9 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.

9.1 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

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

where β_0 is the intercept.

It is the expected value for y when x is 0.

β_1 is the slope.

It is the expected increase in y for every 1 unit increase in x.

ϵ is some error. In fact,

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

(recall checking if the residuals were normally distributed is one of our model assessment techniques)

Goal: We want to use inference to get interval estimates for our ① slope and ② predicted values and significance tests that the slope is not equal to zero.

inference

9.1.1 Variance estimation

What are the parameters in our model, and how do we estimate them?

β_0, β_1 — least squares

$\sigma^2 \leftarrow$?

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

Definition 9.1. 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 $e_i = y_i - \hat{y}_i$,

estimate 2 things (b_0 and b_1)

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

is the *line-fitting sample variance*. Associated with it are $\nu = n - 2$ degrees of freedom and an estimated standard deviation of response $s_{LF} = \sqrt{s_{LF}^2}$.

This is also called the Mean square Error (MSE)

can be found in JMP

It has $\nu = n-2$ degrees of freedom because we must estimate 2 quantities to compute it (β_0 and β_1).

variance of the errors

s_{LF}^2 estimates the level of basic background variation σ^2, whenever the model is an adequate description of the data.

9.1.2 Inference for parameters

true slope

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. $(1-\alpha)100\%$ confidence interval
2. Formal hypothesis (significance) test

Both of these require

① an estimate of β_1 (which is b_1) and ② a standard error for b_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

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

So, a $(1-\alpha)100\%$ CI for β_1 is

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

standard error for b_1

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

$$t = \frac{b_1 - \#}{\left(\frac{S_{LF}}{\sqrt{(x-\bar{x})^2}}\right)} \sim t_{n-2}$$

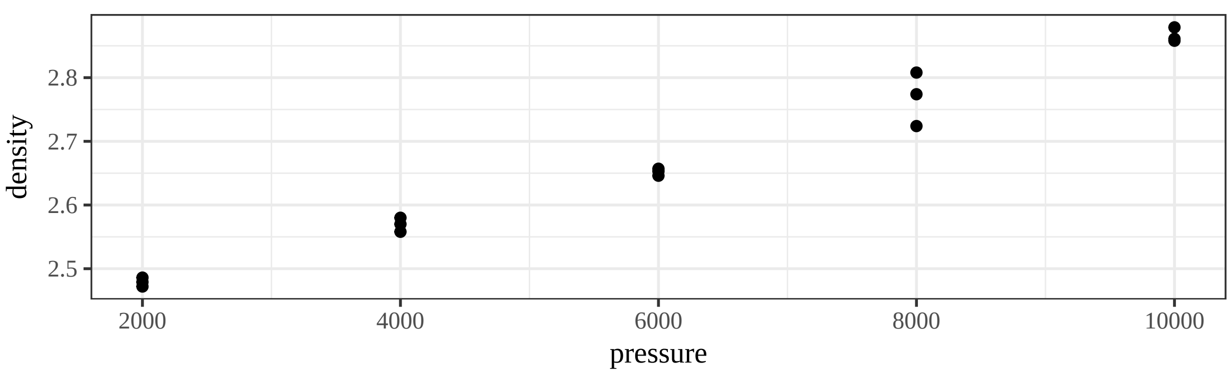
Example 9.1 (Ceramic powder pressing)**.** A mixture of Al_2O_3, polyvinyl alcohol, and water was prepared, dried overnight, crushed, and sieved to obtain 100 mesh size grains. These were pressed into cylinders at pressures from 2,000 psi to 10,000 psi, and cylinder densities were calculated. Consider a pressure/density study of $n = 15$ data pairs representing

$$x = \text{ the pressure setting used (psi)}$$

$$y = \text{ the density obtained (g/cc)}$$

in the dry pressing of a ceramic compound into cylinders.

pressure	density p	ressure d	ensity
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		



