\%$ CI for β_1 is

$$b_1 \pm t_{(n-2, 1-\alpha/2)} \frac{s_{LF}}{\sqrt{\sum(x_i - \bar{x})^2}}$$

and the test statistic for $\text{H}_0 : \beta_1 = \#$ is

$$K = \frac{b_1 - \#}{\frac{s_{LF}}{\sum(x_i - \bar{x})^2}}$$

Example:[Ceramic powder pressing]

A mixture of Al_2O_3, polyvinyl alcohol, and water was prepared, dried overnight, crushed, and sieved to obtain 100 mesh size grains.

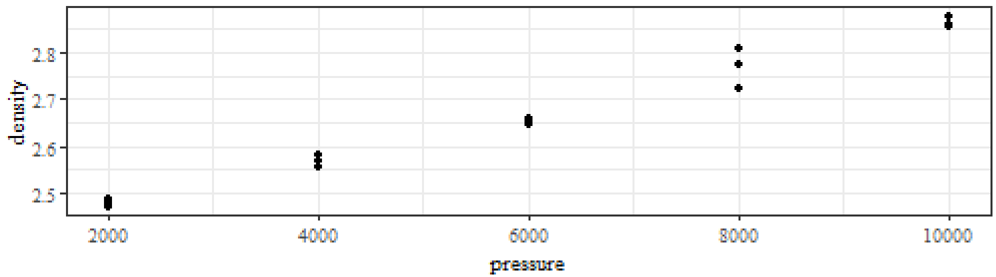
These were pressed into cylinders at pressures from 2,000 psi to 10,000 psi, and cylinder densities were calculated. Consider a pressure/density study of $n = 15$ data pairs representing

$$\begin{aligned} x = & \text{ the pressure setting used (psi)} \\ y = & \text{ the density obtained (g/cc)} \end{aligned}$$

in the dry pressing of a ceramic compound into cylinders.

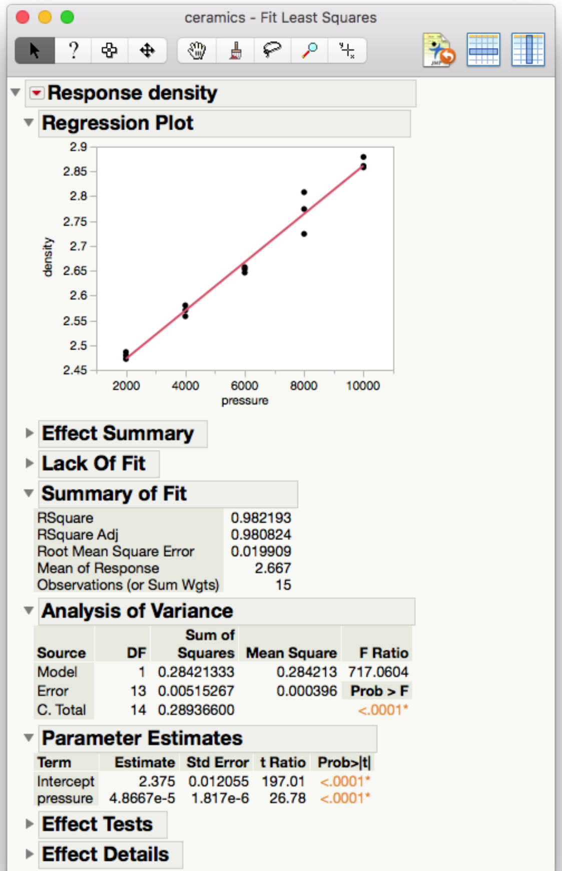
Example:[Ceramic powder pressing]

pressure	density	pressure	density
2000	2.486	6000	2.653
2000	2.479	8000	2.724
2000	2.472	8000	2.774
4000	2.558	8000	2.808
4000	2.570	10000	2.861
4000	2.580	10000	2.879
6000	2.646	10000	2.858
6000	2.657		

