

Simple Linear Regression

Variance Estimation

MSE

Inference for Parameters

Inference for mean response

Inference for mean response

$$\hat{y} = b_0 + b_1 x_i$$

Recall our model

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

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

$$E(Y) = E(\beta_0 + \beta_1 x_i + \epsilon_i) = \underbrace{\beta_0}_{\text{true mean response}} + \underbrace{\beta_1 x_i}_{\mu_{Y|x}} + \underbrace{E(\epsilon_i)}_{=0}$$

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

$$\text{estimate of } \mu_{Y|x} \leftarrow \hat{y} = b_0 + b_1 x$$

the mean response
But how good is the estimate?

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$$\mu_{Y|x} = E(Y)$$

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

$$\text{Note: } \text{Var}(Y) = \sigma^2$$

$$\text{Var}(\hat{\mu}_{Y|x}) = \sigma^2 \left(\frac{1}{n} + \frac{(\underline{x} - \bar{x})^2}{\sum(\underline{x_i} - \bar{x})^2} \right)$$

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

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

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

$$SE(\hat{\mu}_{Y|x})$$

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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

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

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

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

true mean response $\hat{\mu}_{Y|x}$ *estimate of mean response*

$SE(\hat{\mu}_{Y|x}) = \sqrt{\text{var}(\hat{\mu}_{Y|x})}$

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

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$$MSE = \hat{Y}_T = b_0 + b_1 X$$

Inference for Parameters

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$\hat{Y}_{|x}$ Inference for mean response

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

* estimate

$\hat{\mu}_{Y|x}$

dist. quantile

$t_{(n-2, 1-\alpha/2)}$

*

s_{LF}

$\sqrt{(\frac{1}{n} + \frac{(x - \bar{x})^2}{\sum(x_i - \bar{x})^2})}$

SE (estimate)

and the one-sided the CI are analogous.

Note:

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

not given
in JMP

JMP Shortcut Notice

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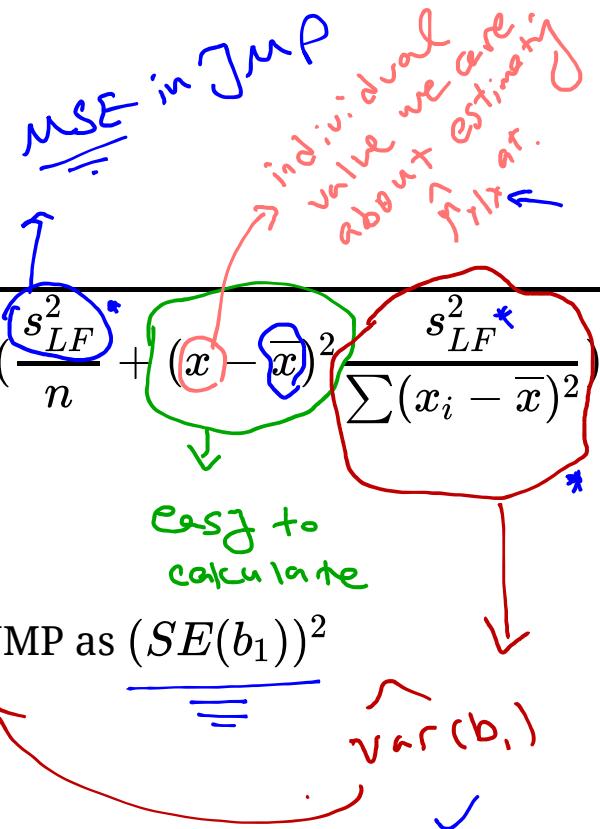
Using JMP we can get

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

Note that:

* not given
in JMP

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



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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: $\bar{x} = 6000$) ✓

solution: first find an estimate for true mean density of ceramics at $x = 4000$.

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

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

and next, find the SE of $\hat{\mu}_{Y|x=4000}$ *

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

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

• 4000

6000

$$\text{var}(b_1) = [SE(b_1)]^2$$

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$$SE(\hat{Y}_{x=4000}) = 0.0062933 \quad \checkmark$$

Inference for Parameters

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Example:[Ceramic powder pressing]

$$\begin{aligned} &= \sqrt{\frac{0.000396}{15} + (4000 - 6000)^2 (1.817 \times 10^{-6})^2} \\ &= \sqrt{0.000039606} \end{aligned}$$

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

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

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

$$= 2.569648 \pm 2.160 \times (0.0062933) = (2.5561, 2.5833)$$

We are 95% confident that the true mean density of the ceramics at 4000 psi is between 2.5561 and 2.5833.

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Example:[Ceramic powder pressing]

Now calculate and interpret a 2-sided 95% confidence interval for the true mean density at $\underline{\underline{x}} = \underline{\underline{5000}}$ psi.