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

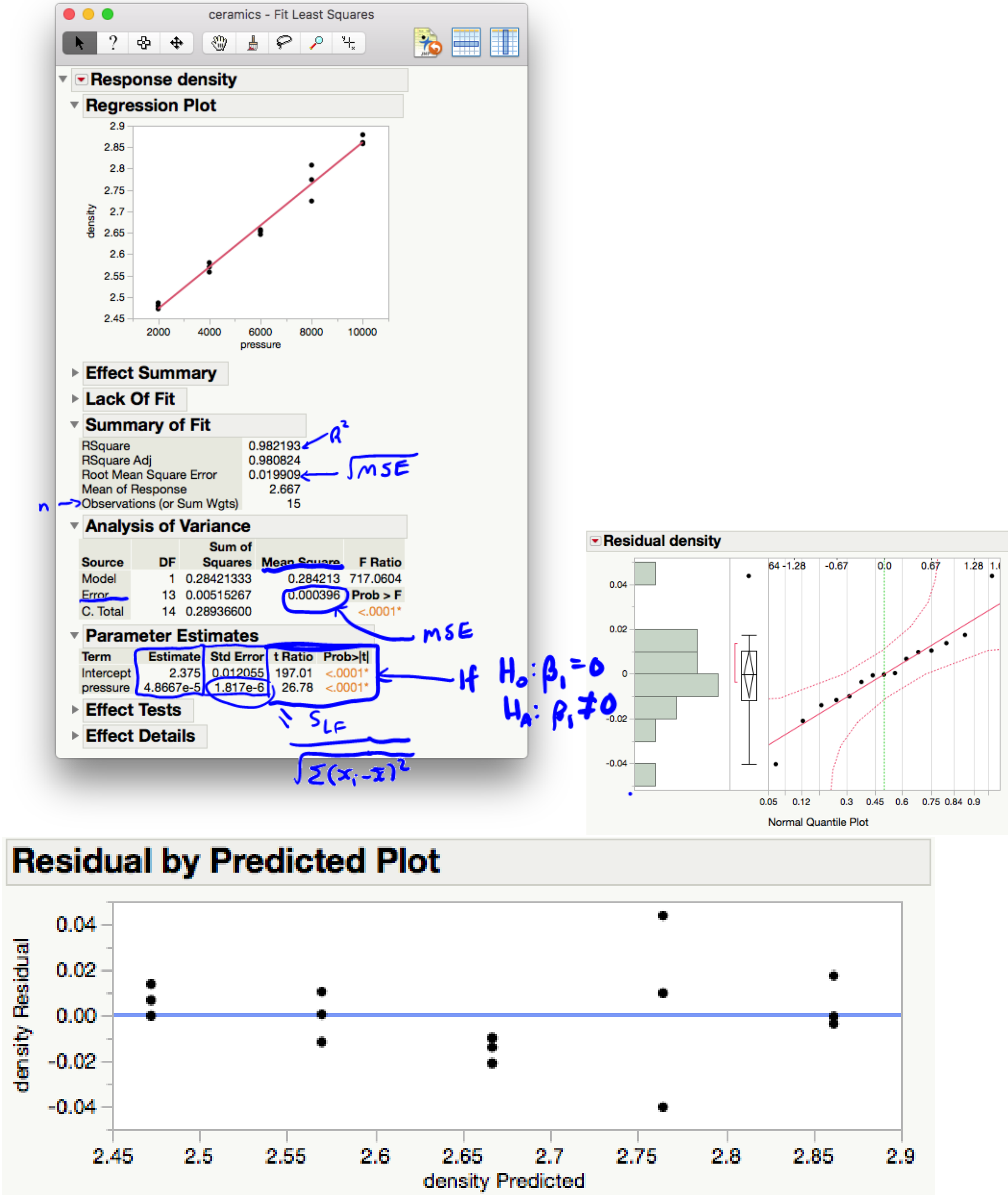


Figure 1: Least squares regression of density on pressure of ceramic cylinders.

1. Write out the model with the appropriate estimates.

$$\hat{y} = 2.375 + 4.8667 \times 10^{-5} x$$

2. Are the assumptions for the model met?

Yes. The residual plot shows random scatter around 0 and the Normal QQ plot of residuals looks linear, indicating they are normally distributed.

