STAT 135 Lab 12
Multiple Linear Regression (Matrix Form), Residual analysis, Inference about $\hat{\beta}$

Rebecca Barter

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Multiple Linear Regression

Simple Linear Regression

Recall simple linear regression, where we had a single variable, x, and we wanted to use it as a predictor for our response, y:

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

So that taking a linear combination of x (with some noise) gives the response y.
For example, we could fit a model for the height of suds (mm) as a function of soap (g) used based on the following 10 observations.

i	1	2	3	4	5	6	7	8	9	10
soap (x)	3.5	4.0	4.5	5.0	5.5	6.0	6.5	7.0	7.5	8.0
suds (y)	24.4	32.1	37.1	40.4	43.3	51.4	61.9	66.1	77.2	79.2

Simple Linear Regression

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suds (y)	24.4	32.1	37.1	40.4	43.3	51.4	61.9	66.1	77.2	79.2

and find that

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x} = -20.2$$

$$\hat{\beta}_1 = cov(x, y)/var(y) = 12.4$$

and conclude that our fitted line is given by:

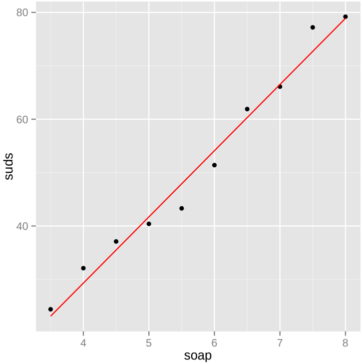
$$\widehat{\text{suds}} = -20.2 + 12.4 \times \text{soap}$$

I

Simple Linear Regression

Our fitted (red) line is given by:

$$\widehat{\text{suds}} = -20.2 + 12.4 \times \text{soap}$$



Multiple Linear Regression

What if we believed that not only the amount of soap used, but also the following variables affected the height of the suds:

- oil level of soap
- acidity of the soap
- amount of water
- hardness of the water

Then we might want to include these predictors in our model:

$$\begin{aligned}\text{suds} \ = \ \beta_0 \ + \ \beta_1 \times (\text{soap}) \ + \ \beta_2 \times (\text{oil}) \ + \ \beta_3 \times (\text{acidity}) \\ + \ \beta_4 \times (\text{water}) \ + \ \beta_5 \times (\text{hardness}) + \epsilon\end{aligned}$$

This is an example of **multiple linear regression*** (linear regression with more than one *predictor* (x)).

*not the same as **multivariate linear regression**: lin. reg. with more than one *response* (y)

Multiple Linear Regression

In multiple linear regression, the **response, $\mathbf{y_i}$**, for subject i ($i = 1, ..., n$) can be modeled as a linear combination of your $p - 1$ **predictors**, $\mathbf{x_{i,j}}$, $j = 0, ..., p - 1$, as follows:

$$\boxed{y_i = \beta_0 \ + \ \beta_1 x_{i,1} \ + \ \beta_2 x_{i,2} \ + ... + \ \beta_{p-1} x_{i,(p-1)} \ + \ \epsilon_i}$$

where the **random error terms**, $\boldsymbol{\epsilon}_i$, are independent random variables such that $E(\epsilon_i) = 0$ and $Var(\epsilon_i) = \sigma^2$.

- Note that we often require that $\epsilon_i \overset{IID}{\sim} N(0, \sigma^2)$, but in general, the normality is not required for unbiased estimates of the β's
- We do require $p < n$ (i.e. the number of predictors is less than the number of observations)

Multiple Linear Regression

Our regression equation is of the form:

$$y_i = \beta_0 \ + \ \beta_1 x_{i,1} \ + \ \beta_2 x_{i,2} \ + ... + \ \beta_{p-1} x_{i,(p-1)} \ + \ \epsilon_i$$

The question is, how do we estimate the β's? We want to minimize the distance from our observed observations y_i to our fitted line. That is, we want to find the values of β_0, β_1, ..., β_{p-1} that minimize

$$S(\beta_0, \beta_1, ..., \beta_{p-1}) = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - ... - \beta_{p-1} x_{i,p-1})^2$$

To do this by differentiating with respect to each β_j separately will be very time consuming.

