## 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

$$y = \beta_0 + \beta_1 x + 6$$

where  $\beta_0$  is the intercept.

 $\beta_1$  is the slope.

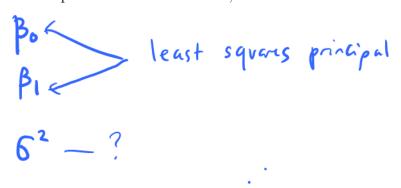
 $\epsilon$  is some error. In fact,

(recall checking it residuals are normally distributed is one of our model assessment techniques)

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.

### 9.1.1 Variance estimation

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



We need an estimate for  $\sigma^2$  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  $e_i = y_i - \hat{y}_i$ ,

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

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

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

#### 9.1.2 Inference for parameters

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-a)100% lonfidence interval
- 2. Formal hypothesis (significance) test

Both of these require

Dan estimate for β, (b,) and ② a "standard error" for β,

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

$$b_1 \sim N\left(\beta_1, \frac{\sigma^2}{\sum (x_i - \bar{x})^2}\right)$$
 we must estimate it using  $\int MSE = SLF$ 

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

$$\sum (x_i - \bar{x})^2$$
standard error for  $\beta_1$ 

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

$$K = \frac{b_1 - \#}{\left(\frac{S_{LF}}{\sqrt{\sum_i (x_i - \bar{x})^2}}\right)} \sim t_{h-2} \quad \text{if } H_0 \text{ is true}$$

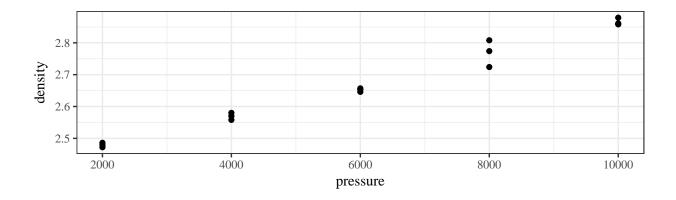
**Example 9.1** (Ceramic powder pressing). A mixture of  $Al_2O_3$ , polyvinyl alcohol, and water was prepared, dried overnight, crushed, and sieved to obtain 100 mesh size grains. These were pressed into cylinders at pressures from 2,000 psi to 10,000 psi, and cylinder densities were calculated. Consider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

x = the pressure setting used (psi)

y = 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.

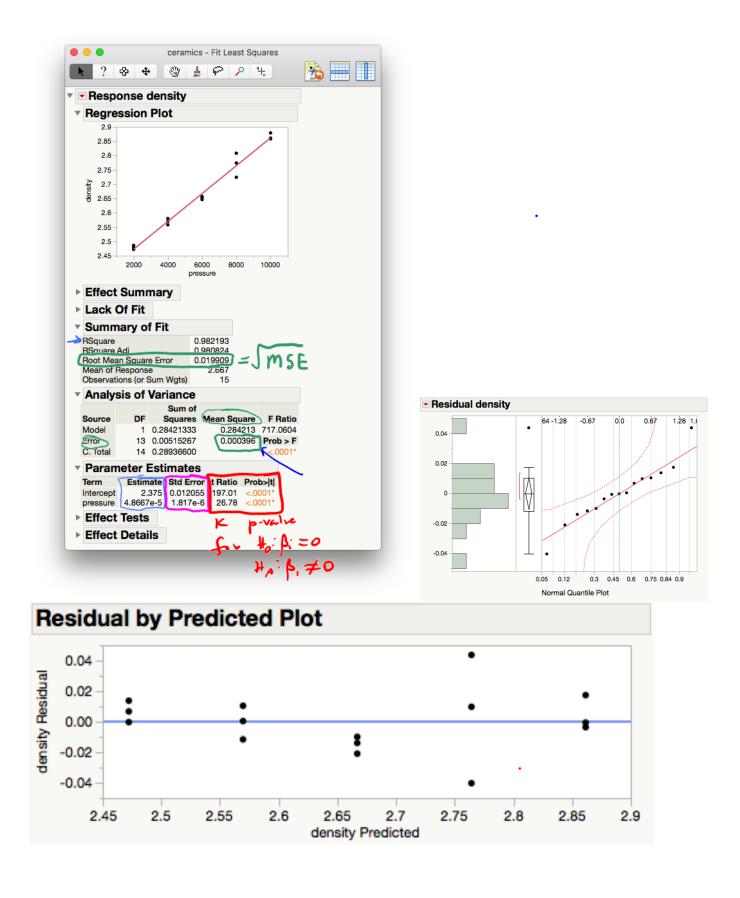


Figure 1: Least squares regression of density on pressure of ceramic cylinders.