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

$$R^2 = 0.9821$$

4. What is the correlation between x and y?

For SLR,

$$r = \sqrt{R^2} = \sqrt{0.9821} = 0.9911$$

5. Estimate σ^2.

$$\hat{\sigma}^2 = s_{LF}^2 = MSE = .000396$$

$$s_{LF}^2 = \frac{1}{n-2} \sum_{i=1}^{n} \hat{e}_i^2$$

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

$$\widehat{\text{Var}}(b_1) = \frac{s_{LF}^2}{\sum (x_i - \bar{x})^2} = \left(SE(b_1)\right)^2 = (1.817 \times 10^{-6})^2 = 3.3015 \times 10^{-12}$$

7. Calculate and interpret the two-sided 95% CI for β_1

$$b_1 \pm t_{n-2,1-\alpha/2} \frac{s_{\varepsilon}}{\sqrt{\Sigma(x_i-\bar{x})^2}} = 4.8667\times10^{-5} \pm t_{15-2,.975}\,(1.817\times10^{-6})$$

$$= 4.8667\times10 \pm 2.160\,(1.817\times10^{-6})$$

$$= (.00004479, .00005259)$$

We are 95% confident that [for every 1 psi increase in pressure, we expect density to increase between .00004479 g/cc and .00005259 g/cc.]

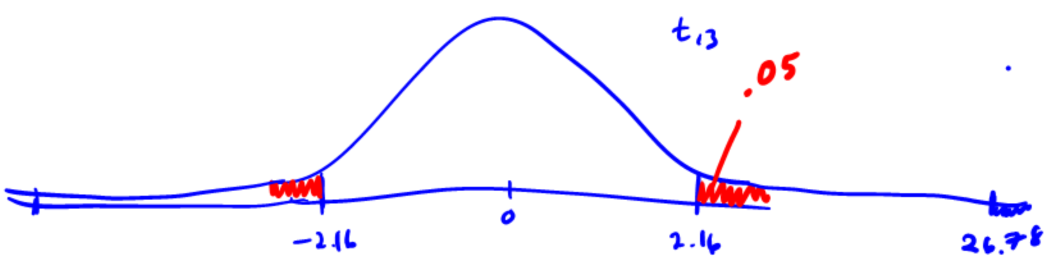
8. Conduct a formal hypothesis test at the $\alpha = .05$ significance level to determine if the relationship between density and pressure is significant.

1. $H_0: \beta_1 = 0 \quad H_A: \beta_1 \neq 0$

2. $\alpha = .05$

3. I will use the test statistic $K = \dfrac{b_1 - 0}{\frac{s_{\varepsilon}}{\sqrt{\Sigma(x_i-\bar{x})^2}}}$ which has a t_{n-2} distribution assuming H_0 is true and the regression model is valid.

4. $K = \dfrac{4.8667\times10^{-5}}{1.817\times10^{-6}} = 26.7843 > t_{13,.975} = 2.160$



5. Since $K = 26.7843 > 2.16 = t_{13,.975} \Rightarrow$ p-value $< \alpha \Rightarrow$ we reject H_0.

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

7. Calculate and interpret the two-sided 95% CI for β_1

$$b_1 \pm t_{n-2,1-\alpha/2} \frac{s_e}{\sqrt{\Sigma(x_i-\bar{x})^2}} = 4.8667\times10^{-5} \pm t_{15-2,.975}(1.817\times10^{-6})$$

$$= 4.8667\times10 \pm 2.160\ (1.817\times10^{-6})$$

$$= (.00004479, .00005259)$$

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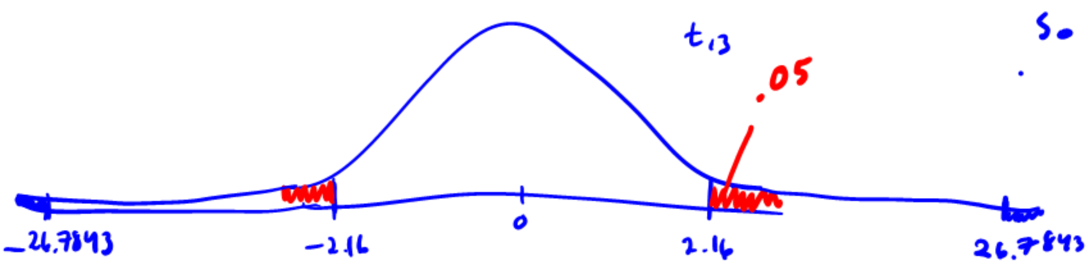
4. $K = \dfrac{4.8667\times10^{-5}}{1.817\times10^{-6}} = 26.7843 > t_{13,.975} = 2.160$