Multiple Linear Regression

We want to find the values of β_0, β_1, ..., β_{p-1} that minimize

$$S(\beta_0, \beta_1, ..., \beta_{p-1}) = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - ... - \beta_{p-1} x_{i,p-1})^2$$

At this point, it's time to introduce the much more convenient **matrix notation** for linear regression.

Matrix Notation for Multiple Linear Regression

Multiple Linear Regression

Our regression equation for each subject ($i = 1, ..., n$) are of the form:

subject 1: $y_1 = \beta_0 + \beta_1 x_{1,1} + \beta_2 x_{1,2} + ... + \beta_{p-1} x_{1,(p-1)} + \epsilon_1$

subject 2: $y_2 = \beta_0 + \beta_1 x_{2,1} + \beta_2 x_{2,2} + ... + \beta_{p-1} x_{2,(p-1)} + \epsilon_2$

$$\vdots$$

subject n: $y_n = \beta_0 + \beta_1 x_{n,1} + \beta_2 x_{n,2} + ... + \beta_{p-1} x_{n,(p-1)} + \epsilon_n$

Multiple Linear Regression

subject 1: $y_1 = \beta_0 \times 1 + \beta_1 x_{1,1} + \beta_2 x_{1,2} + ... + \beta_{p-1} x_{1,(p-1)} + \epsilon_1$

subject 2: $y_2 = \beta_0 \times 1 + \beta_1 x_{2,1} + \beta_2 x_{2,2} + ... + \beta_{p-1} x_{2,(p-1)} + \epsilon_2$

$$\vdots$$

subject n: $y_n = \beta_0 \times 1 + \beta_1 x_{n,1} + \beta_2 x_{n,2} + ... + \beta_{p-1} x_{n,(p-1)} + \epsilon_n$

This can be written in matrix form as follows

$$\underset{(n\times 1)}{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}} = \underset{(n\times p)}{\begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,p-1} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,p-1} \\ 1 & x_{3,1} & x_{3,2} & \dots & x_{3,p-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n,1} & x_{n,2} & \dots & x_{n,p-1} \end{bmatrix}} \underset{(p\times 1)}{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix}} + \underset{(n\times 1)}{\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \vdots \\ \epsilon_n \end{bmatrix}}$$

Multiple Linear Regression

Multiple regression equations in matrix form:

$$Y = X\beta + \epsilon$$

$$\underset{(n\times 1)}{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}} = \underset{(n\times p)}{\begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,p-1} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,p-1} \\ 1 & x_{3,1} & x_{3,2} & \dots & x_{3,p-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n,1} & x_{n,2} & \dots & x_{n,p-1} \end{bmatrix}} \underset{(p\times 1)}{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix}} + \underset{(n\times 1)}{\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \vdots \\ \epsilon_n \end{bmatrix}}$$

- Y is the $(n \times 1)$ (observed) **response vector**
- X is the $(n \times p)$ (observed) **design matrix**
- β is the $(p \times 1)$ (unobserved) **coefficient vector**
- ϵ is the $(n \times 1)$ (unobserved) **error vector**

Multiple Linear Regression

$$Y = X\beta + \epsilon$$

and we have the following assumptions on the error term:

$$E[\epsilon] = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad Cov(\epsilon) = \sigma^2 I_{n\times n} = \begin{bmatrix} \sigma^2 & 0 & \dots & 0 \\ 0 & \sigma^2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \sigma^2 \end{bmatrix}$$

Moreover, we need ϵ to be independent of X.