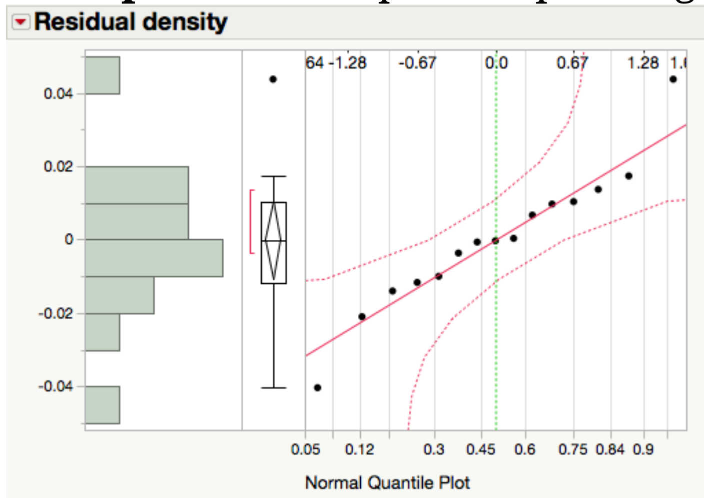


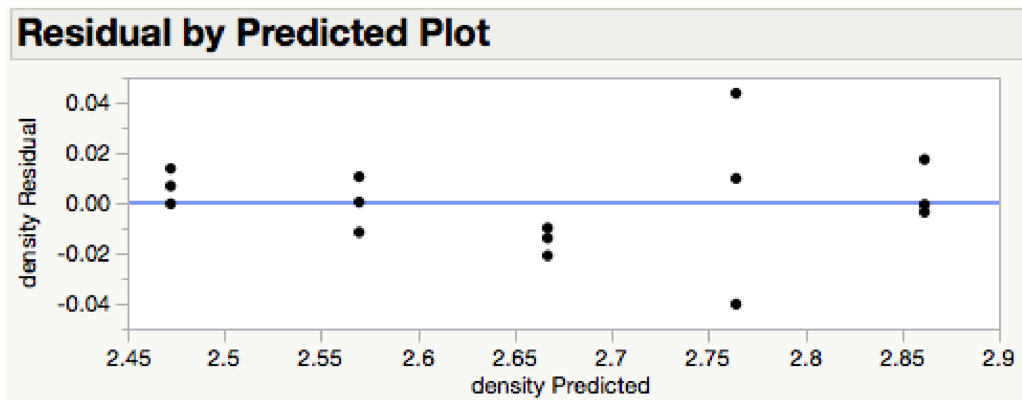
Example:[Ceramic powder pressing]

A line has been fit in JMP using the method of least squares.



Example:[Ceramic powder pressing]





Least squares regression of density on pressure of ceramic cylinders

Example:[Ceramic powder pressing]

1.Write out the model with the appropriate estimates.

2.Are the assumptions for the model met?

3.What is the fraction of raw variation in y accounted for by the fitted equation?

Example:[Ceramic powder pressing]

4.What is the correlation between x and y?

5.Estimate σ^2.

6.Estimate $\mathrm{Var}(b_1)$.

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Example:[Ceramic powder pressing]

7.Calculate and interpret the 95% CI for β_1

8.Conduct a formal hypothesis test at the $\alpha = .05$ significance level to determine if the relationship between density and pressure is significant.

> 1- $H_0: \quad \beta_1 = 0 \; vs. \quad H_1: \quad \beta_1 \neq 0$
>
> 2- $\alpha = 0.05$
>
> 3- I will use the test statistics $K = \frac{b_1 - \#}{\frac{s_{LF}}{\sum (x_i - \bar{x})^2}}$
>
> which has a t_{n-2} distribution assuming that
>
> - H_0 is true and
> - The regression model is valid

Example:[Ceramic powder pressing]

4-
$K = \frac{4.8667 \exp -5}{1.817 \exp -6} = 26.7843 > t_{(13,.975)=2.160}.$
So,

p-value $= P(|T| > K) < 0.05 = \alpha$

5- Since $K = 26.7843 > 2.160 = t_{(13,.975)}$, we **reject** H_0.