So p-value $< .05 = \alpha$



9.1.3 Inference for mean response

Recall our model

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

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

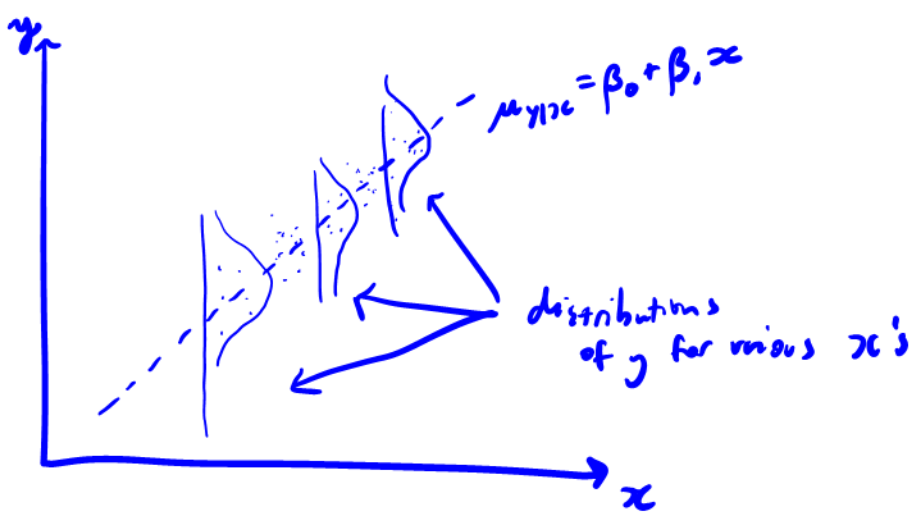
$$\mu_{y|x_i} = E(y_i) = E(\beta_0 + \beta_1 x_i + \varepsilon_i) = \beta_0 + \beta_1 x_i + \overset{=0}{E(\varepsilon_i)}$$
$$= \beta_0 + \beta_1 x_i$$

Now, if some new covariate value x is within the range of the x_i's, we can estimate the true mean response at this new x

interpolation

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

But how good is the estimate?



Under the model,

$\hat{\mu}_{y|x}$ is Normally distributed with

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

individual value of x that we care about

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

sample mean x_i values from data.

all x_i's in the data

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

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

And when σ is unknown (i.e. basically always),

replace σ with $S_{LF} = \sqrt{\frac{1}{n-2} \sum_i (y_i - \hat{y}_i)^2}$

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

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

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

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

$\underbrace{\hspace{6cm}}_{\text{assumptions}}$

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

$$\hat{\mu}_{y|x} \pm t_{n-2,1-\alpha/2} \cdot \boxed{S_{LF}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum_i (x_i-\bar{x})^2}}}$$

(can also make one-sided CI's)

A note on calculating $S_{LF}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum_i (x_i-\bar{x})^2}}$ ← this could take some time

[Shortcut when we have JMP output]