Note that we still need to figure out how to estimate our β's

Multiple Linear Regression

Note that finding the values of $\beta_0, \beta_1, ...\beta_{p-1}$ that minimizes

$$S(\beta_0, \beta_1, ..., \beta_{p-1}) = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - ... - \beta_{p-1} x_{i,p-1})^2$$

is the same as finding the vector $\boldsymbol{\beta}$ that minimizes

$$\boxed{S(\boldsymbol{\beta}) = \|Y - X\boldsymbol{\beta}\|_2^2 = (Y - X\boldsymbol{\beta})^T (Y - X\boldsymbol{\beta})}$$

(this is just a number: $(Y - X\boldsymbol{\beta})^T (Y - X\boldsymbol{\beta})$ has dim (1×1))

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where $\| \cdot \|_2$ is the L^2-norm which is defined for a vector $\mathbf{x} = (x_1, ..., x_n)$ by

$$\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2} = \sqrt{\mathbf{x}^T \mathbf{x}}$$

Multiple Linear Regression

We want to find the vector $\boldsymbol{\beta} = (\beta_0, \beta_1, ..., \beta_{p-1})$ that minimizes

$$S(\boldsymbol{\beta}) = \|Y - X\boldsymbol{\beta}\|_2^2 = (Y - X\boldsymbol{\beta})^T(Y - X\boldsymbol{\beta})$$

We will show that our optimal $\boldsymbol{\beta}$ is given by

$$\boxed{\widehat{\boldsymbol{\beta}} = \left(X^T X\right)^{-1} X^T Y}$$

Where $\widehat{\boldsymbol{\beta}}$ is estimated vector of coefficients for our predictors in our fitted regression line

Multiple Linear Regression

To show that $\widehat{\boldsymbol{\beta}} = \left(X^T X\right)^{-1} X^T Y$, we want to find the vector $\boldsymbol{\beta}$ that satisfies

$$\frac{\partial S(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = 0$$

where

$$\begin{aligned}
\frac{\partial S(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} &= \frac{\partial}{\partial \boldsymbol{\beta}} (Y - X\boldsymbol{\beta})^T (Y - X\boldsymbol{\beta}) \\
&= \frac{\partial}{\partial \boldsymbol{\beta}} \left[Y^T Y - \boldsymbol{\beta}^T X^T Y - Y^T X \boldsymbol{\beta} + \boldsymbol{\beta}^T X^T X \boldsymbol{\beta} \right] \\
&= -X^T Y - X^T Y + 2 X^T X \boldsymbol{\beta}
\end{aligned}$$

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where we have used the following differentiation identities ($\mathbf{x}$ and $\mathbf{a}$ are both $(p \times 1)$ vectors and A is a symmetric $(p \times p)$ matrix):

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{a}^T \mathbf{x} = \frac{\partial}{\partial \mathbf{x}} \mathbf{x}^T \mathbf{a} = \mathbf{a} \qquad \frac{\partial}{\partial \mathbf{x}} \mathbf{x}^{\mathbf{T}} A \mathbf{x} = 2A\mathbf{x} = 2\mathbf{x}^T A$$

Multiple Linear Regression

Thus we need to solve for $\widehat{\boldsymbol{\beta}}$ in:

$$-X^T Y - X^T Y + 2X^T X\widehat{\boldsymbol{\beta}} = 0$$

rearranging gives the **normal equations**

$$X^T X\widehat{\boldsymbol{\beta}} = X^T Y$$

so that if $(X^T X)$ is invertible gives

$$\boxed{\widehat{\boldsymbol{\beta}} = \left(X^T X\right)^{-1} X^T Y}$$

and thus our **fitted model** is given by

$$\boxed{\widehat{Y} = X\widehat{\boldsymbol{\beta}} = X\left(X^T X\right)^{-1} X^T Y}$$

Exercise

Exercise: Multiple Linear Regression

Show that when we have simple linear regression ($p = 2$), i.e.

$$\underset{(n\times 1)}{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}} = \underset{(n\times 2)}{\begin{bmatrix} 1 & x_{1,1} \\ 1 & x_{2,1} \\ 1 & x_{3,1} \\ \vdots & \vdots \\ 1 & x_{n,1} \end{bmatrix}} \underset{(2\times 1)}{\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}} + \underset{(n\times 1)}{\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \vdots \\ \epsilon_n \end{bmatrix}}$$

that

$$\widehat{\boldsymbol{\beta}} = \left(X^T X\right)^{-1} X^T Y$$

yields the same estimates as when we solved for β_0 and β_1 individually.

