multiple_polynomial_regression

September 9, 2019

0.1 Multiple regression

Lets look at a dataset made up of 4 variables: x, y, z, and r.

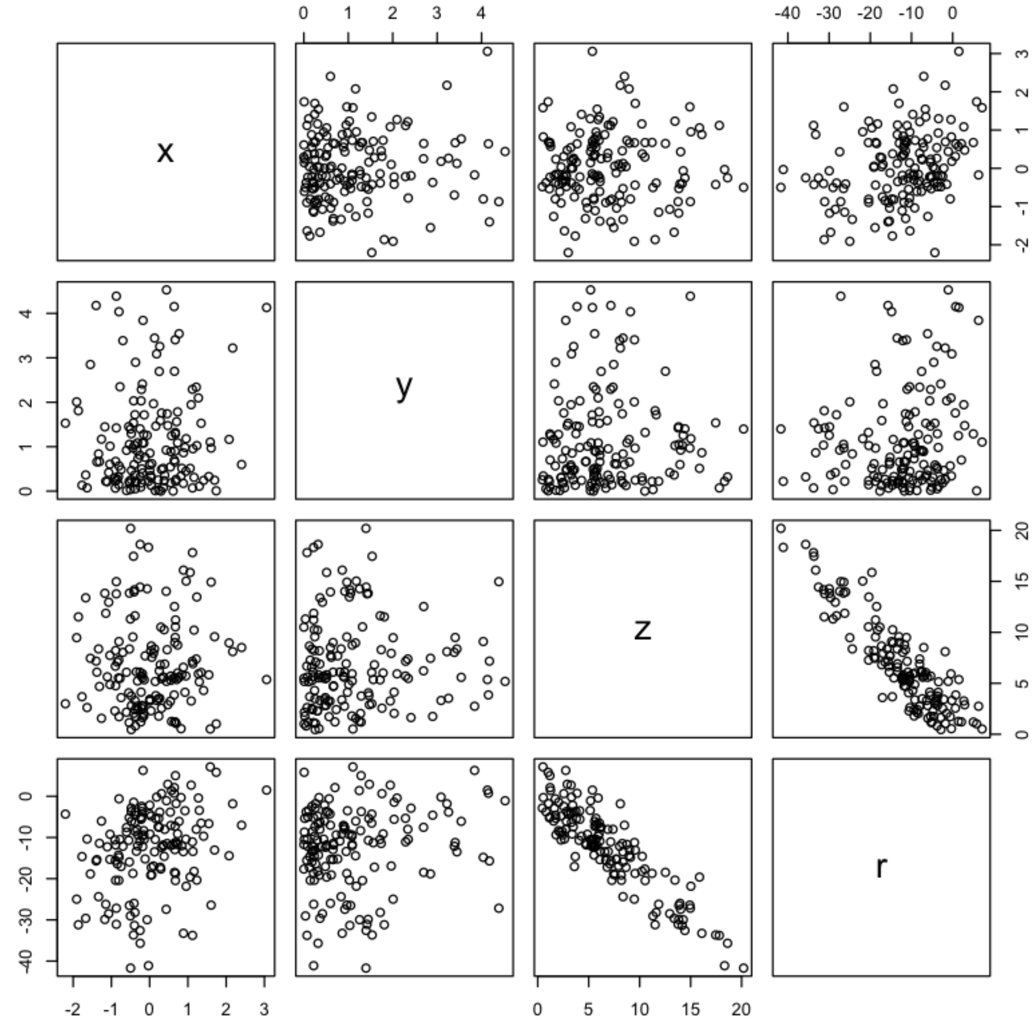
[2]:
```
dta <- read.csv('multipleData.csv')
head(dta)
```

A data.frame: 6 × 4

x	y	z	r
<dbl>	<dbl>	<dbl>	<dbl>
-0.9082393	0.30143444	2.287881	-10.61071
-0.2554406	0.80946626	6.093306	-10.86466
1.2185192	2.33952550	7.383286	-8.01159
-1.3996301	4.17670312	7.174199	-15.69763
0.9467331	0.44573692	5.719590	-10.40901
-0.2311548	0.08942789	1.201217	-5.03375

Just like simple linear regression, we can gain intuition by plotting all variables in a multiple linear regression to one another.