1. Write out the model with the appropriate estimates.

$$\hat{y} = 2.375 + 4.8667 \times 10^{-5} 20$$

2. Are the assumptions for the model met?

Yes. The residual plot shows random scatter around O and the Normal QQ plot looks relatively linear, indicating the residuals are Normally distributed.

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

4. What is the correlation between x and y?

For SLR, 
$$r = \int R^2 = \int .9821 = .9911$$

5. Estimate  $\sigma^2$ .

$$\hat{6}^2 = S_{LF}^2 = MSE = .000396$$

6. Estimate 
$$Var(b_1)$$

$$\sqrt{a_r(b_1)} = \frac{5_{LF}^2}{5(x_i - \overline{x})^2} = \left(5E(b_1)\right)^2 = (1.817 \times 10^{-6})^2$$

$$= 3.3015 \times 10^{-12}$$

2-gided

7. Calculate and interpret the 95% CI for  $\beta_1$ 

$$b_{1} = 4.8667 \times 10^{-5} + t_{15-2,.975} (1.817 \times 10^{-6})$$

$$= 4.8667 \times 10^{5} + 2.160 (1.817 \times 10^{-6})$$

$$= (.60004474, .60005254)$$

We are 95% confident that for every 2 psi increase in pressure density will increase between . 00004474 g/cc and . 00005259g/a on average.

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

3) I will use the test statistic 
$$K = \frac{6,-0}{SLE}$$
 which has a  $t_{n-1}$  dsn assuming to is true and the

regassion model is valid.

$$4 \text{ K} = \frac{4.8667 \times 10^{-5}}{1.817 \times 10^{-6}} = 26.7843 > t_{13,.975} = 2.160$$

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

#### 9.1.3 Inference for mean response

Recall our model

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

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

$$E(\beta_0 + \beta_1 \times i + \xi_i) = \beta_0 + \beta_1 \times i + E\xi_i^{-0}$$

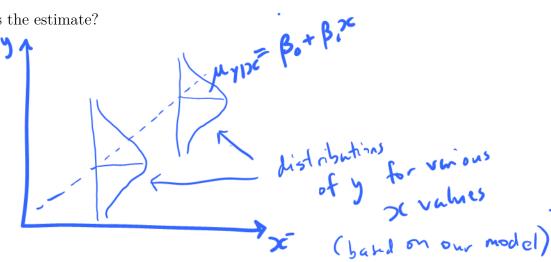
$$M_{Y|X_i} = \beta_0 + \beta_1 \times i$$

$$pure don't extrapolate extrapolate$$

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

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

But how good is the estimate?



Under the model,

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

$$E(\hat{\mu}_{Y|x}) = \mu_{Y|x} = \beta_0 + \beta_1 x \quad \text{individual value of } x$$

that we are about estimating that we are about estimating that we have a for the state of the state

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

And when  $\sigma$  is unknown (i.e. basically always),

replace 6 with 
$$\frac{1}{S_{LF}} = \int_{h-2}^{L} \frac{1}{2} \frac{$$

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

$$K = \frac{\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{\xi_{:}(x-\bar{x})^2}}}{\frac{1}{\xi_{:}(x-\bar{x})^2}}$$

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

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

$$\int_{\text{Mylox}} \frac{1}{z} + \int_{\text{min}} \frac{1}{z_{i}(x_{i}-\overline{x})^{2}} \int_{\text{malogous}} \frac{1}{z_{i}(x_{i}-\overline{x})^{2}} \int_{\text{malogous}} \frac{1}{z_{i}(x_{i}-\overline{x})^{2}} \int_{\text{malogous}} \frac{1}{z_{i}(x_{i}-\overline{x})^{2}} \int_{\text{min}} \frac{1}{z$$

**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 density of ceramics at 4000 psi and interpret it. Note: 5 = 6000

$$\int_{LF} \frac{1}{n} + \frac{(x-\overline{x})^2}{E_1(x_1-\overline{x})^2} = \int_{\overline{x}} \frac{S_{LF}}{n} + (x-\overline{x})^2 \frac{S_{LF}}{E_2(x_1-\overline{x})^2} = (SE(I_1)^2)^2$$

$$= \int_{0.00376} \frac{0.000376}{15} + (9000-6000)^2 (1.817 \times 166)^2$$

$$= \int_{0.000376} \frac{0.000376}{15} + (9000-6000)^2 (1.817 \times 166)^2$$

$$= \int_{0.000376} \frac{0.000376}{15} + (9000-6000)^2 (1.817 \times 166)^2$$

$$= \int_{0.000376} \frac{0.00007}{15} + (9000-6000)^2 (1.817 \times 166)^2$$

$$= \int_{0.000376} \frac{0.0007}{15} + (9000-6000)^2 (1.817 \times 166)^2$$

$$= \int_{0.000376}$$

on page 4, he range of X's is 2000 to 10000 So both 4000 and 5000 are reasonable values to either the bree response for we are not extrapolating.