Exercise

Exercise: Multiple Linear Regression

The file cigarete_dat.txt contains measurements of weight and tar, nicotine, and carbon monoxide content for 25 brands of domestic cigarettes. We want to use this dataset to define a model for the carbon monoxide level as a function of the other variables.

- Identify the correlation between all pairs of variables. If we find two variables are highly correlated, should we use only one of them?
- Choose the variables to include in the linear model, and identify the design matrix, X.
- Fit a multiple linear regression model to CO levels and report the fitted model.

Inference about $\widehat{\boldsymbol{\beta}}$

Inference about $\widehat{\boldsymbol{\beta}}$

We now turn to examining properties of our estimator (a random vector), $\hat{\boldsymbol{\beta}}$, in particular, calculating its expected value and covariance matrix. Recall that

- X and $\boldsymbol{\beta}$ are fixed
- $Y = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$ is random (but only through epsilon)
- $E(\boldsymbol{\epsilon}) = 0$ and $Cov(\boldsymbol{\epsilon}) = \sigma^2 I_{n\times n}$

$$\begin{aligned}
E\left(\widehat{\boldsymbol{\beta}}\right) &= E\left(\left(X^T X\right)^{-1} X^T Y\right) \\
&= \left(X^T X\right)^{-1} X^T E\left(Y\right) \\
&= \left(X^T X\right)^{-1} X^T E\left(X\boldsymbol{\beta} + \boldsymbol{\epsilon}\right) \\
&= \left(X^T X\right)^{-1} X^T X\boldsymbol{\beta} \\
&= \boldsymbol{\beta}
\end{aligned}$$

Thus $\widehat{\boldsymbol{\beta}}$ is an unbiased estimator for $\boldsymbol{\beta}$

Inference about $\widehat{\boldsymbol{\beta}}$

Recall that

- X and $\boldsymbol{\beta}$ are fixed
- $Y = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$ is random (but only through epsilon)
- $E(\boldsymbol{\epsilon}) = 0$ and $Cov(\boldsymbol{\epsilon}) = \sigma^2 I_{n\times n}$

$$
\begin{aligned}
Cov\left(\widehat{\boldsymbol{\beta}}\right) &= Cov\left(\left(X^T X\right)^{-1} X^T Y\right) \\
&= \left(X^T X\right)^{-1} X^T Cov(Y) X \left(X^T X\right)^{-1} \\
&= \left(X^T X\right)^{-1} X^T Cov(X\boldsymbol{\beta} + \boldsymbol{\epsilon}) X \left(X^T X\right)^{-1} \\
&= \left(X^T X\right)^{-1} X^T Cov(\boldsymbol{\epsilon}) X \left(X^T X\right)^{-1} \\
&= \left(X^T X\right)^{-1} X^T \sigma^2 I_{n\times n} X \left(X^T X\right)^{-1} \\
&= \sigma^2 \left(X^T X\right)^{-1}
\end{aligned}
$$

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where we have used the formula that if A is a constant matrix then $Cov(AY) = ACov(Y)A^T$ and $Cov(A+Y) = cov(A)$

Inference about $\widehat{\boldsymbol{\beta}}$

$$Cov\left(\widehat{\boldsymbol{\beta}}\right) = \sigma^2 \left(X^T X\right)^{-1}$$

We don't know σ^2, but we can estimate it using:

$$\hat{\sigma}^2 = \frac{RSS}{n-p} = \frac{\|Y - X\hat{\beta}\|_2^2}{n-p} = \frac{\|e\|_2^2}{n-p}$$

where $e = Y - X\hat{\beta}$ is the vector of residuals.*

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*See last week's slides.