[3]:
```
plot(dta)
```



Sometimes this plot is call a **draftsman plot**. We notice a few interesting relationships * r and z are related negatively. Increasing values of z correspond to decreasing values of r * x is modestly related to r, y, and z positively. Increasing values of x corrspond to increasing values of y, z, and r

A **multiple linear regression (sometimes called a multivariate regression)** relates changes in \$>\$1 variable (the right-hand side of the equals signs) to a response variable, or variable to predict, or variable to explain (the left hand side of the equals sign). We can write this down in model form as

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in} + \epsilon_i \tag{1}$$
$$\epsilon \sim N(0, \sigma^2), \tag{2}$$

and using matrices and vectors,

$$
\begin{aligned}
y &= X\beta + \epsilon && (3)\\
\epsilon &\sim N(0, \sigma^2), && (4)
\end{aligned}
$$

where

$$
\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix}; X = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \cdots & x_{1,n} \\ 1 & x_{2,1} & x_{2,2} & \cdots & x_{2,n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{i,1} & x_{i,2} & \cdots & x_{i,n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{M,1} & x_{M,2} & \cdots & x_{M,N} \end{bmatrix}
$$

The parameters for each variable (β) are stacked into a single vector.

The Matrix X assigns one column per variable, and a column of 1s to represent the intercept.

We can also write the above multiple regression in probabilistic form

$$
y \sim N(X\beta, \sigma^2)
$$

Notice the same equation is used to represent simple linear regression and multiple linear regression. The differences between simple and multiple regression are folded into X and β.

0.2 Polynomial regression

We've discussed simple and multiple linear regression. Now lets discuss how linear regression can apply to nonlinear relationships.

Polynomial regression supposes the functional form relating y and x is a polynomial

$$
\begin{aligned}
y_i &= f(x_i|\beta)\\
&= \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \cdots \beta_n x_i^n + \epsilon_i\\
\epsilon_i &\sim N(0, \sigma^2)
\end{aligned}
$$

We can rewrite this equation in matrix form

$$
\begin{aligned}
y_i &= f(x_i|\beta)\\
&= X\beta + \epsilon\\
\epsilon &\sim N(0, \sigma^2)
\end{aligned}
$$

where

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix}; X = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_i & x_i^2 & \cdots & x_i^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_M & x_M^2 & \cdots & x_M^N \end{bmatrix}$$

Here the matrix X looks slightly different than in multiple regression. The first column of 1s is a place-holder for an intercept. The second column is the linear term x_i, the next column a quadratic term x_i^2, next column a cubic term x_i^3 and so on. The same observation x is raised to higher powers as we move across columns.

Now lets look at an example.