① find an estimate
For true mean density
at $x=5000$.

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

and

② find $SE(\hat{y}|x=5000)$

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

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

$$= \sqrt{\frac{0.00395}{15} + (5000 - 6000)^2 (1.817 \times 10^{-6})^2}$$

$$= \sqrt{0.00002970} = 0.005449 = SE(\hat{y}|x=5000) \quad 27 / 53$$

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Example: [Ceramic powder pressing]

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

$$\hat{\mu}_{Y|x=4000} \pm t_{(n-2, 1-\alpha/2)} \times s_{LF} \sqrt{\left(\frac{1}{n} + \frac{(x - \bar{x})^2}{\sum(x_i - \bar{x})^2}\right)}$$
$$= 2.618335 \pm t_{(15-2, 0.975)} \times (0.005449) \quad SE(\hat{\mu}_{Y|x=4000})$$
$$= 2.618335 \pm 2.160 \times (0.005449)$$
$$= (2.60656, 2.63011) *$$

We are 95% confident that the true mean density of the ceramics at 4000 psi is between 2.60656 and 2.63011

Multiple Linear Regression

Simple Linear Regression

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Multiple linear regression

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

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

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

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

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

We can formalize this now as

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

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

Variance Estimation in MLR

Simple Linear Regression

Variance Estimation

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Variance estimation

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

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

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

Definition:

For a set of n data vectors

$(x_{11}, x_{21}, \dots, x_{p-11}, y), \dots, (x_{1n}, x_{2n}, \dots, x_{p-1n}, y)$
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 $s_{SF} = \sqrt{s_{SF}^2}$.

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Variance estimation

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



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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%) $\times 10$

$$\rightarrow y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$$

$$\begin{aligned} P &=? \\ P-1 &= 3 \Rightarrow P=4 \end{aligned}$$

$$t_{(n-P)}$$

Simple Linear Regression

Variance Estimation

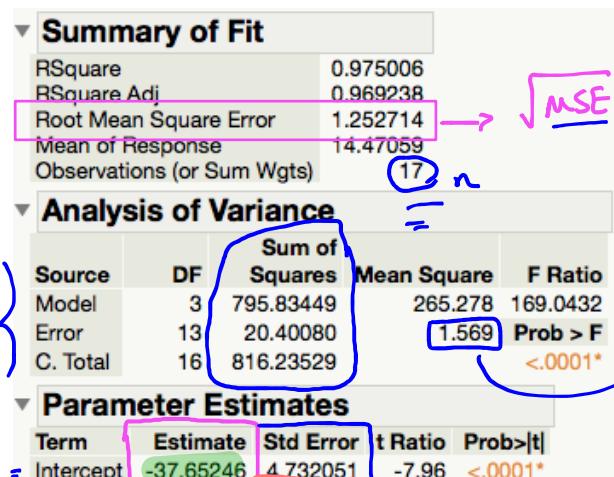
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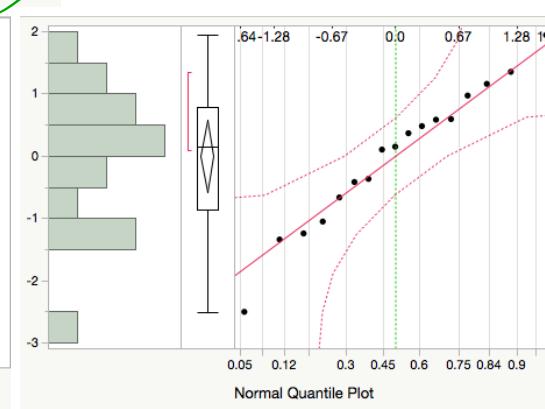
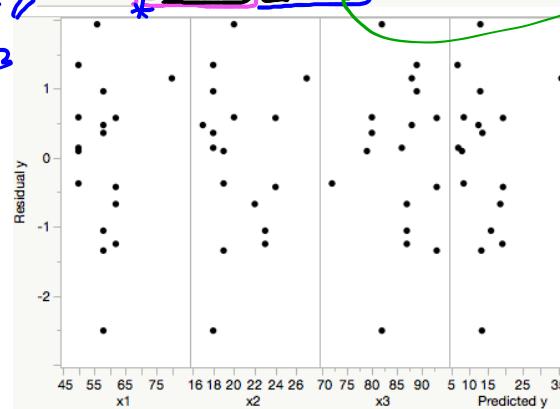
Example:[Stack loss]



$$\sqrt{\frac{MSE}{S^2_{SF}}} = \sqrt{\frac{S^2}{S^2_{SF}}} = \frac{S}{S_{SF}}$$

$$MSE = S_{SE}^2$$

$\sec(b_i)$; $i = 1, 2, 3$



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Example:[Stack loss]