Notice $S_{LF}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum (x_i-\bar{x})^2}} = \sqrt{\frac{S_{LF}^2}{n} + \underbrace{(x-\bar{x})^2}_{\text{easy to calculate}} \boxed{\frac{S_{LF}^2}{\sum(x_i-\bar{x})^2}}}$ ← $\hat{Var}(b_1)$ can get from JMP as $(\hat{SE}(b_1))^2$

can get from JMP as MSE

Example 9.2 (Ceramic powder pressing). Return to the ceramic density problem. We will make a 2-sided 95% confidence interval for the true mean $\mu_{y|x}$ density of ceramics at 4000 psi and interpret it. Note $\bar{x} = 6000$ $x = 4000$

$$\hat{\mu}_{y|x=4000} = 2.375 + 4.8667 \times 10^{-5}(4000) = 2.569668 \text{ g/cc}$$

$$s_{LF}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{\Sigma(x_i-\bar{x})^2}} = \sqrt{\frac{s_{LF}^2}{n} + (x-\bar{x})^2 \frac{s_{LF}^2}{\Sigma(x_i-\bar{x})^2}} \leftarrow (SE(b_1))^2$$

MSE

$$= \sqrt{\frac{.000396}{15} + (4000-6000)^2(1.817\times10^{-6})^2}$$

$$= \sqrt{.00003960 6}$$

$$= .006293 3$$

The $\hat{\mu}_{y|x} \pm t_{n-2,1-\alpha/2}\, s_{LF}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{\Sigma_i(x_i-\bar{x})^2}}$

$$= 2.569668 \pm t_{13,.975}(.0062933)$$

$$= 2.569668 \pm 2.160(.0062933)$$

$$= 2.569668 \pm 0.01359$$

$$= (2.5561, 2.5833)$$

We are 95% confident that the true mean density of the ceramics at 4000 psi is between 2.5561 g/cc and 2.5833 g/cc. $\mu_{y|x=4000}$

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

$$\hat{\mu}_{y|x=5000} = 2.375 + 4.8667 \times 10^{-5}(5000) = 2.618335 \text{ g/cc}$$

$$s_{LF}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum_i (x_i-\bar{x})^2}} = \sqrt{\frac{.000396}{15} + (5000-6000)^2 (1.817 \times 10^{-6})^2}$$

$$= .0054499$$

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

$$= 2.618335 \pm t_{13,.975}(.0054499)$$

$$= 2.618335 \pm 2.160(.0054499)$$

$$= (2.60656, 2.63011)$$

We are 95% confident that the true mean density at 5000 psi falls between 2.60656 g/cc and 2.63011 g/cc.

9.2 Multiple regression

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

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

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

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

(use JMP)

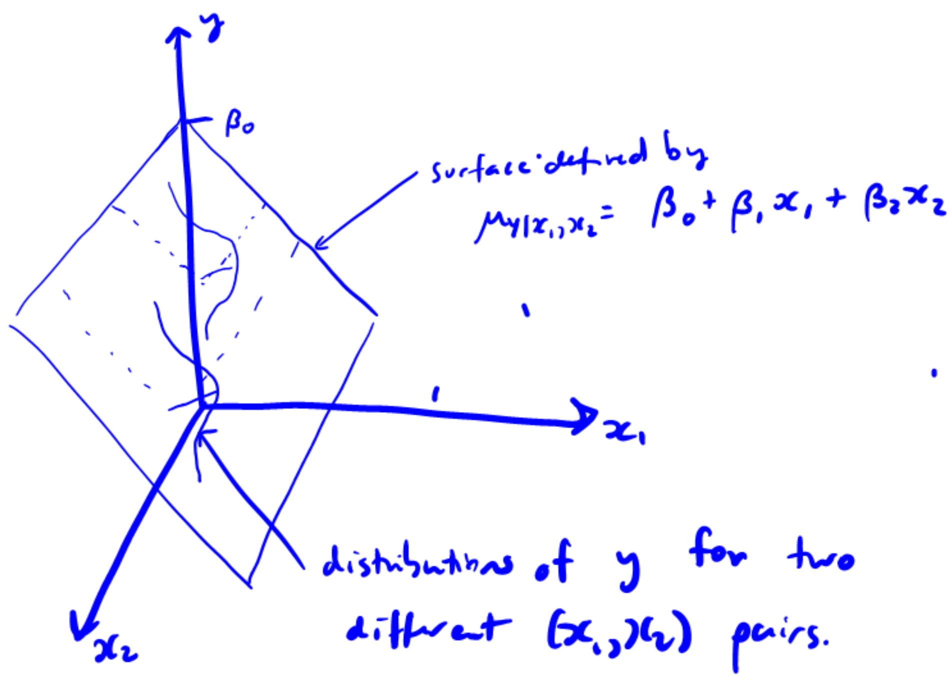
to find the estimates $b_0, \dots, b_{p-1}$.

