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

$$y = eta_0 + eta_1 x + \epsilon$$
 $\varepsilon \stackrel{\text{iid}}{\sim} N(\circ, \sigma^2)$

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,

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

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.

Note, in SLRE $y = \beta_0 + \beta_1 \times + \epsilon_1$ if $\beta_1 = \rho_0$, $y = \beta_0 + \epsilon_1$ i.e there's no relationship between $x, y = \beta_0 + \epsilon_1$ in the state $\beta_1 = \rho_0$ and $\beta_2 = \beta_0 + \epsilon_1$ i.e.

Lest if $\beta_1 = \rho_0$.

Variance Estimation

Variance estimation

unichown Parameter

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 $e_i = y_i - \hat{y}_i$,

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

is the line-fitting sample variance.

because there are

By, By in the model

6/45

Variance estimation

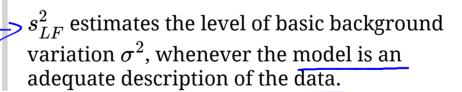
Variance Estimation

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

MSE

This is also called **Mean Square Error (MSE)** and can be found in *JMP* output.

It has $\nu=\underline{n-2}$ degrees of freedom because we must estimate 2 quantities $\underline{\beta_0}$ and $\underline{\beta_1}$ to calculate it.

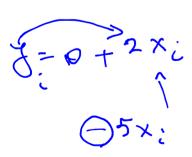


Inference for Parameter / 0 In / 1

Variance **Estimation**

MSE

Inference for **Parameters**



Inference for parameters

Inference for
$$\beta_1$$
:

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

$$\star$$
 1. 100* $(1-\alpha)$ % confidence interval

2.Formal hypothesis tests

Both of these require

1. An estimate for
$$\beta_1$$
 and β_1 and β_1 . 2. a **standard error** for β_1

Inference for β_1 :

Variance Estimation

It can be shown that since $y_i = eta_0 + eta_1 x_i + \epsilon_i$ and $\langle \epsilon_i \rangle \stackrel{ ext{iid}}{\sim} N(0,\sigma^2)$, then

 $\sqrt{ ext{MSE}} = S_{LF}.$

Ebi=Bi

$$V(0,\sigma^2)$$
, then
$$V(0,\sigma^2) = b_1 \sim N(\beta_1) \left(\frac{\sigma^2}{\sum (x-\bar{x})^2}\right)$$

MSE

Note that we never know σ^2 , so we must estimate it using

Inference for **Parameters**

So, a
$$(1-lpha)100$$
% CI for eta_1 is

$$b_1 \pm t_{(n-2,1-lpha/2)} \sqrt{rac{s_{LF}}{\sqrt{\sum (x_i-\overline{x})^2}}}$$

and the test statistic for $H_0: \beta_1 = \#$ is

$$SE(b_1) = \frac{b_1 - \#^{2}}{\overline{\sum_{(x_i - \overline{x})^2}}} \sim t$$

$$vale(H_0)$$

Example: [Ceramic powder pressing]