6- There is enough evidence to conclude that there is **a linear relationship between density and pressure**

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Inference for mean response

Recall our model

$$y_1 = \beta_0 + \beta_1 x_i + \epsilon_i, \quad \epsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2).$$

Under the model, the true mean response at some observed covariate value x_i is

$$E(\beta_0 + \beta_1 x_i + \epsilon_i) = \beta_0 + \beta_1 x_i + E(\epsilon_i)$$
$$\Rightarrow \mu_{Y|x} = \beta_0 + \beta_1 x_i$$

Now, if some new covariate value x is within the range of the x_i's (we don't extrapolate), we can estimate the true mean response at this new x. i.e

$$\hat{\mu}_{Y|x} = \hat{y} = b_0 + b_1 x$$

But how good is the estimate?

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Inference for mean response

Under the model, $\hat{\mu}_{Y|x}$ is Normally distributed with

$$E(\hat{\mu}_{Y|x}) = \mu_{Y|x} = \beta_0 + \beta_1 x$$

and

$$\mathrm{Var}\hat{\mu}_{Y|x} = \sigma^2 (\frac{1}{n} + \frac{(x - \overline{x})^2}{\sum (x_i - \overline{x})^2})$$

Where x is the individual value of x that we care about estimating $\mu_{Y|x}$ at, and x_i are all x_i's in our data.

So we can construct a $N(0,1)$ random variable by standardizing.

$$Z = \frac{\hat{\mu}_{Y|x} - \mu_{Y|x}}{\sigma \sqrt{(\frac{1}{n} + \frac{(x-\overline{x})^2}{\sum (x_i - \overline{x})^2})}} \sim N(0,1)$$

Inference for mean response

And when σ is unknown (i.e. basically always), we replace σ with $S_{LF} = \sqrt{\frac{1}{n-2}\sum(y_i - \hat{y}_i)^2}$ where we can get from JMP as **root mean square error (MSE)**. Then

$$T = \frac{\hat{\mu}_{Y|x} - \mu_{Y|x}}{s_{LF}\sqrt{\left(\frac{1}{n} + \frac{(x-\overline{x})^2}{\sum(x_i-\overline{x})^2}\right)}} \sim t_{(n-2)}$$

To test $H_0 : \mu_{y|x} = \#$, we can use the test statistics

$$K = \frac{\hat{\mu}_{Y|x} - \#}{s_{LF}\sqrt{\left(\frac{1}{n} + \frac{(x-\overline{x})^2}{\sum(x_i-\overline{x})^2}\right)}}$$

which has a t_{n-2} distribution if 1) H_0 is true and 2) the model is correct.

Inference for mean response

A 2-sided $(1-\alpha)100\%$ CI for $\mu_{y|x}$ is

$$\hat{\mu}_{Y|x} \pm t_{(n-2,1-\alpha/2)} \ * \ s_{LF}\sqrt{(\frac{1}{n} + \frac{(x-\overline{x})^2}{\sum(x_i-\overline{x})^2})}$$

and the one-sided the CI are analogous.

Note:

> in the above formula, $\sum(x_i-\overline{x})^2$ is not given by default in JMP.

JMP Shortcut Notice

Inference for mean response

Using JMP we can get

$$s_{LF}\sqrt{(\frac{1}{n}+\frac{(x-\overline{x})^2}{\sum(x_i-\overline{x})^2})}=\sqrt{(\frac{s_{LF}^2}{n}+(x-\overline{x})^2\frac{s_{LF}^2}{\sum(x_i-\overline{x})^2})}$$
$$=\hat{Var}(b_1)$$

Note that:

> We can get $\hat{Var}(b_0)$ from JMP as $(SE(b_1))^2$

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Example:[Ceramic powder pressing]

Return to the ceramic density problem. We will make a 2-sided 95% confidence interval for the true mean density of ceramics at 4000 psi and interpret it. (Note: $\overline{x} = 6000$)

solution:

$$\hat{\mu}_{Y|x=4000} = \hat{y} = b_0 + b_1 x$$

$$= 2.375 + 4.8667 \times 10^{-5} \times (4000) = 2.569668$$

and

$$s_{LF}\sqrt{\left(\frac{1}{n} + \frac{(x-\overline{x})^2}{\sum(x_i-\overline{x})^2}\right)}$$

$$= \sqrt{\left(\frac{s_{LF}^2}{n} + (x-\overline{x})^2\frac{s_{LF}^2}{\sum(x_i-\overline{x})^2}\right)}$$