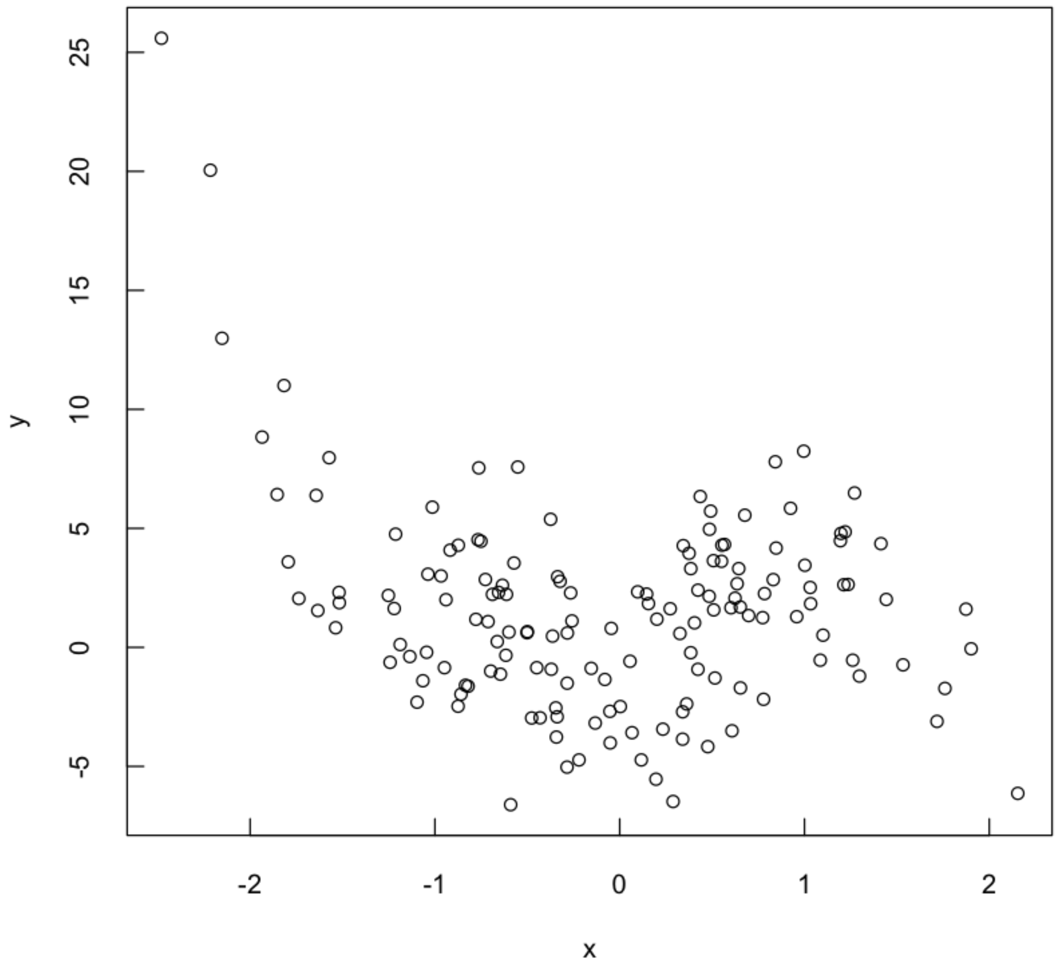
[4]:
```
data <- read.csv('polynomialData.csv')
head(data)
```

A data.frame: 6 × 2

x	y
<dbl>	<dbl>
0.9958723	8.2420054
-0.6556163	2.3114202
-0.9176787	4.0842076
0.1963727	-5.5386897
1.0309346	2.5166174
1.2610719	-0.5388713

Here we just have x values and y values. The difference, they're not related to each other linearly.

[5]:
```
plot(data$x,data$y
      ,xlab="x"
      ,ylab="y"
      ,tck=0.02
)
```



The variable x does not relate to y linearly; fitting a straight line to this data may under-represent the more complicated relationship.

Lets fit three different models: a linear model, a quadratic model, and a cubic model. We can plot each model fit and evaluate which model looks like it best represents the relationship between x and y.

[6]:
```
simpleLinearRegression <- lm(y~x,data=data)
print(simpleLinearRegression)

quadraticRegression <- lm(y~x+I(x^2),data=data)
print(quadraticRegression)

cubicRegression <- lm(y~x+I(x^2)+I(x^3),data=data)
```