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

MSE

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

Inference for Parameters

```
\begin{cases} x = \text{ the pressure setting used } (\underline{\underline{psi}}) \\ y = \text{ the density obtained } (\underline{g/cc}) \end{cases}
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in the dry pressing of a ceramic compound into cylinders.

Example:[Ceramic powder pressing]

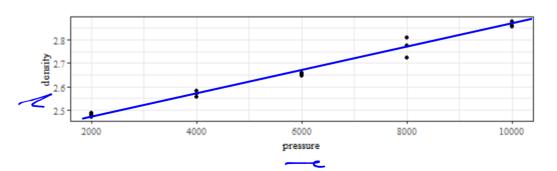
Variance
Estimation

MSE

Inference for Parameters

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		





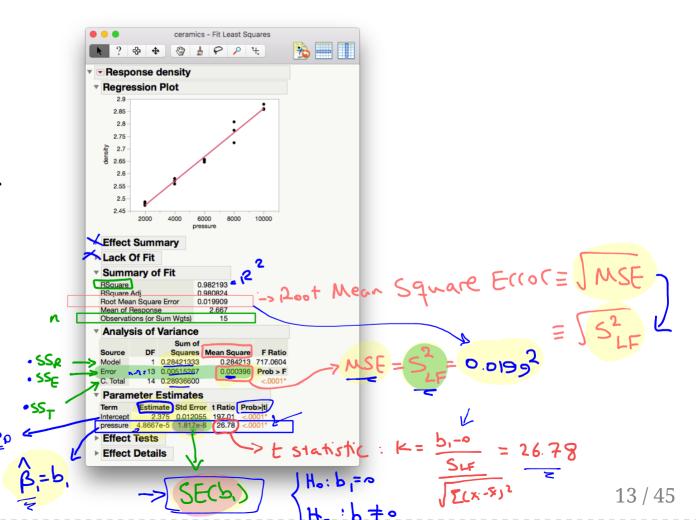
Example: [Ceramic powder pressing]

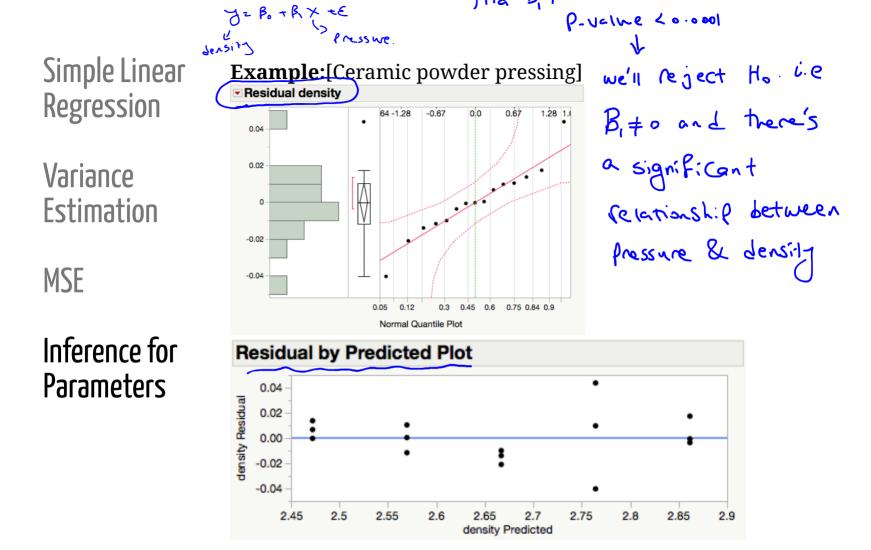
A line has been fit in JMP using the method of least squares.

Variance Estimation

MSE

Inference for Parameters





Least squares regression of density on pressure of ceramic cylinders

Variance Estimation

MSE

Inference for Parameters

Example: [Ceramic powder pressing]

1. Write out the model with the appropriate estimates.

$$\hat{\beta} = \hat{\beta}_0 + \hat{\beta}_1 \times = b_0 + b_1 \times = 2.375 + 4.8667 \times 10^{-5} \times 10^{-5$$

2.Are the assumptions for the model met?

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

$$p^2 = 98.21/$$

Example: [Ceramic powder pressing]

4. What is the correlation between x and y?

5. Estimate σ^2 .

$$6^2 = 5^2_1 = MSE = 0.000396$$

Inference for Parameters

6.Estimate $Var(b_1)$.

$$Vor(b) = \frac{S_{LF}^2}{\sum (x_i - \bar{x})^2} = (SE(b_i))^2$$

$$= (1.817 \times 1.6)^2$$

$$= (3.3015 \times 1.6)^2$$
This.

Example: [Ceramic powder pressing]

7.Calculate and interpret the 95% CI for β_1

Variance Estimation

MSE

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

Inference for Parameters

$$egin{aligned} extstyle 1 extstyle H_0: & eta_1 = 0 \ vs. & H_1: & eta_1
eq 0 \end{aligned} \ \ extstyle 2 extstyle lpha = 0.05 \end{aligned}$$

3- I will use the test statistics $K=\frac{b_1-\#}{s_{LF}}$ which has a t_{n-2} distribution assuming that

-)ullet H_0 is true and
 - The regression model is valid

Variance Estimation

MSE

Inference for Parameters

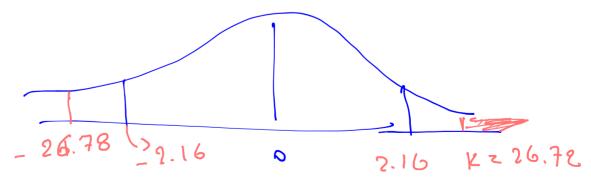
Example: [Ceramic powder pressing]

$$K = \underbrace{\frac{4.8667 \exp -5}{1.817 \exp -6}}_{\text{So,}} = \underbrace{26.7843}_{\text{$1.817 \exp -6$}} = \underbrace{\frac{26.7843}{1.817 \exp -6}}_{\text{$1.817 \exp -6$}}} = \underbrace{\frac{26.7843}_{\text{$1.817 \exp -6$}}}}_{\text{$1.817 \exp -6$}}} = \underbrace{\frac{26.7$$

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

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



Inference for mean response

Variance Estimation

Recall our model

$$y_1 = eta_0 + eta_1 x_i + \epsilon_i, \quad \epsilon_i \stackrel{ ext{iid}}{\sim} N(0,\sigma^2).$$

Inference for Parameters

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

Inference for mean response

$$E(eta_0 + eta_1 x_i + \epsilon_i) = eta_0 + eta_1 x_i + E(\epsilon_i) \ \Rightarrow \mu_{Y|x} = eta_0 + eta_1 x_i$$

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

$$\hat{\mu}_{Y|x}=\hat{y}=b_0+b_1x$$

But how good is the estimate?

Inference for mean response

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

$$E(\hat{\mu}_{Y|x})=\mu_{Y|x}=eta_0+eta_1 x$$

MSE

and

Inference for Parameters

 $ext{Var}\hat{\mu}_{Y|x} = \sigma^2(rac{1}{n} + rac{(oldsymbol{x} - \overline{x})^2}{\sum (oldsymbol{x}_i - \overline{x})^2})$

Inference for mean response

Where \mathbf{x} is the individual value of \mathbf{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.

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

Inference for mean response