Then we have the fitted model as

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

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

Simple Linear Regression

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Inference for parameters

We are often interested in answering questions (doing formal inference) for $\beta_0, \dots, \beta_{p-1}$ 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)~~

previously, in SLR:

Under our model assumptions,

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

$b_i \sim N(\beta_i, d_i \sigma^2)$ $\text{var}(b_i) \rightarrow \sum (x_i - \bar{x})^2$

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

That means

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

$\sqrt{\text{var}(b_i)} \rightarrow s_{\text{SE}}$ JMP

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So, a test statistic for $H_0 : \beta_i = \#$ is

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

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

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

\uparrow
 $s_{\text{Ec } b_i})$

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

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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:

$$1 - H_0 : \beta_1 = 1 \text{ vs. } H_1 : \beta_1 < 1$$

$$2 - \alpha = 0.1$$

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

- ① • H_0 is true and
- ② • The regression model $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \epsilon_i$ is valid

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Example:[Stack loss, cont'd]

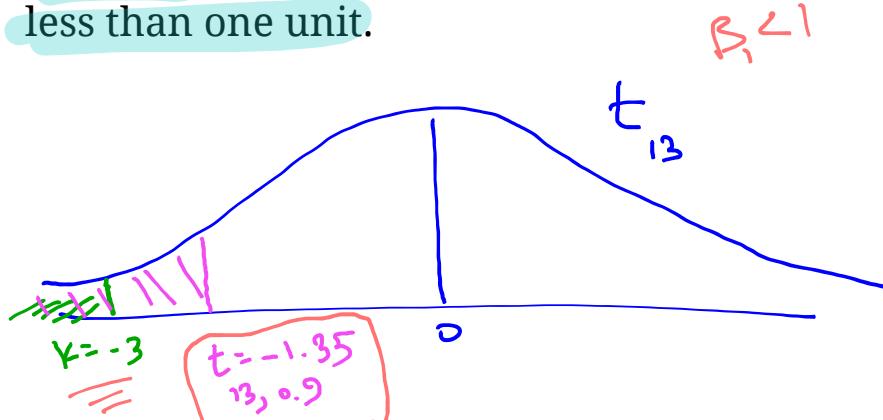
$$4- K = \frac{0.7977 - 1}{0.06744} = -3 \text{ and } t_{(13,9)} = 1.35. \text{ So,}$$

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.



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Example:[Stack loss, cont'd]

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

solution:

$$1 - H_0 : \beta_3 = 0 \text{ vs. } H_1 : \beta_3 \neq 0$$

$$2 - \alpha = 0.05$$

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 $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \epsilon_i$ is valid

is the slope for β_3

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Example: [Stack loss, cont'd]

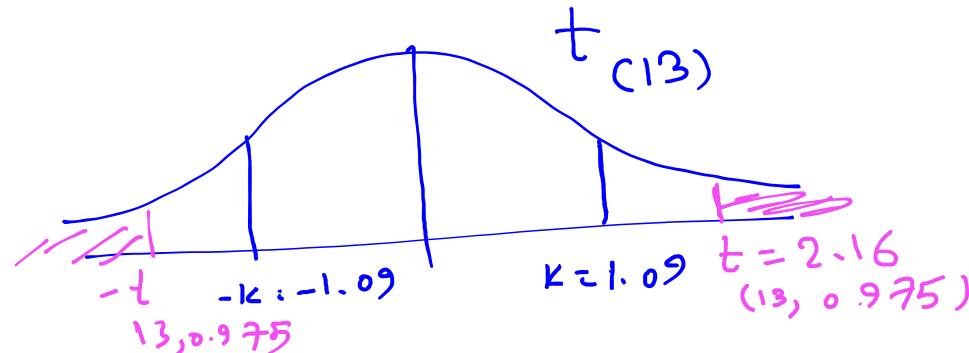
→ 4- $K = \frac{-0.06706 - 0}{0.0616} = -1.09$ and
 $t_{(13,.975)} = 2.16$. So,

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

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

5- Since p-value > α , we fail to reject H_0 .

6- There is **not enough evidence** to conclude that, with all other covariates held constant, there is a significant **linear** relationship between stack loss and acid concentration.



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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

$$\hat{b}_3 \pm t_{(n-p, 1-\alpha/2)} \overbrace{SE(\hat{b}_3)}^{\text{JMP}} = -.06706 \pm 3.62(0.0616) \\ = (-0.2525 \ 0.1185)$$

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.

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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

$$b_2 \pm t_{(n-p, 1-\alpha/2)} \times \overbrace{SE(b_2)}^{\text{JMP}} = 0.5773 \pm 1.77(0.166) \\ = (0.2834 \ 0.87127)$$

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

Inference for Mean Response

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Previously we fit $y|x$ only one x .
Inference for mean response $\hat{y}|x \rightarrow$ multiple x_i 's.