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Example:[Ceramic powder pressing]

$$= \sqrt{\frac{0.000396}{15} + (4000 - 6000)^2 (1.817 \times 10^{-6})^2}$$

$$= \sqrt{0.000039606}$$

$$= 0.0062933$$

Therefore, a two-sided 95% confidence interval for the true mean density at 4000 psi is

$$\hat{\mu}_{Y|x=4000} \pm t_{(n-2, 1-\alpha/2)} \; \times \; s_{LF} \sqrt{\left(\frac{1}{n} + \frac{(x - \overline{x})^2}{\sum (x_i - \overline{x})^2}\right)}$$

$$= 2.569648 \pm t_{(15-2, 0.975)} \times (0.0062933)$$

$$= 2.569648 \pm 2.160 \times (0.0062933)$$

$$= (2.5561 \; , \; 2.5833)$$

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Example:[Ceramic powder pressing]

Now calculate and interpret a 2-sided 95% confidence interval for the true mean density at 5000 psi.

$$\hat{\mu}_{Y|x=5000} = \hat{y} = b_0 + b_1 x$$
$$= 2.375 + 4.8667 \times 10^{-5} \times (5000) = 2.618335$$

and

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Example:[Ceramic powder pressing]

Therefore, a two-sided 95% confidence interval for the true mean density at 4000 psi is

$$\hat{\mu}_{Y|x=5000} \pm t_{(n-2,1-\alpha/2)} \times s_{LF}\sqrt{(\frac{1}{n} + \frac{(x-\overline{x})^2}{\sum(x_i-\overline{x})^2})}$$

$$= 2.618335 \pm t_{(15-2,0.975)} \times (0.005449)$$

$$= 2.618335 \pm 2.160 \times (0.005449)$$

$$= (2.60656\ ,\ 2.63011)$$

We are 95% cofident that the true mean density of the ceramics at 5000 psi is between 2.60656 and 2.63011

Multiple Linear Regression

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

MLR

Multiple linear regression

Recall the summarization the effects of several different quantitative variables $x_1, \ldots, x_{p-1}$ on a response y.

$$y_i \approx \beta_0 + \beta_1 x_{1i} + \cdots + \beta_{p-1} x_{p-1,i}$$

Where we estimate $\beta_0, \ldots, \beta_{p-1}$ using the *least squares principle* by minimizing the function

$$S(b_0, \ldots, b_{p-1}) = \sum_{i=1}^{n} (y_i - \hat{y})^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{1,i} - \cdots - \beta$$

to find the estimates $b_0, \ldots, b_{p-1}$.

We can formalize this now as

$$Y_i = \beta_0 + \beta_1 x_{1i} + \cdots + \beta_{p-1} x_{p-1,i} + \epsilon_i$$

where we assume $\epsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2)$.

Variance Estimation in MLR

Variance estimation

Based on our multiple regression model, the residuals are of the form

$$e_i = y_i - \hat{y}_i = y_i - (b_0 + b_1 x_{1\,i} + \cdots + b_{p-1} x_{p-1\,i}$$

And we can estimate the variance similarly to the SLR case.

Definition:

For a set of n data vectors $(x_{11}, x_{21}, \ldots, x_{p-11}, y), \ldots, (x_{1n}, x_{2n}, \ldots, x_{p-1n}, y)$ where least squares fitting is used to fit a surface,

$$s_{SF}^2 = \frac{1}{n-p} \sum (y - \hat{y})^2 = \frac{1}{n-p} \sum e_i^2$$

is the **surface-fitting sample variance** (also called mean square error, MSE). Associated with it are $\nu = n - p$ degrees of freedom and an estimated standard deviation of response $s_{SF} = \sqrt{s_{SF}^2}$.

Variance estimation

Note: the SLR fitting sample variance s^2_{LF} is the special case of s^2_{SF} for $p = 2$.