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

for $p=3$



9.2.1 Variance estimation

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

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

$$= y_i - (b_0 + b_1 x_{1i} + \dots + b_{p-1} x_{p-1,i})$$

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

σ^2

Definition 9.2. 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,

also called mean square error (MSE)

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

there are p terms that are estimated $(b_0, \dots, b_{p-1})$ so we divide by $n-p$

is the *surface-fitting sample variance*. Associated with it are $\nu = n - p$ degrees of freedom and an estimated standard deviation of response $s_{SF} = \sqrt{s_{SF}^2}$.

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

Example 9.3 (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

Summary of Fit

RSquare	0.975006
RSquare Adj	0.969238
Root Mean Square Error	1.252714 ← S_{SF}
Mean of Response	14.47059
Observations (or Sum Wgts)	17

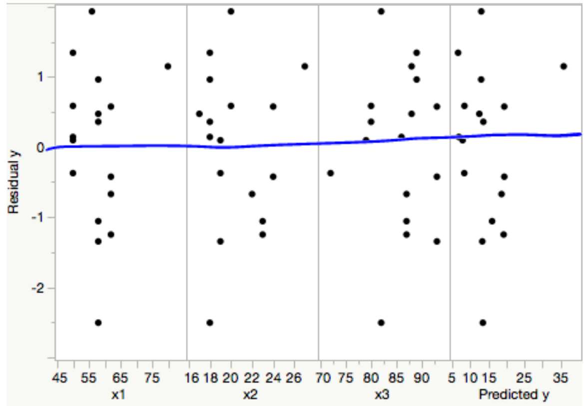
Analysis of Variance

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*

$S_{SF}^2 = MSE$

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



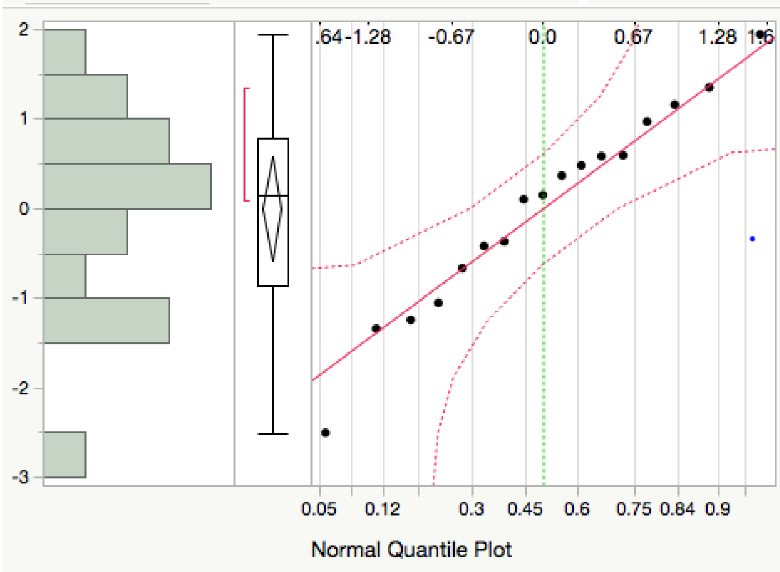


Figure 2: Least squares regression of stack loss on air flow, inlet temperature, and modified acid concentration.

$\hat{y} = -37.65246 + 0.7977x_1 + 0.5773x_2 - 0.0671x_3$

The residual plots vs. x_1, x_2, x_3, and $\hat{y}$ look like random scatter around 0 and the QQ-plot of residuals looks linear, indicating the residuals are normally distributed.

The model is valid.

9.2.2 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).