We can also estimate the mean response at the set of covariate values, $(x_1, x_2, \dots, x_{p-1})$. Under the model assumptions, the estimated mean response, $\hat{\mu}_{y|x}$, at $\mathbf{x} = (x_1, x_2, \dots, x_{p-1})$ is **Normally distributed** with:

$$\mathbb{E}(\hat{\mu}_{y|x}) = \mu_{y|x} = \beta_0 + \beta_1 x_1 + \cdots + \beta_{p-1} x_{p-1}$$

and

$$Var(\hat{\mu}_{y|x}) = \sigma^2 A^2$$

for some constant A, that is hard to compute by hand.

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$\mu_{y|x}$ ← vector.

Then, under the model assumptions

$$Z = \frac{\hat{\mu}_{y|x} - \mu_{y|x}}{\sigma A} \sim N(0, 1)$$

and

$$S_{SF} \quad T = \frac{\hat{\mu}_{y|x} - \mu_{y|x}}{s_{SF} A}$$

And a test statistic for testing $H_0 : \mu_{y|x} = \#$ is

$$K = \frac{\hat{\mu}_{y|x} - \#}{s_{SF} A}$$

which has a $t_{(n-p)}$ distribution under H_0 if the model holds true. \sim

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

$$\hat{\mu}_{y|x} \pm t_{(n-p, 1-\alpha/2)} \times s_{\text{CFA}}$$

Note that the one-sided CI will be analogous.

Note: $S_{\text{CFA}} = SE(\hat{\mu}_{y|x})$, and we can use JMP to get this.

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Example:[Stack loss, cont'd]

We can use JMP to compute a 2-sided 95% CI around the mean response at point 3:

$$x_1 = 62, x_2 = 23, x_3 = 87, y = 18$$

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Example:[Stack loss, cont'd]

The screenshot shows the JMP software interface for a "stackloss - Fit Least Squares" model. A context menu is open under the "Save Columns" option. The menu includes options like "Regression Reports", "Estimates", "Effect Screening", "Factor Profiling", "Row Diagnostics", "Save Columns", "Model Dialog", "Effect Summary", "Local Data Filter", "Redo", and "Save Script". Under "Save Columns", a sub-menu is displayed with the following items: "Prediction Formula", "Predicted Values" (which is circled in blue), "Residuals", "Mean Confidence Interval", "Indiv Confidence Interval", "Studentized Residuals", "Hats", "Std Error of Predicted" (which is also circled in blue), "Std Error of Residual", "Std Error of Individual", "Effect Leverage Pairs", "Cook's D Influence", "StdErr Pred Formula", "Mean Confidence Limit Formula", "Indiv Confidence Limit Formula", "Save Coding Table", "Publish Prediction Formula", "Publish Standard Error Formula", "Publish Mean Confid Limit Formula", and "Publish Indiv Confid Limit Formula".

How to get predicted values and standard errors

Simple Linear Regression

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Example:[Stack loss, cont'd]

Source	x1	x2	x3	y	Predicted y	StdErr Pred y
stackloss	1	80	27	88	37	35.849282687
	2	62	22	87	18	18.671300496
	3	62	23	87	18	19.248640953
	4	62	24	93	19	19.423620349
	5	62	24	93	20	19.423620349
	6	58	23	87	15	16.057898713
	7	58	18	80	14	13.640617664
	8	58	18	89	14	13.037076072
	9	58	17	88	13	12.526795792
	10	58	18	82	11	13.50649731
	11	58	19	93	12	13.346175822
	12	50	18	89	8	6.6555915917
	13	50	18	86	7	6.8567721223
	14	50	19	72	8	8.3729550563
	15	50	19	79	8	7.903533818
	16	50	20	80	9	8.4138140985
	17	56	20	82	15	13.065807105
Rows	All rows	17				
	Selected	1				
	Excluded	0				
	Hidden	0				
	Labelled	0				

Predicted values and standard errors.

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Example:[Stack loss, cont'd]

With $t_{(n-p,1-\alpha/2)} = t_{(13,975)} = \underline{2.16}$, the 95% confidence interval is

$$\hat{\mu}_{y|x}$$

$$\rightarrow \hat{\mu}_{y|x} \pm t_{(n-p,1-\alpha/2)} SE(\hat{\mu}_{y|x})$$

$$= \underline{19.2486} \pm \underline{2.16} \times \underline{(0.41785)}$$

$$= \underline{(18.343, 20.151)}$$

We are 95% confident that when air flow is 62 units, temperature is 23 degrees and the adjusted percentage of circulating acid is 87 units, the true mean stack loss is between 18.343 and 20.151 units.