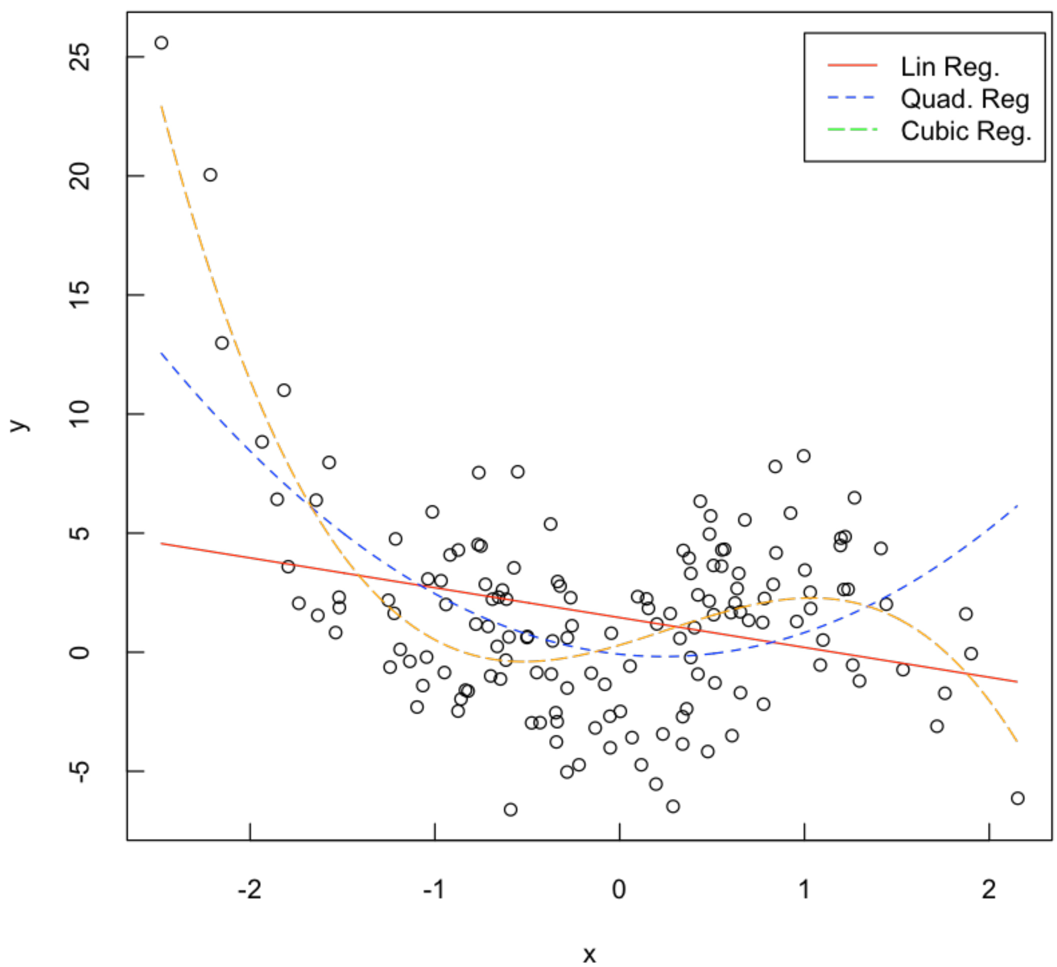
```
print(cubicRegression)
```

```
Call:
lm(formula = y ~ x, data = data)

Coefficients:
(Intercept)            x
      1.453       -1.253


Call:
lm(formula = y ~ x + I(x^2), data = data)

Coefficients:
(Intercept)            x       I(x^2)
   -0.08514     -0.81522      1.72492


Call:
lm(formula = y ~ x + I(x^2) + I(x^3), data = data)

Coefficients:
(Intercept)            x       I(x^2)       I(x^3)
     0.2994       2.2877       1.0962      -1.4120
```

[7]:

```
plot(data$x,data$y
     ,xlab="x"
     ,ylab="y"
     ,tck=0.02
)

minX <- min(data$x)
maxX <- max(data$x)

#linear regression
betas <- coef(simpleLinearRegression)
beta0 <- betas[1]
beta1 <- betas[2]

xVals <- seq(minX,maxX,0.01)
linearYPredictions <- beta0 + beta1*xVals
lines(xVals,linearYPredictions,col='red')

#quadratic regression
betas <- coef(quadraticRegression)
```

```
beta0 <- betas[1]
beta1 <- betas[2]
beta2 <- betas[3]

xVals <- seq(minX,maxX,0.01)
quadraticYPredictions <- beta0 + beta1*xVals + beta2*xVals^2
lines(xVals,quadraticYPredictions,col='blue', lty=2)

#cubic regression
betas <- coef(cubicRegression)
beta0 <- betas[1]
beta1 <- betas[2]
beta2 <- betas[3]
beta3 <- betas[4]

xVals <- seq(minX,maxX,0.01)
cubicYPredictions <- beta0 + beta1*xVals + beta2*xVals^2 + beta3*xVals^3
lines(xVals,cubicYPredictions,col='orange',lty=5)


legend(1,26,legend=c("Lin Reg.","Quad. Reg", "Cubic Reg.")
                     ,col=c('red','blue','green')
                     ,lty=c(1,2,5)
)
```



What fit looks best?

0.3 Optimization and assessing error

We can look at the three model fits to the data and visually assess fit, but a quantitative method for evaluating model fit is likely more convincing. A quantitative fit allows us to numerically compare model fits.