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

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

$$S_{F} \int_{\Lambda}^{\frac{1}{2}} + \frac{(x-\bar{x})^{2}}{\Sigma_{i}(x_{i}-\bar{x})^{2}} = \int_{\Lambda}^{\frac{2}{2}} + (x-\bar{x})^{2} \frac{S_{i}e^{2}}{\Sigma_{i}(x_{i}-\bar{x})^{2}} = (SE(i,))^{2}$$

$$MSE \int_{15}^{\frac{1}{2}} + (5000 - 6000)^{2} (1.817 \times 10^{-6})^{2}$$

$$= 2.6(8335) = 2.160(.00341)$$

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We are 95% confident that he true mean dentity of the caranics at 5000 psi is between 2.60656g/cc and 2.63011 g/cc.

# 9.2 Multiple regression

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

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

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

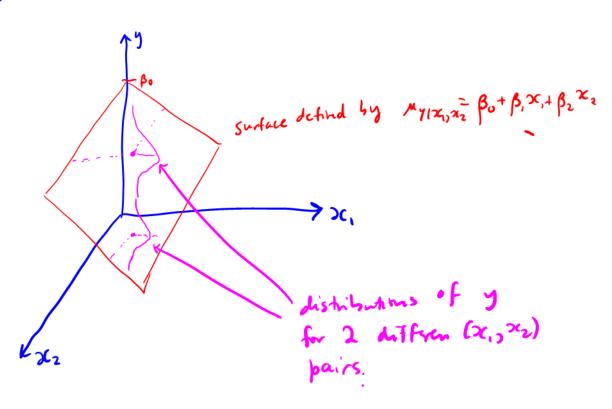
$$S(b_0, \dots, b_{p-1}) = \sum_{i=1}^{n} (y_i - \hat{y})^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{1,i} - \dots - \beta_{p-1} x_{p-1,i})^2$$

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

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



#### 9.2.1 Variance estimation

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

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

$$= y_i - (b_0 + b_1 x_i + ... + b_{p-1} x_{p-1})$$

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

**Definition 9.2.** 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. 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%) × 10

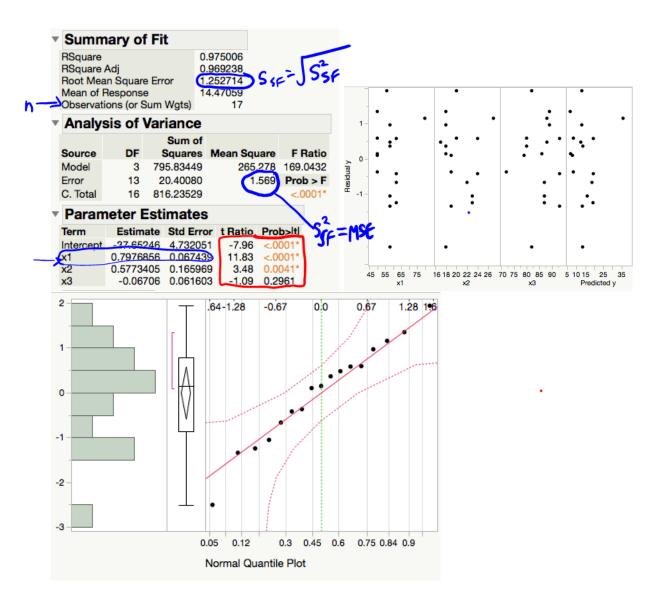


Figure 2: Least squares regression of stack loss on air flow, inlet temperature, and modified acid concentration.

The residual plats to  $x_0, x_1, x_2, x_3$ , and g look like random scather around 0 and the QQ-plot of the residuals looks linear, indicating the residuals are Normally distributed.

This 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  $d_i, i=0,1,\ldots,p-1$ . (that are hard to longule/describe analytically. But JMP can help).

That means

$$\frac{b_i - \beta_i}{S_{SF} \int_{a_i}^{a_i}} = \frac{b_i - \beta_i}{SE(b_i)} \sim t_{n-p}$$

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

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

**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  $\beta_3$ .
- 4. Construct and interpret a 90% confidence interval for  $\beta_2$ .