Inference about $\widehat{\boldsymbol{\beta}}$

We can also test hypotheses about our true parameters, β_j. It is common to test the hypothesis that

$$H_0 : \beta_j = 0$$

for each $j = 0, .., p-1$, since if we have that $\beta_j = 0$, then the variable to which it corresponds has no effect on our response.

Note that if we assumed, $\epsilon \sim N(0, \sigma^2 I_{n\times n})$ then we have shown that

$$\widehat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, \sigma^2 (X^T X)^{-1})$$

where we can estimate our variance by $\hat{\sigma}^2 (X^T X)^{-1}$

Inference about $\widehat{\boldsymbol{\beta}}$

$$H_0 : \beta_j = 0$$

$$\widehat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, \sigma^2 (X^T X)^{-1})$$

So

$$\frac{\hat{\beta}_k - \beta_k}{\hat{\sigma}\sqrt{(X^T X)^{-1}_{k,k}}} \sim t_{n-p}$$

so our p-value is given by

$$P_{H_0}\left(|t_{n-p}| \geq \left| \frac{\hat{\beta}_k - \beta_k}{\hat{\sigma}\sqrt{(X^T X)^{-1}_{k,k}}} \right| \right)$$

where $(X^T X)^{-1}_{k,k}$ is the kth diagnoal entry of the matrix $(X^T X)^{-1}$

Exercise

Exercise: Inference about $\widehat{\boldsymbol{\beta}}$

For our previous example, test the hypothesis that the coefficient (β_{tar}) of Tar is zero.

Model Diagnostics

Model Diagnostics

How can we tell if our model is a good fit for the data?

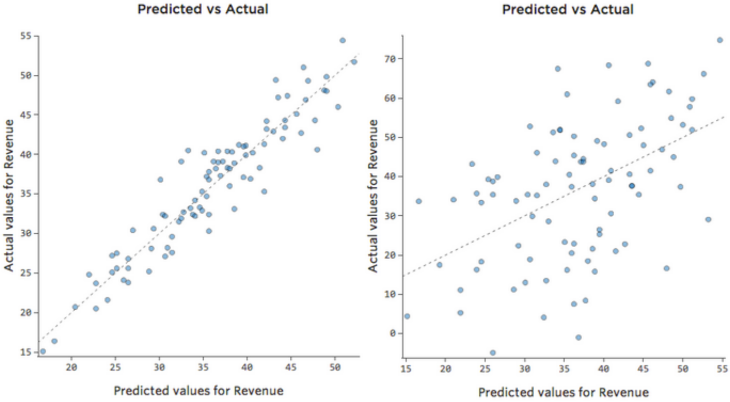
- Fitted-versus-observed plot
- Standardized residual versus fitted values plot

Model Diagnostics

We can look at a fitted-versus-observed plot

- We hope to see that the fitted values are very similar to the observed (true) values
- This corresponds to a diagonal line.

Model Diagnostics



The fitted/predicted values for the model on the left are closer to the true values than for the model on the right.

Model Diagnostics

We can look at a standardized residual versus fitted values plot

- We hope to see that the residuals are randomly scattered about $y = 0$
- We don't want to see any clear pattern

Note that the standardized residuals are

$$\frac{e_i}{\sqrt{Var(e_i)}}$$

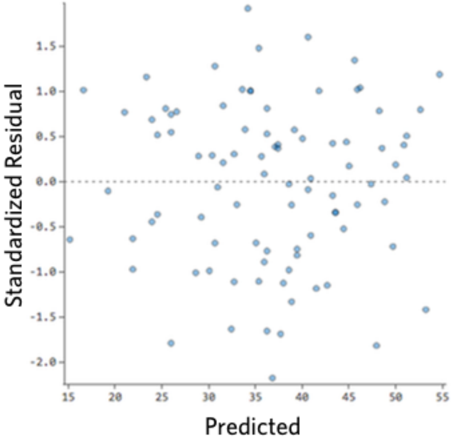
where

$$\begin{aligned}
Cov(e) &= Var(Y - X\hat{\beta}) \\
&= Var(Y - X(X^TX)^{-1}X^TY) \\
&= Var((I - X(X^TX)^{-1}X^T)Y) \\
&= (I - X(X^TX)^{-1}X^T)Var(Y)(I - X(X^TX)^{-1}X^T) \\
&= \sigma^2(I - X(X^TX)^{-1}X^T)
\end{aligned}$$

where the last equality follows from
$(I - X(X^TX)^{-1}X^T)^2 = (I - X(X^TX)^{-1}X^T)$