Variance Estimation

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

MSE

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

Inference for Parameters

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

Inference for mean response

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

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

Inference for mean response

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

MSE

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

Inference for Parameters

and the one-sided the CI are analogous.

Inference for mean response

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

Variance Estimation Using JMP we can get

MSE

$$egin{aligned} s_{LF} \sqrt{(rac{1}{n} + rac{(x-\overline{x})^2}{\sum (x_i - \overline{x})^2})} = \sqrt{(rac{s_{LF}^2}{n} + (x-\overline{x})^2)} & \stackrel{s_{LF}}{\sum (x_i - \overline{x})^2} \end{aligned}$$

Inference for Parameters

Note that:

Inference for mean response

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

Example: [Ceramic powder pressing]

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

solution:

MSE

$$egin{aligned} \hat{\mu}_{Y|x=4000} &= \hat{y} = b_0 + b_1 x \ &= 2.375 + 4.8667 imes 10^{-5} imes (4000) = 2.569668 \end{aligned}$$

Inference for **Parameters**

and

Inference for mean response

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

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

Example:[Ceramic powder pressing]

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

$$= \sqrt{0.000039606}$$

Variance **Estimation**

$$=\sqrt{0.000039606}$$

MSE

= 0.0062933

Inference for **Parameters**

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

$$\hat{\mu}_{Y|x=4000} \pm t_{(n-2,1-lpha/2)} \, imes \, s_{LF} \sqrt{(rac{1}{n} + rac{(x-\overline{x})^2}{\sum (x_i - \overline{x})^2})}$$

Inference for mean response

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

$$=2.569648\pm2.160 imes(0.0062933)$$

$$=(2.5561,\ 2.5833)$$

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.

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

and

$$S_{LF} \int (\frac{1}{n} + \frac{(x-\widehat{x})^2}{\mathbb{E}(x_i-\widehat{x})^2} =$$

Example:[Ceramic powder pressing]

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

Variance Estimation

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

MSE

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

Inference for Parameters

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

Inference for mean response

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

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

Multiple linear regression

Variance Estimation

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

$$y_i pprox eta_0 + eta_1 x_{1i} + \dots + eta_{p-1} x_{p-1,i}$$

MSE

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

Inference for Parameters

$$S(b_0,\ldots,b_{p-1})=\sum_{i=1}^n(y_i-\hat{y})^2=\sum_{i=1}^n(y_i-eta_0-eta_1x_{1,i}-\cdots$$
 و جنرنام to find the estimates b_i ...

Inference for mean response

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

We can formalize this now as

$$Y_i = eta_0 + eta_1 x_{1i} + \dots + eta_{p-1} x_{p-1,i} + \epsilon_i$$

MLR

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

Variance Estimation in MLR

Variance estimation

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

$$egin{aligned} e_i = y_i - \hat{y}_i = y_i - (b_0 + b_1 x_{1\,i} + \dots + b_{p-1} x_{p-1\,i}) \end{aligned}$$

MSE

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

Inference for Parameters

Definition:

Inference for mean response