Under our model assumptions,

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

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

That means

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

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

$$K = \frac{b_i - \#}{s_{SF}\sqrt{d_i}} = \frac{b_i - \#}{SE(b_i)} \sim t_{n-p} \text{ if } ① \ H_0 \text{ is true and } ② \text{ the model is valid.}$$

and a 2-sided $(1-\alpha)100\%$ CI for β_i is

$$b_i \pm t_{n-p,1-\alpha/2}\, s_{SF}\sqrt{d_i}$$

i.e. $$b_i \pm t_{n-p,1-\alpha/2}\, \underline{SE(b_i)}$$

given in JMP.

Example 9.4 (Stack loss, cont'd)**.** Using the model fit on page 15, 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 $\alpha = .1$.
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 $\alpha = .05$.
3. Construct and interpret a 99% confidence interval for β_3.
4. Construct and interpret a 90% confidence interval for β_2.

9.2.3 Inference for mean response

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

with:

Then, under the model assumptions

And a test statistic for testing $\mathrm{H}_0 : \mu_{y|\boldsymbol{x}} = \#$ is

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

Example 9.5 (Stack loss, cont'd)**.** We can use JMP to compute a 2-sided 95% CI around the mean response at point 3:

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

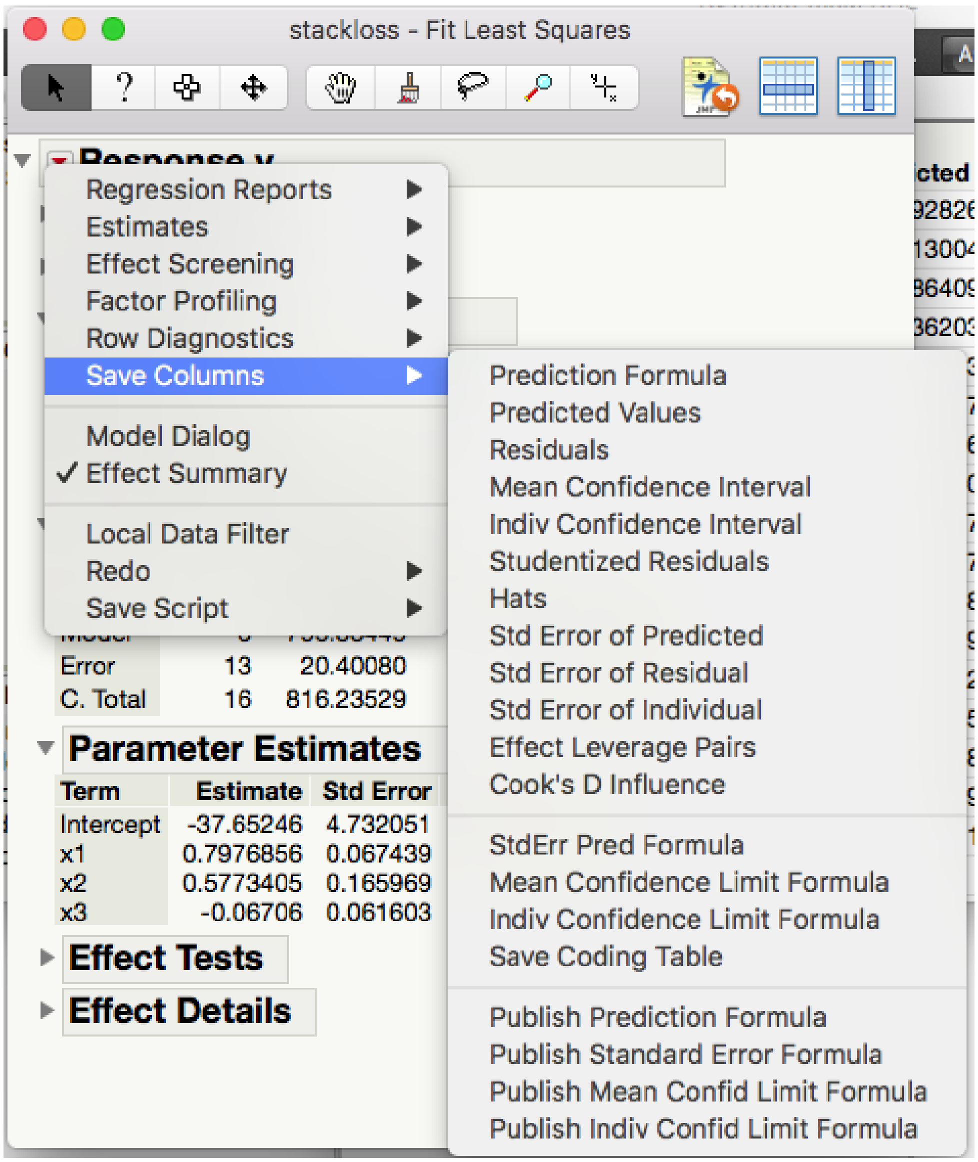
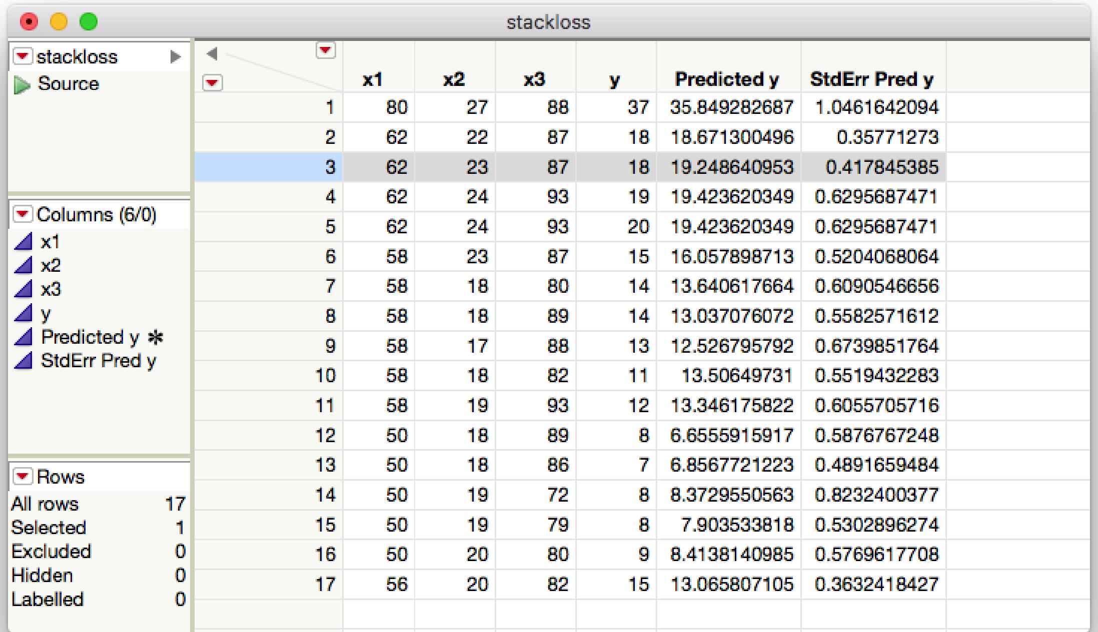


Figure 3: How to get predicted values and standard errors.



	x1	x2	x3	y	Predicted y	StdErr Pred y
1	80	27	88	37	35.849282687	1.0461642094
2	62	22	87	18	18.671300496	0.35771273
3	62	23	87	18	19.248640953	0.417845385
4	62	24	93	19	19.423620349	0.6295687471
5	62	24	93	20	19.423620349	0.6295687471
6	58	23	87	15	16.057898713	0.5204068064
7	58	18	80	14	13.640617664	0.6090546656
8	58	18	89	14	13.037076072	0.5582571612
9	58	17	88	13	12.526795792	0.6739851764
10	58	18	82	11	13.50649731	0.5519432283
11	58	19	93	12	13.346175822	0.6055705716
12	50	18	89	8	6.6555915917	0.5876767248
13	50	18	86	7	6.8567721223	0.4891659484
14	50	19	72	8	8.3729550563	0.8232400377
15	50	19	79	8	7.903533818	0.5302896274
16	50	20	80	9	8.4138140985	0.5769617708
17	56	20	82	15	13.065807105	0.3632418427

Figure 4: Predicted values and standard errors.