The most common metric for evaluating model fit is the **s**um **s**quares **r**rror (SSE). Given a data set, the **SSE** sums over all observations $(y_i, x_{i1}, x_{i2}, \cdots, x_{im})$ the squared difference between (y_i) and model predictions $[\hat{y}_i = f(x_i|\beta)]$

$$\mathrm{SSE}(y, \hat{y}) = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2,$$

or in vector form,

$$\mathrm{SSE}(y, \hat{y}) = (y - \hat{y})'(y - \hat{y})$$

where

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \tag{5}$$

and

$$y' = \begin{bmatrix} y'_1 \\ y'_2 \\ \vdots \\ y'_n \end{bmatrix} \tag{6}$$

Intuitively, SSE is a measure of the distance between your data and model. We can compute the SSE for the three above models fit to our non-linear data.

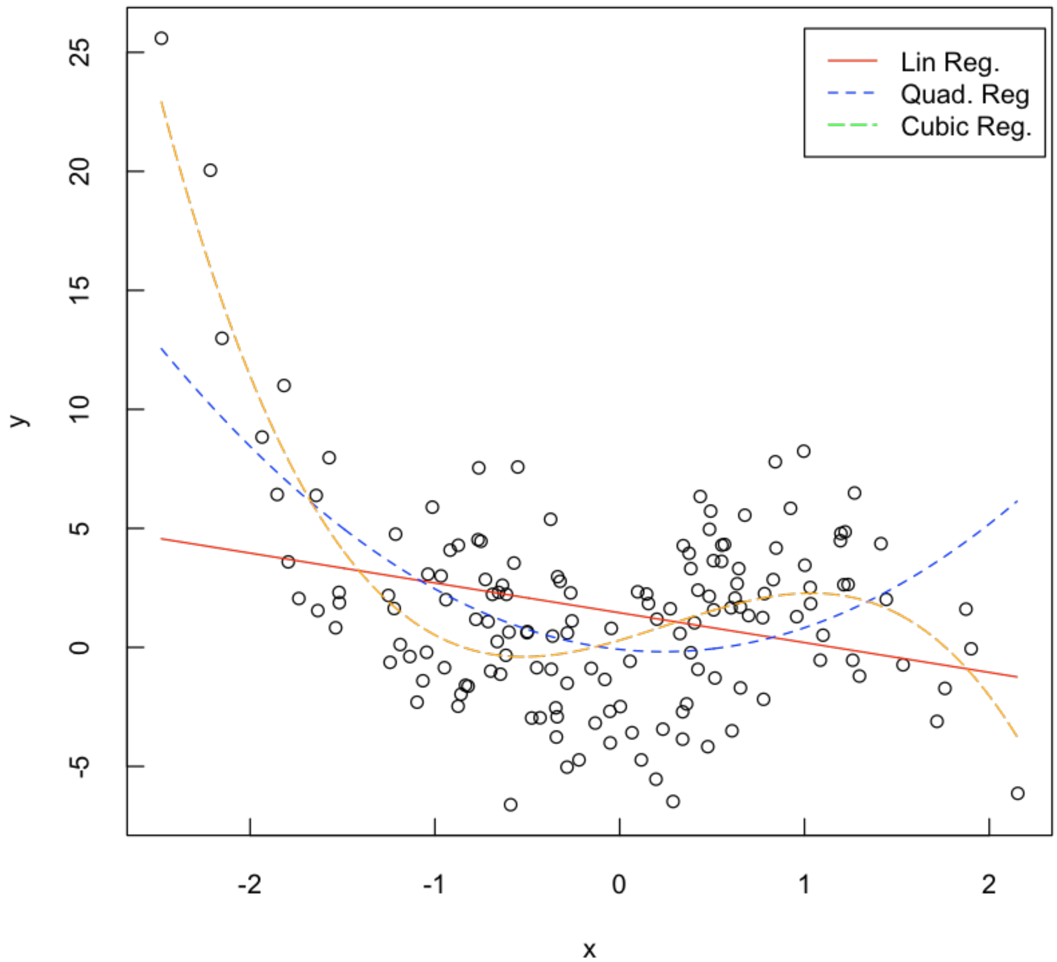
[10]:
```
plot(data$x,data$y
     ,xlab="x"
     ,ylab="y"
     ,tck=0.02
)

minX <- min(data$x)
maxX <- max(data$x)

#linear regression
betas <- coef(simpleLinearRegression)
beta0 <- betas[1]
beta1 <- betas[2]

xVals <- seq(minX,maxX,0.01)
linearYPredictions <- beta0 + beta1*xVals
lines(xVals,linearYPredictions,col='red')

ssr_SLR = sum((fitted(simpleLinearRegression) - data$y)^2) #NEW
```

```r
#quadratic regression
betas <- coef(quadraticRegression)
beta0 <- betas[1]
beta1 <- betas[2]
beta2 <- betas[3]

xVals <- seq(minX,maxX,0.01)
quadraticYPredictions <- beta0 + beta1*xVals + beta2*xVals^2
lines(xVals,quadraticYPredictions,col='blue', lty=2)

ssr_QR = sum((fitted(quadraticRegression) - data$y)^2) #NEW


#cubic regression
betas <- coef(cubicRegression)
beta0 <- betas[1]
beta1 <- betas[2]
beta2 <- betas[3]
beta3 <- betas[4]

xVals <- seq(minX,maxX,0.01)
cubicYPredictions <- beta0 + beta1*xVals + beta2*xVals^2 + beta3*xVals^3
lines(xVals,cubicYPredictions,col='orange',lty=5)

ssr_CR = sum((fitted(cubicRegression) - data$y)^2) #NEW


legend(1,26,legend=c("Lin Reg.","Quad. Reg", "Cubic Reg.")
                     ,col=c('red','blue','green')
                     ,lty=c(1,2,5)
)

sprintf("SSR Simple Linear Regression = %.2f",ssr_SLR)
sprintf("SSR Quadratic Regression = %.2f",ssr_QR)
sprintf("SSR Cubic Regression = %.2f",ssr_CR)
```