- 2 d=,1
- 2) x=,1
  3) I will have he test statistic K=  $\frac{b_1-1}{SE(b_1)}$  which, mode the assumption state  $O(b_1)$  is true and The model  $Y_1 = β_0 + β_1 x_3 + β_2 x_2 + β_3 x_3 + ε_{ij} ε_i^{N}N(0,6^2)$ is correct, is distributed ta-p = t17-4 = t13
- $4 \text{ K} = \frac{6.7977-1}{0.06344} = -3.00 \text{ and } t_{13..9} = 1.35$

produ: P(T < K) = P(T < - 3)

<.1 = d -3 -1,35

- € With K=-3 < -1.35 = -t<sub>13,9</sub> => p-value < α => We reject the and conclude in favor of the
- @ There is enough evidence that he true slope on airflow is less than I unit stackloss/unit airflow. With each unit increase in airflow and all other covariates held constant, we expect stuck loss to insease by less Im I unit.

2. (1) 
$$H_0: \beta_3 = 0$$
  $H_A: \beta_3 \neq 0$ 

2 d= 0.05

where E; id NCO,62) i=1,...,17 holds, then K~th-p= t14-4= t13.

$$4) K = \frac{-0.06706-0}{0.0616} = -1.09$$

p-value = P(ITI > |KI) = P(ITI > 1.09)

1 + 13,975 = 2.16

- 5) Since our p-value 7d => we shail to reject Ho
- 6 The is not enough evidence to conclude that, with all other committees held constant, there is a significant below relationship between stackloss and acid concentration.

Then 
$$b_s \pm t_{n-p,1-\alpha/4}$$
 SE(b<sub>3</sub>) = -0.06706 ± 3.612 (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 invease anywhere from -0,2525 units to 0.1165 units.

4 For a 90% two sided CI for 
$$\beta_2$$
,  $\alpha = .1$ ,  $t_{h-\rho, 1-\alpha/2}^{-1} t_{18, .95} = 1.77$   
Then  $b_2 \pm t_{n-\rho, 1-\alpha/2}$  SE( $b_2$ ) = 0.8773 ± 1.77 (0.166)

We are 90%, confident that for exp 1 degree insease in temperature up all other covariates held constant, stack loss is expected to invease by anywhere times 0. 2934 units to 0.8713 units.

#### 9.2.3 Inference for mean response

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

with

Then, under the model assumptions

$$Z = \frac{\hat{\mu}_{y|x} - \mu_{y|x}}{\sigma A} \sim N(0,1)$$
 and  $T = \frac{\hat{\mu}_{y|x} - \mu_{y|x}}{S_{s_F} A} \sim t_{n-p}$ 

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

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

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

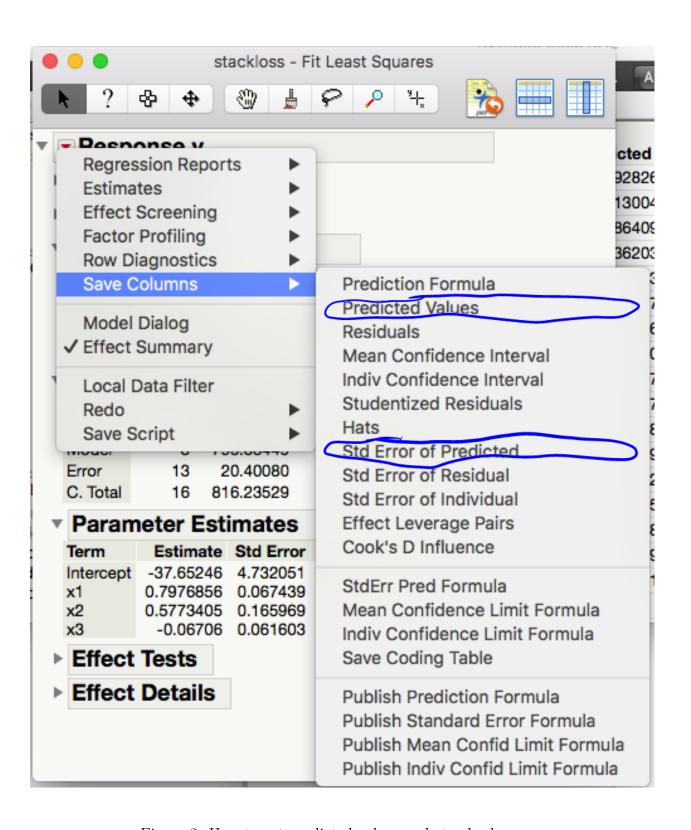


Figure 3: How to get predicted values and standard errors.

• •				stackloss	6			
▼ stackloss ▶	■ •							
Source	•	x1	x2	x3	У	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	
Columns (6/0)  x1  x2  x3  y Predicted y *  StdErr Pred y	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	
Rows All rows 17 Selected 1 Excluded 0 Hidden 0 Labelled 0	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.

the true mean stack loss is between 18.343 and 20. 151 units.