Example:[Stack loss]

Consider a chemical plant that makes nitric acid from ammonia. We want to predict stack loss (\$y\$, 10 times the \% of ammonia lost) using

> x_1: air flow into the plant
>
> x_2: inlet temperature of the cooling water
>
> x_3: modified acid concentration (% circulating acid -50%) $\times$ 10

Example:[Stack loss]

Summary of Fit

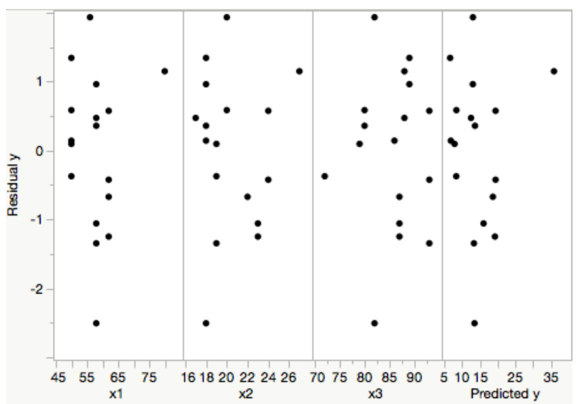
RSquare	0.975006
RSquare Adj	0.969238
Root Mean Square Error	1.252714
Mean of Response	14.47059
Observations (or Sum Wgts)	17

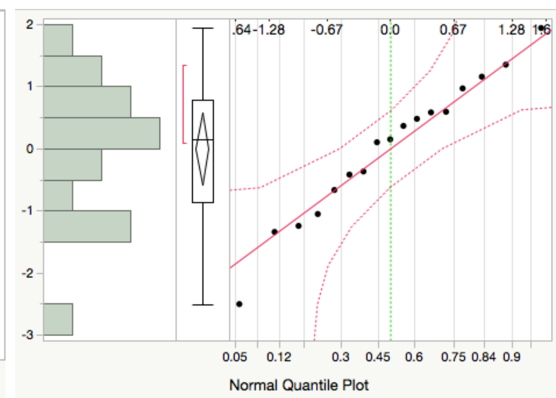
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	3	795.83449	265.278	169.0432
Error	13	20.40080	1.569	Prob > F
C. Total	16	816.23529		<.0001*

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-37.65246	4.732051	-7.96	<.0001*
x1	0.7976856	0.067439	11.83	<.0001*
x2	0.5773405	0.165969	3.48	0.0041*
x3	-0.06706	0.061603	-1.09	0.2961





Example:[Stack loss]

Then we have the fitted model as

$$\hat{y} = -37.65246 + 0.7977x_1 + 0.5773x_2 - 0.0971x_3$$

> The residual plots VS. x_1 , x_2 x_3 and $\hat{y}$ look like random scatter around zero.
>
> The QQ-plot of the residuals looks linear, indicating that the residuals are Normally distributed.
>
> This model is valid.

Inference for Parameters in MLR

Inference for parameters

We are often interested in answering questions (doing formal inference) for $\beta_0, \ldots, \beta_{p-1}$ individually. For example, we may want to know if there is a significant relationship between y and x_2 (holding all else constant).

\vspace{.2in}

Under our model assumptions,

$$b_i \sim N(\beta_i, d_i \sigma^2)$$

for some positive constant $d_i, i = 0, 1, \ldots, p-1$. That are hard to compute analytically, but JMP can help)

That means

$$\frac{b_i - \beta_i}{s_{LF}\sqrt{d_i}} = \frac{b_i - \beta_i}{SE(b_i)} \sim t_{(n-p)}$$

Inference for parameters

So, a test statistic for $\mathrm{H}_0 : \beta_i = \#$ is

$$K = \frac{b_i - \#}{s_{LF}\sqrt{d_i}} = \frac{b_i - \#}{SE(b_i)} \sim t_{(n-p)}$$

if 1) H_0 is true and 2) the model is valid, and a 2-sided $(1-\alpha)100\%$ CI for β_i is

$$b_i \pm t_{(n-p,1-\alpha/2)} \times s_{LF}\sqrt{d_i}$$

or

$$b_i \pm t_{(n-p,1-\alpha/2)} \times SE(b_i)$$

Example:[Stack loss, cont'd]