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,

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

MLR

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

Variance Estimation **Note:** the SLR fitting sample variance s_{LF}^2 is the special case of s_{SF}^2 for p=2.

MSE

Inference for Parameters

Inference for mean response

MLR

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Example:[Stack loss]

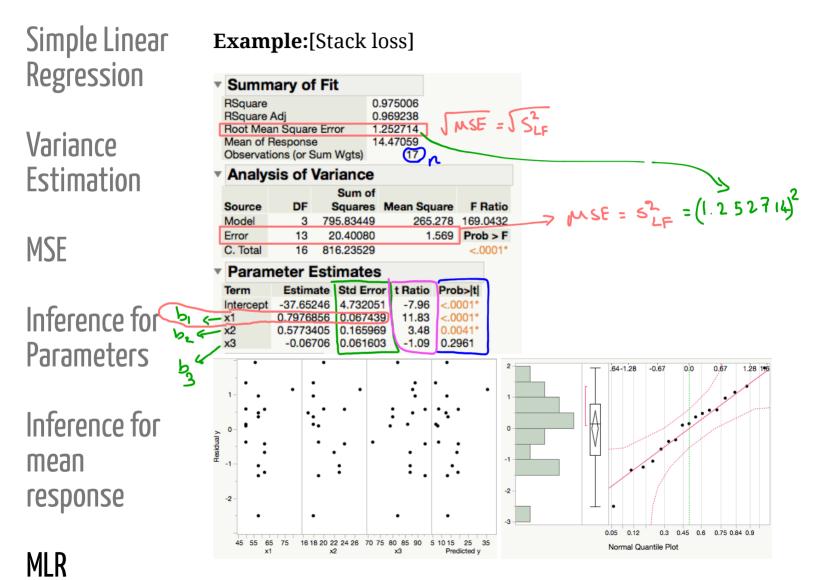
Consider a chemical plant that makes nitric acid from ammonia. We want to predict stack loss (y), 10 times the \% of ammonia lost) using

 x_1 : air flow into the plant

 x_2 : inlet temperature of the cooling water

 x_3 : modified acid concentration (% circulating acid -50%) imes 10

MLR



Variance Estimation

MSE

Inference for Parameters

Inference for mean response

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

Variance Estimation 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).

MSE

\vspace{.2in}

Inference for Parameters

Under our model assumptions,

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

Inference for mean response

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

That means

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

MLR

Inference for parameters

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

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

MSE

if 1) H_0 is true and 2) the model is valid, and a 2-sided (1-lpha)100% CI for eta_i is

Inference for Parameters

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

or

Inference for mean response

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

Example:[Stack loss, cont'd]

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

MSE

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 $\alpha = .1$. By is associated with X,

Inference for

solution:

Parameters

1-
$$H_0: \;\; eta_1 = 1 \; vs. \;\;\; H_1: \;\; eta_1 < 1$$

$$2$$
- $\alpha=0.1$

Inference for mean response

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

MLR

• The regression model
$$y_i=eta_0+eta_1x_{i\ 1}+eta_2x_{i\ 2}+eta_3x_{i\ 3}+\epsilon_i$$
 is valid

Example:[Stack loss, cont'd]



MSE

Inference for **Parameters**

Inference for mean response

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.

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

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-
$$H_0:~eta_3=0~vs.~~H_1:~eta_3
eq 0$$

2-
$$lpha=0.05$$

3- I will use the test statistics $K=rac{b_3-1}{SE(b_3)}$ which has a $t_{n-p}=t_{17-4}$ distribution assuming that

- H_0 is true and
- The regression model $y_i=eta_0+eta_1x_{i\ 1}+eta_2x_{i\ 2}+eta_3x_{i\ 3}+\epsilon_i$ is valid

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Example:[Stack loss, cont'd]

4-
$$K=rac{-0.06706-0}{0.0616}=-1.09$$
 and $t_{(13,.975)}=2.16$. So,

$$\operatorname{p-value} = P(|T| > |K|) =$$

$$P(|T| > 1.09) > P(|T| > t_{(13,.975)}) = 0.05\alpha$$

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 .

Variance Estimation

solution:

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

MSE

then

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

Inference for mean response

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

Example:[Stack loss, cont'd]

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

Variance Estimation

solution:

For a 90% two-sided CI for β_2 ,

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

Inference for Parameters

Then

$$b_2 \pm t_{(n-p,1-lpha/2)} imes SE(b_2) = 0.5773 \pm 1.77 (0.166) \ = (0.2834 \ 0.87.127)$$

Inference for mean response

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.