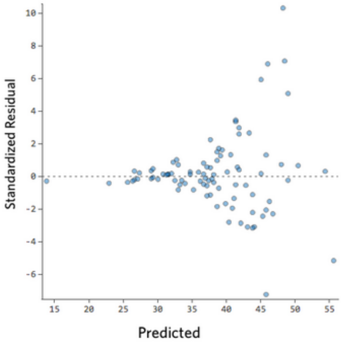
Model Diagnostics

This is an example of a good residual plot



Model Diagnostics

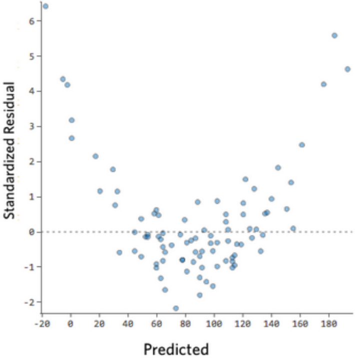
This is an example of a residual plot where there is heteroscedasticity (the variance is not the same for all observations)



A common solution is to transform a variable (most often a log-transform). Sometimes heteroscedasticity indicates that an important variable is missing.

Model Diagnostics

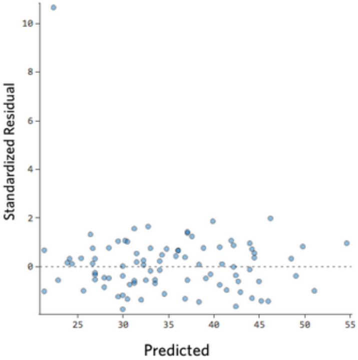
This is an example of a residual plot where there is a non linear relationship between variable and response



We might include a non-linear variable in our model. For example if the above model corresponded to $y = x + 1$, we might instead use $y = x^2 + x + 1$ (define a new predictor equal to x^2)

Model Diagnostics

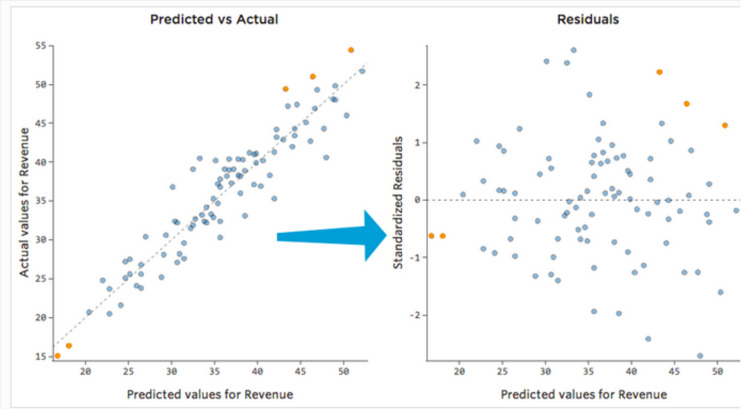
This is an example of a residual plot where there is an outlier



If we have an outlier, it is important to try to identify *why* the observation is an outlier (it could actually be informative). If the point corresponds to a genuine measurement error, then you should remove the outlier, otherwise, see if a transformation (e.g. square-root or log) diminishes the impact of the outlier.

Model Diagnostics

Here we can see how the predicted/fitted versus observed plot is transformed into a residual plot



Note that we've colored in a few dots in orange so you can get the sense of how this transformation works.

Exercise

Exercise: Model Diagnostics

For our cigarette example, plot a fitted versus observed plot as well as a residual plot. Do you think the model is fitting well?