'SSR Simple Linear Regression = 2519.69'

'SSR Quadratic Regression = 1972.54'

'SSR Cubic Regression = 1362.07'



We see the the model with smallest sum square residual is the cubic model. The difference between model predictions made by the cubic model and the empirical data is smallest. In fact, the cubic model's SSR is 1.0-(1362.07/2519.69) 45% smaller than simple linear regression, and 1.0-(1972.54/2519.69) 21% smaller than quadratic regression.

0.4 Minimizing SSE

0.4.1 optimal within a model

We can take the idea that a smaller SSE suggests a better model fit further. Instead of using SSE to compare different models, we can use the SSE to evaluate different parameter values inside the same model.

Consider the same dataset as above and suppose we're fitting a simple linear regression. Then our SSE becomes

$$\text{SSE}(y, \hat{y}_i) = \sum_{i=1}^{N} [y_i - \hat{y}_i]^2 \tag{7}$$

$$\text{SSE}(y, x, \beta_0, \beta_1) = \sum_{i=1}^{N} [y_i - (\beta_0 + \beta_1 x_i)]^2 \tag{8}$$

$$\tag{9}$$

where y and x are vectors of data. Step two in above equation replaced the predicted value $\hat{y}$ with the linear model used to make this prediction $\beta_0 + \beta_1 x$.

Now our SSE is a function of the data, that cannot be changed, and the parameters of our model β_0 and β_1. Changing β_0 or β_1 will change the value of the SSE. One way to find a best fit model is to find those parameters value that make the SSE as small as possible.

0.4.2 derivative

SSE is a function of β_0 and β_1, and can be optimized by taking the derivative with respect to both parameters and finding the point where the derivative of these two equations equals zero simultaneously.

We take the derivative with respect to β_0

$$\frac{d\text{SSE}(\beta_0, \beta_1)}{d\beta_0} = \sum_{i=1}^{N} [y_i - (\beta_0 + \beta_1 x_i)]^2 \tag{10}$$

$$\frac{d\text{SSE}(\beta_0, \beta_1)}{d\beta_0} = \sum_{i=1}^{N} \frac{d}{d\beta_0} [y_i - (\beta_0 + \beta_1 x_i)]^2 \tag{11}$$

$$\frac{d\text{SSE}(\beta_0, \beta_1)}{d\beta_0} = \sum_{i=1}^{N} -2[y_i - (\beta_0 + \beta_1 x_i)] \tag{12}$$

$$\tag{13}$$

The above derivative can be set to zero and solved for β_0, our variable.