Using the model fit on slide 35, answer the following questions:

1.Is the average change in stack loss (y) for a one unit change in air flow into the plant (x_1) less than 1 (holding all else constant)? Use a significance testing framework with $\alpha = .1$.

solution:

> 1- $H_0: \quad \beta_1 = 1 \; vs. \quad H_1: \quad \beta_1 < 1$
>
> 2- $\alpha = 0.1$
>
> 3- I will use the test statistics $K = \frac{b_1 - 1}{SE(b_1)}$ which has a $t_{n-p} = t_{17-4}$ distribution assuming that
>
> - H_0 is true and
> - The regression model $y_i = \beta_0 + \beta_1 x_{i\,1} + \beta_2 x_{i\,2} + \beta_3 x_{i\,3} + \epsilon_i$ is valid

Example:[Stack loss, cont'd]

4- $K = \frac{0.7977-1}{0.06744} = -3$ and $t_{(13,.9)} = 1.35$. So,

p-value
$= P(T < K) < P(T < -3) < 0.1 = \alpha$

5- Since $K = -3 < -1.35 = -t_{(13,.9)}$, we **reject** H_0.

6- There is enough evidence to conclude that the slope on airflow is less than one unit stackloss/unit airflow. With each unit increase in airflow and all other covariates held constant, we expect stack loss to increase by less than one unit.

Example:[Stack loss, cont'd]

2.Is the there a significant relationship between stack loss (y) and modified acid concentation (x_3) (holding all else constant)? Use a significance testing framework with $\alpha = .05$.

solution:

> 1- $H_0: \quad \beta_3 = 0 \; vs. \quad H_1: \quad \beta_3 \neq 0$
>
> 2- $\alpha = 0.05$
>
> 3- I will use the test statistics $K = \frac{b_3 - 1}{SE(b_3)}$ which has a $t_{n-p} = t_{17-4}$ distribution assuming that
>
> - H_0 is true and
> - The regression model $y_i = \beta_0 + \beta_1 x_{i\,1} + \beta_2 x_{i\,2} + \beta_3 x_{i\,3} + \epsilon_i$ is valid

Example:[Stack loss, cont'd]

> 4- $K = \frac{-0.06706-0}{0.0616} = -1.09$ and $t_{(13,.975)} = 2.16$. So,
>
> p-value $= P(|T| > |K|) =$
>
> $P(|T| > 1.09) > P(|T| > t_{(13,.975)}) = 0.05\alpha$
>
> 5- Since p-value $> \alpha$, we **fail to reject** H_0.
>
> 6- There is not enough evidence to conclude that, with all other covarates held constant, there is a significant linear relatinoship between stack loss and acid concentration.

Example:[Stack loss, cont'd]

3.Construct and interpret a 99% two-sided confidence interval for β_3.

solution:

$$t_{(n-p,1-\alpha/2)} = t_{(13,.995)} = 3.012$$

then

$$\begin{aligned} b_3 \pm t_{(n-p,1-\alpha/2)}\, SE(b_3) &= -.0.06706 \pm 3.62(0.0616) \\ &= (-0.2525 \;\; 0.1185) \end{aligned}$$

We are 99% confident that for every unit increase in acid concentration, **with all other covariates held constant**, we expect stack loss to increase anywehre from -0.2525 units to 0.1185 units.

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

MLR

Example:[Stack loss, cont'd]

4.Construct and interpret a two-sided 90% confidence interval for β_2

solution:

For a 90% two-sided CI for β_2,

$$\alpha = 0.1 \ , \ t_{(n-p, 1-\alpha/2)} = t_{(13, 0.95)} = 1.77$$

Then

$$\begin{aligned} b_2 \pm t_{(n-p,1-\alpha/2)} \times SE(b_2) &= 0.5773 \pm 1.77(0.166) \\ &= (0.2834 \ \ 0.87.127) \end{aligned}$$

We are 90% confident that for every one degree increase in temprature **with all other covariates held constant**, stack loss is expected to increase by anywhere from 0.2834 units to 0.8713 units.