$$\sum_{i=1}^{N} -2[y_i - (\beta_0 + \beta_1 x_i)] = 0 \tag{14}$$

$$\sum_{i=1}^{N} y_i - N\beta_0 - \beta_1 \sum_{i=1}^{N} x_i = 0 \tag{15}$$

$$N\beta_0 = \sum_{i=1}^{N} y_i - \beta_1 \sum_{i=1}^{N} x_i \tag{16}$$

$$\beta_0 = \bar{y} - \beta_1 \bar{x} \tag{17}$$

$$\tag{18}$$

The value for β_0 that optimizes the SSE is the average of our y values minus the optimal β_1 times the average of our x values.

We must also take the derivative with respect to β_1.

$$\frac{d\text{SSE}(\beta_0, \beta_1)}{d\beta_1} = \sum_{i=1}^{N} [y_i - (\beta_0 + \beta_1 x_i)]^2 \tag{19}$$

$$\frac{d\text{SSE}(\beta_0, \beta_1)}{d\beta_1} = \sum_{i=1}^{N} -2x_i[y_i - (\beta_0 + \beta_1 x_i)] \tag{20}$$

$$\tag{21}$$

The above equation can also be set to zero and solved for β_1.

$$\sum_{i=1}^{N} -2x_i[y_i - (\beta_0 + \beta_1 x_i)] = 0 \tag{22}$$

$$\sum_{i=1}^{N} x_i y_i - x_i\beta_0 - \beta_1 x_i^2 = 0 \tag{23}$$

$$\tag{24}$$

At this point we can substitute the optimal value for β_0 we derived.

$$\sum_{i=1}^{N} x_i y_i - x_i(\bar{y} - \beta_1 \bar{x}) - \beta_1 x_i^2 = 0 \tag{25}$$

$$\sum_{i=1}^{N} x_i y_i - \sum_{i=1}^{N} x_i \bar{y} + \sum_{i=1}^{N} x_i \beta_1 \bar{x} - \beta_1 x_i^2 = 0 \tag{26}$$

$$\beta_1 \left(x_i^2 - \sum_{i=1}^{N} x_i \bar{x} \right) = \sum_{i=1}^{N} x_i y_i - \sum_{i=1}^{N} x_i \bar{y} \tag{27}$$

$$\beta_1 = \frac{\sum_{i=1}^{N} x_i y_i - \sum_{i=1}^{N} x_i \bar{y}}{\left(x_i^2 - \sum_{i=1}^{N} x_i \bar{x} \right)} \tag{28}$$

This equation for β_1 doesn't look like anything we can recognize, but we can change the SSE we optimized to make this equation look more familiar. The equation we optimized was a function of β_0 and β_1, and so adding a constant value that does not include β_0 or β_1 would not change the optimal β.

From each data point, lets subtract $\bar{x}$ and $\bar{y}$, called centering our data. Then the above equation becomes

$$\begin{aligned}
\beta_1 &= \frac{\sum_{i=1}^{N} x_i y_i - \sum_{i=1}^{N} x_i \bar{y}}{\left(x_i^2 - \sum_{i=1}^{N} x_i \bar{x} \right)} && (29) \\
&= \frac{\sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y}) - \sum_{i=1}^{N} (x_i - \bar{x})\bar{y}}{\sum_{i=1}^{N} (x_i - \bar{x})^2 - \bar{x} \sum_{i=1}^{N} (x_i - \bar{x})} && (30) \\
&= \frac{\sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{N} (x_i - \bar{x})^2} && (31) \\
&= \frac{Cov(X, Y)}{Var(X)} && (32)
\end{aligned}$$

Centering our data, we see the optimal β_1 is the covariance between y and x divided by the variance of x.

We can also right the above in matrix form. The covariance between X and Y is written

$$Cov(X, Y) = X'y$$

where $X = x - \bar{x}$ and $Y = y - \bar{y}$, and the variance of X is written

$$Var(X) = X'X.$$

Then the expression for β_1 is

$$\beta_1 = (X'X)^{-1}(X'y)$$

But by adding a column of 1s to X, we can see that the above expression works for both β_1 and β_0. In fact, this expression will work for any design matrix X.

So we can write

$$\beta = (X'X)^{-1}(X'y)$$

To see this more clearly, let's generalize our derivations of β_0 and β_1 to multiple βs.

We first form our SSE for multiple linear regression

$$\text{SSE}(y, X, \beta_0, \beta_1) = \sum_{i=1}^{N} [y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in})]^2$$

where x_{ij} is observation i for variable j. Taking the derivative for every β and setting equal to 0 we have

For β_0

$$\sum_{i=1}^{N} 1[y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in})] = 0 \tag{33}$$

$$\sum_{i=1}^{N} (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in}) = \sum_{i=1}^{N} 1 y_i \tag{34}$$

$$\tag{35}$$

For β_1

$$\sum_{i=1}^{N} x_{i1}[y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in})] = 0 \tag{36}$$

$$\sum_{i=1}^{N} x_{i1}(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in}) = \sum_{i=1}^{N} x_{i1} y_i \tag{37}$$

$$\tag{38}$$

For β_2

$$\sum_{i=1}^{N} x_{i2}[y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in})] = 0 \tag{39}$$

$$\sum_{i=1}^{N} x_{i2}(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in}) = \sum_{i=1}^{N} x_{i2} y_i \tag{40}$$

$$\tag{41}$$

For β_n

$$\sum_{i=1}^{N} x_{in}[y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in})] = 0 \tag{42}$$
$$\sum_{i=1}^{N} x_{in}(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots \beta_n x_{in}) = \sum_{i=1}^{N} x_{in} y_i \tag{43}$$
$$\tag{44}$$

The right hand side of this system of equations can be rewritten as

$$X'y,$$

and the left hand side can be rewritten as

$$(X'X)\beta.$$

Our system of equations is then

$$(X'X)\beta = X'y.$$

We can solve for β by left multiplying each side by $(X'X)^{-1}$

$$\beta = (X'X)^{-1}X'y$$

and arriving at the same solution for multiple linear regression that we found with simple linear regression.

We can verify that the above equation $(X'X)^{-1}X'y$ recovers the optimal βs using R.

[25]:
```
print(cubicRegression)

y <- data$y
ones = rep(1,length(data$x))
x    = data$x
x2   = data$x^2
x3   = data$x^3

X = cbind(ones,x,x2,x3)
print(head(X))

optimalBetas <- solve(t(X)%*%X,t(X)%*%y)  # this is the same as solving our␣
 ↪system of equatons.
print(round(optimalBetas,4))
```

```
Call:
lm(formula = y ~ x + I(x^2) + I(x^3), data = data)

Coefficients:
(Intercept)            x       I(x^2)       I(x^3)
     0.2994       2.2877       1.0962      -1.4120

     ones          x         x2           x3
[1,]    1  0.9958723 0.99176166  0.987667975
[2,]    1 -0.6556163 0.42983269 -0.281805304
[3,]    1 -0.9176787 0.84213426 -0.772808705
[4,]    1  0.1963727 0.03856225  0.007572574
[5,]    1  1.0309346 1.06282620  1.095704329
[6,]    1  1.2610719 1.59030227  2.005485460
        [,1]
ones  0.2994
x     2.2877
x2    1.0962
x3   -1.4120
```

The beta coefficients we found from running a cubic regression match the beta coefficients from solving the system of equations above that minimize the SSE.

0.4.3 the linear in linear regression

Note that all the relationships linking x and y could be expressed using the same equation

$$y \sim N(X\beta, \sigma^2)$$

Why then is this called **linear** regression?

The **linear** in linear regression refers to the parameters. Lets look a the model form of a cubic regression.

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 \tag{45}$$
$$\epsilon \sim N(0, \sigma^2) \tag{46}$$

We can rewrite the above equation, so that it looks a bit more like multiple regression.

$$y = \beta_0 + \beta_1 x + \beta_2 q + \beta_3 r \tag{47}$$
$$q = x^2 \tag{48}$$
$$r = x^3 \tag{49}$$
$$\epsilon \sim N(0, \sigma^2) \tag{50}$$

Our equation now is linear in β and in reference to three variables: x, q, and r. We can do this with any functional form for x. The “linear” refers to the parameters.